



## Full wwPDB EM Validation Report ⓘ

Jul 28, 2025 – 05:40 PM EDT

PDB ID : 9CWM / pdb\_00009cwm  
EMDB ID : EMD-45967  
Title : Cryo-EM structure of human Low-density lipoprotein receptor-related protein 2  
Authors : Zhang, Z.; Lyu, M.  
Deposited on : 2024-07-29  
Resolution : 3.30 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

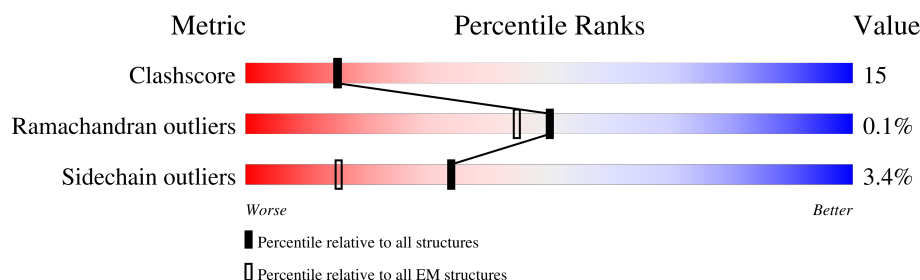
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




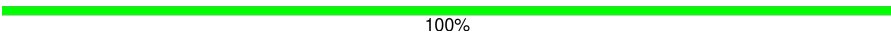
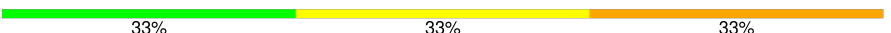



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4655	
1	B	4655	
2	C	3	
2	D	3	
2	E	3	
2	F	3	
2	I	3	
2	J	3	

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Mol	Chain	Length	Quality of chain
2	K	3	 67% 33%
2	L	3	 100%
2	N	3	 33% 33% 33%
3	G	2	 50% 50%
3	H	2	 50% 50%
3	M	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	-	-	X	-

## 2 Entry composition [i](#)

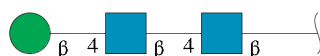
There are 4 unique types of molecules in this entry. The entry contains 58072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Low-density lipoprotein receptor-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3695	Total	C	N	O	S	0	0
			28662	17831	4991	5563	277		
1	B	3692	Total	C	N	O	S	0	0
			28653	17828	4988	5560	277		

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



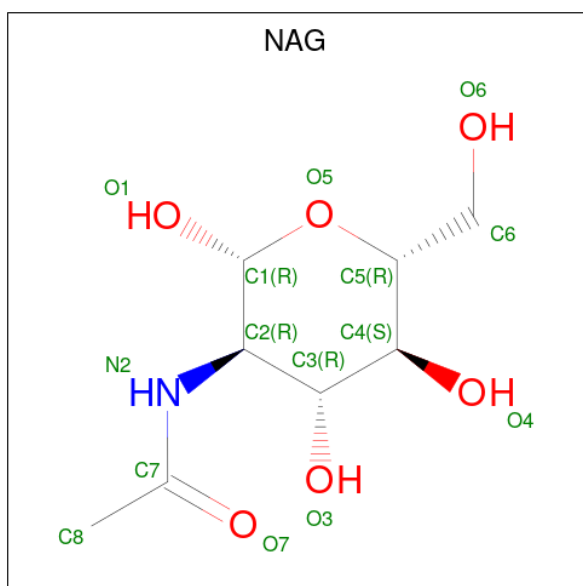
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	N	O	0	0
			39	22	2	15		
2	N	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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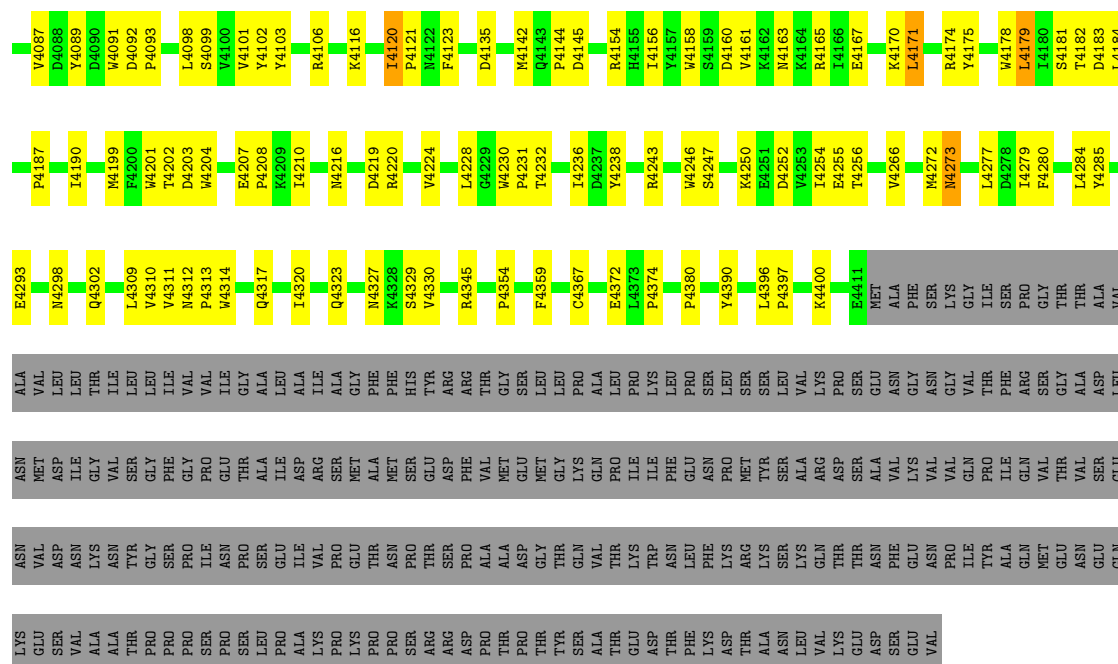
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	





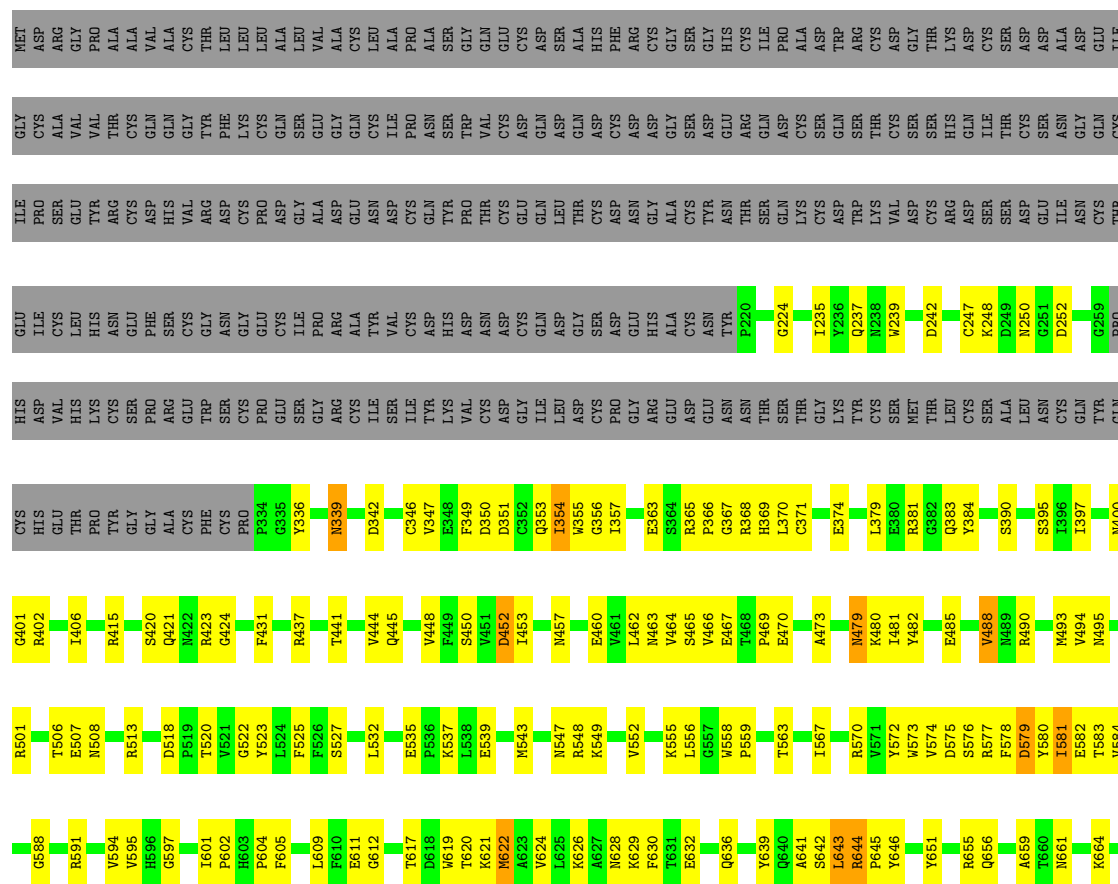






# • Molecule 1: Low-density lipoprotein receptor-related protein 2

Chain B:  53% 25% 21%





D3747	Q3612	D3496	T3362	L3265	E3053	ASP	GLY	ASN	PRO	R2711	Y2607	V9513	S2409
D3750	C3613	L3502	A3363	R3288	D3054	VAL	GLY	PRO	ARG	C2712	T2608	L2614	S2414
S3773	D3614	Y3507	L3364	L3269	N3055	CYS	ARG	THR	GLU	I2713	R2614	D2615	T2414
S3774	C3619	C3508	P3367	P3270	D3056	THR	CYS	CYS	ILE	S2714	I2615	P2516	
R3775	N3622	M3509	T3371	A3271	E3063	ASP	PRO	THR	CYS	D2724	A2618	G2519	V2417
W3776	D3626	P3510	I3372	A3272	L3087	GLY	SER	THR	ASN	C2725	C2725	Y2520	V2421
I3777	D3626	C3512	N3376	E3273	P3073	THR	GLU	HIS	GLY	C2726	A2619	L2521	
H3780	H3629	C3512	N3376	V3277	T3074	ASP	THR	THR	VAL	G2728	R2620	W2523	L2424
Y3781	H3629	S3513	Y3380	D3278	C3075	ASN	CYS	CYS	ASN	S2729	G2623	Y2426	L2425
N3782	R3633	Q3516	Y3380	S3281	C3075	GLN	ASP	SER	ASN	E2733	H2629	K2531	Y2427
D3783	F3617	R3282	R3192	R3282	H3078	CYS	ASP	GLY	ASP	A2737	L2633	I2532	S2428
C3784	F3640	K3283	Q3193	E3079	E3079	THR	ASN	PHE	ASN	L2737	L2633	E2533	S2429
D3789	R3641	E3390	N3194	F3080	A3088	ARG	GLN	ASP	ASN	L2738	L2634	R2534	
E3790	N3644	N3522	S3195	K3081	C3082	THR	CYS	CYS	THR	H2739	P2637	T2536	R2432
R3791	C3647	I3526	P3199	P3199	C3082	CYS	GLY	SER	ALA	T2740	P2637	R2542	I2433
T3797	D3657	R3280	Y3200	Y3200	R3086	SER	MET	GLY	GLU	T2747	I2640	V2543	Y2434
C3798	K3531	L3294	F3203	F3203	C3087	GLU	SER	ARG	LYS	CYS	I2641	P2544	F2435
H3799	D3662	S3297	S3204	E3089	E3089	GLU	GLU	ILE	CYS	ASN	T2642	I2545	N2438
P3800	D3533	D3298	Y3208	M3090	M3090	PHE	LYS	PRO	PRO	GLY	V2644	V2546	L2439
E3801	D3665	G3302	N3211	K3091	K3091	THR	THR	GLN	ASP	ARG	K2648	S2548	A2440
Y3802	E3666	H3303	N3211	K3091	K3091	CYS	ARG	HIS	ARG	CYS	Q2649	S2549	S2441
Q3804	P3667	R3304	S3220	C3094	C3094	TYR	HIS	TRP	THR	VAL	Q2649	L2550	Y2448
E3808	E3670	C3311	L3221	D3099	D3099	GLY	GLN	CYS	CYS	GLN	C2651	P2553	A2449
H3809	T3682	V3312	L3226	N3103	N3103	ILE	GLN	ASP	SER	S2757	N2652	L2556	T2450
C3810	T3688	F3318	V3229	S3104	S3104	ILE	CYS	ASP	ASN	R2758	N2653	L2557	S2453
G3811	R3691	C3318	V3229	D3106	D3106	PHE	SER	PHE	HIS	R2759	C2655	H2456	H2457
G3818	R3691	T3570	N3446	K3107	K3107	ARG	SER	ALA	ASN	C2760	E2656	P2458	T2457
S3819	C3692	P3323	D3233	G3110	G3110	CYS	GLU	ASP	ASN	Y2763	I2665	G2466	G2466
S3820	R3324	R3324	R3236	I3111	I3111	ASP	PHE	SER	ASN	R2764	N2664	V2567	D2474
A3821	A3574	G3325	R3236	N3112	N3112	ARG	LEU	SER	ILE	C2774	H2679	L2572	W2475
D3822	H3675	L3326	K3239	E3113	E3113	HIS	CYS	GLU	ASP	C2775	Q2573	R2574	I2476
C3823	D3453	A3327	R3240	C3114	C3114	ASN	VAL	PRO	ILE	L2776	Y2683	I2575	
L3824	I3454	L3328	R3240	H3115	H3115	ASP	ASN	ALA	PRO	F2777	Y2684	E2576	L2486
D3825	H3455	H3329	W3243	R3115	R3115	ASP	ASP	SER	ARG	ARG	L2685		
E3829	H3458	Q3331	I3244	H3124	H3124	ARG	ARG	CYS	VAL	ASP	A2686	M2489	T2489
C3832	D3583	Y3332	D3245	T3129	T3129	PRO	PRO	GLY	TYR	CYS	R2689	R2585	I2490
P3833	Y3460	L3335	Q3249	L3130	L3130	ASN	THR	HIS	LEU	ASN	E2586	W2491	S2491
T3834	R3461	L3335	Q3249	L3130	L3130	ASP	ARG	SER	CYS	ALA	V2587	S2492	W2492
R3835	N3467	W3337	I3251	C3135	C3135	ARG	ARG	GLU	ASP	THR	H2691	C2692	W2493
F3836	F3468	W3337	E3252	S3136	S3136	CYS	CYS	THR	GLY	GLU	C2692	L2494	E2495
P3837	C3469	Y3345	R3253	F3255	F3255	ILE	ILE	CYS	ASN	PHE	V2694	L2598	T2501
G3838	L3479	I3346	F3255	K3142	K3142	PRO	GLN	ALA	CYS	MET	S2704	T2599	I2502
A3840	G3485	K3356	T3259	D3146	D3146	ASP	PRO	ALA	GLY	ASN	T2705	CYS	Y2601
Y3841	G3486	K3261	N3260	K3147	K3147	THR	THR	GLY	ASP	ASN	T2706	G2603	L2563
C3842	E3492	I3360	K3261	R3148	R3148	VAL	VAL	PHE	ASN	ARG	C2707	A2504	R2505
Q3843	E3492	I3360	K3261	R3148	R3148	CYS	CYS	LYS	SER	ARG	S2708	Y2604	R2505
M3846	W3611	S3361	I3264	V3151	V3151	ASP	GLY	ASP	GLU	ILE	I2710	Y2606	R2510

Chain E:  67% 33%



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111811	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.033	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	5/29362 (0.0%)	0.43	4/39957 (0.0%)
1	B	0.25	6/29354 (0.0%)	0.43	7/39946 (0.0%)
All	All	0.26	11/58716 (0.0%)	0.43	11/79903 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	LYS	C-N	9.10	1.44	1.33
1	B	842	PHE	C-N	8.55	1.44	1.33
1	B	995	GLN	C-N	8.00	1.45	1.33
1	A	995	GLN	C-N	7.15	1.44	1.33
1	A	843	THR	C-N	6.31	1.41	1.33
1	B	841	PHE	C-N	-6.12	1.25	1.33
1	B	843	THR	C-N	6.04	1.42	1.33
1	A	481	ILE	C-N	5.63	1.41	1.33
1	B	367	GLY	C-N	5.59	1.41	1.33
1	B	996	ARG	C-N	5.46	1.40	1.33
1	A	996	ARG	C-N	5.04	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2726	GLY	N-CA-C	-9.85	102.41	115.32
1	A	2726	GLY	N-CA-C	-9.74	102.56	115.32
1	B	3819	GLY	N-CA-C	-6.17	107.74	115.08
1	B	842	PHE	O-C-N	5.58	129.92	123.17
1	A	480	LYS	O-C-N	5.54	130.43	123.23
1	B	995	GLN	O-C-N	5.45	130.23	123.15
1	B	1132	ASN	N-CA-C	-5.32	105.96	113.20
1	B	611	GLU	CB-CA-C	-5.17	110.59	116.54
1	A	995	GLN	O-C-N	5.16	129.46	122.96
1	B	3613	CYS	N-CA-C	-5.04	104.39	110.44
1	A	3881	VAL	CB-CA-C	-5.02	109.02	114.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	819	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28662	0	26485	823	0
1	B	28653	0	26477	829	0
2	C	39	0	34	2	0
2	D	39	0	34	2	0
2	E	39	0	34	5	0
2	F	39	0	34	0	0
2	I	39	0	34	3	0
2	J	39	0	34	3	0
2	K	39	0	34	6	0
2	L	39	0	34	0	0
2	N	39	0	34	2	0
3	G	28	0	25	7	0
3	H	28	0	25	1	0
3	M	28	0	25	1	0
4	A	168	0	156	1	0
4	B	154	0	143	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	58072	0	53642	1640	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4329:SER:HB2	3:G:1:NAG:C1	1.75	1.16
1:A:4007:ASP:HA	1:A:4025:LYS:HA	1.10	1.09
1:B:1228:GLY:HA3	1:B:3195:SER:HA	1.51	0.91
1:A:4007:ASP:HA	1:A:4025:LYS:CA	2.00	0.90
1:B:3611:TRP:HA	1:B:3614:ASP:HB3	1.55	0.88
1:B:3239:LYS:HB2	2:K:1:NAG:H62	1.56	0.87
1:A:339:ASN:HB2	1:A:342:ASP:HB2	1.55	0.87
1:A:3239:LYS:HB2	2:E:1:NAG:H62	1.58	0.83
1:B:4208:PRO:HB2	1:B:4228:LEU:HB2	1.61	0.83
1:A:4007:ASP:CA	1:A:4025:LYS:HA	2.02	0.83
1:A:1228:GLY:HA3	1:A:3195:SER:HA	1.59	0.83
1:B:4293:GLU:HG2	1:B:4310:VAL:HG22	1.61	0.82
1:B:1352:SER:HA	1:B:1355:ASP:HB2	1.60	0.82
1:A:3255:PHE:HD2	2:E:1:NAG:H5	1.42	0.82
1:B:3998:ASN:HB2	1:B:4001:ASP:HB2	1.60	0.82
1:B:1159:HIS:HB2	1:B:1175:VAL:HG13	1.60	0.81
1:A:911:GLU:HG2	1:A:912:GLN:HG3	1.63	0.81
1:A:3255:PHE:CD2	2:E:1:NAG:H5	2.15	0.81
1:B:3255:PHE:HD2	2:K:1:NAG:H5	1.45	0.80
1:B:354:ILE:HG23	1:B:357:ILE:HB	1.62	0.80
1:B:3255:PHE:CD2	2:K:1:NAG:H5	2.17	0.80
1:B:2758:TYR:HB3	1:B:2763:TYR:HB2	1.66	0.78
1:B:4124:GLU:HG3	3:M:1:NAG:H83	1.66	0.78
1:B:1172:LYS:HE2	1:B:1177:GLY:HA3	1.64	0.78
1:B:3244:ILE:HG12	1:B:3251:ILE:HG12	1.67	0.77
1:B:3287:LEU:HD13	1:B:3323:PRO:HB2	1.65	0.77
1:A:1349:ASN:HB3	1:A:1370:GLY:HA3	1.67	0.76
1:A:4179:LEU:HD13	1:A:4199:MET:HE1	1.66	0.76
1:B:2398:LEU:HD22	1:B:2424:LEU:HD21	1.68	0.76
1:A:3063:GLU:HB2	1:A:3067:LEU:HB2	1.67	0.75
1:B:2489:MET:HA	1:B:2505:ARG:HA	1.67	0.75
1:B:2475:TRP:HZ2	1:B:2649:GLN:HB2	1.50	0.75
1:B:3063:GLU:HB2	1:B:3067:LEU:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3244:ILE:HG12	1:A:3251:ILE:HG12	1.68	0.74
1:B:3819:GLY:H	1:B:3835:ARG:HH21	1.32	0.74
1:A:3287:LEU:HD13	1:A:3323:PRO:HB2	1.69	0.74
1:A:3791:ARG:HH21	1:B:4142:MET:HG3	1.52	0.74
1:B:3326:LEU:HG	1:B:3335:LEU:HD11	1.69	0.73
1:A:2489:MET:HA	1:A:2505:ARG:HA	1.68	0.73
1:B:2686:ALA:HB2	1:B:2693:ILE:HD11	1.69	0.73
1:A:363:GLU:HB2	1:A:370:LEU:HB3	1.71	0.73
1:A:1461:LEU:HD23	1:A:1462:VAL:HG23	1.71	0.73
1:B:363:GLU:HB2	1:B:370:LEU:HB3	1.69	0.73
1:A:2707:CYS:HB3	1:A:2729:SER:HB3	1.71	0.73
1:A:4329:SER:CB	3:G:1:NAG:C1	2.62	0.73
1:A:1074:CYS:HB2	1:A:1078:GLU:HB2	1.71	0.72
1:B:4179:LEU:HD13	1:B:4199:MET:HE1	1.70	0.72
1:B:1461:LEU:HD23	1:B:1462:VAL:HG23	1.71	0.72
1:B:2759:ARG:NH1	1:B:2760:CYS:SG	2.63	0.72
1:A:3326:LEU:HG	1:A:3335:LEU:HD11	1.69	0.72
1:B:578:PHE:HB3	1:B:1175:VAL:HG12	1.71	0.72
1:A:1254:PRO:HG2	4:A:4702:NAG:H83	1.70	0.71
1:B:3104:SER:HA	1:B:3107:LYS:HB3	1.72	0.71
1:A:466:VAL:HB	1:A:469:PRO:HG3	1.73	0.71
1:B:1354:SER:H	1:B:1366:GLN:HE21	1.37	0.71
1:B:3836:PHE:HD2	1:B:3838:ASP:HB3	1.55	0.71
1:A:911:GLU:HB3	1:A:947:MET:HE2	1.72	0.71
1:B:817:THR:HG23	1:B:1001:PRO:HB3	1.71	0.71
1:A:4022:ARG:HB3	1:A:4029:GLU:HB3	1.73	0.71
1:A:3423:THR:HB	1:A:3451:PRO:HB2	1.73	0.71
1:A:1352:SER:HA	1:A:1355:ASP:HB2	1.73	0.71
1:A:481:ILE:HG13	1:A:496:LEU:HD23	1.73	0.70
1:B:1364:CYS:HA	1:B:1373:CYS:HA	1.73	0.70
1:B:3364:LEU:HD11	1:B:3367:PRO:HB3	1.71	0.70
1:A:2686:ALA:HB2	1:A:2693:ILE:HD11	1.71	0.70
1:A:883:ARG:HE	1:A:896:HIS:HD2	1.38	0.70
1:B:237:GLN:HB2	1:B:549:LYS:HD2	1.74	0.70
1:A:3364:LEU:HD11	1:A:3367:PRO:HB3	1.74	0.70
1:A:4208:PRO:HB2	1:A:4228:LEU:HB2	1.72	0.70
1:B:2707:CYS:HB3	1:B:2729:SER:HB3	1.72	0.70
1:B:1353:CYS:SG	1:B:1364:CYS:HB2	2.32	0.70
1:A:4142:MET:HG3	1:B:3791:ARG:HH21	1.57	0.70
1:A:991:VAL:HG23	1:A:995:GLN:HG3	1.73	0.69
1:B:1160:ARG:HE	1:B:1162:ILE:HG22	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2475:TRP:HZ2	1:A:2649:GLN:HB2	1.55	0.69
1:A:3796:ARG:NH2	1:A:3810:CYS:SG	2.65	0.69
1:B:1658:THR:HB	1:B:1686:PRO:HB2	1.73	0.69
1:A:744:VAL:HG22	1:A:958:LEU:HD13	1.74	0.69
1:B:3423:THR:HB	1:B:3451:PRO:HB2	1.73	0.69
1:B:3875:LEU:HB3	1:B:3879:LEU:HA	1.74	0.69
1:A:582:GLU:HG2	1:A:591:ARG:HE	1.58	0.69
1:B:4204:TRP:HA	1:B:4231:PRO:HD2	1.74	0.69
1:B:3796:ARG:NH2	1:B:3810:CYS:SG	2.66	0.69
1:B:395:SER:HB2	1:B:651:TYR:HB3	1.74	0.68
1:A:1826:LEU:HD22	1:A:1835:LEU:HD21	1.76	0.68
1:A:1658:THR:HB	1:A:1686:PRO:HB2	1.75	0.68
1:A:1435:SER:HB2	1:A:1452:THR:HB	1.75	0.68
1:B:911:GLU:HG2	1:B:912:GLN:HG3	1.76	0.68
1:A:829:ARG:NH1	1:A:873:ASN:OD1	2.27	0.67
1:A:1588:MET:SD	1:A:1718:GLN:NE2	2.66	0.67
1:B:1435:SER:HB2	1:B:1452:THR:HB	1.76	0.67
1:B:2608:THR:HG22	1:B:2615:ILE:HG12	1.75	0.67
1:A:3264:ILE:HG22	1:A:3265:ILE:HG13	1.77	0.67
1:B:847:ARG:NH2	1:B:1251:ASP:OD2	2.28	0.67
1:B:3578:CYS:HB3	1:B:3583:ASP:HB2	1.77	0.67
1:B:1114:TYR:N	1:B:1122:ILE:O	2.27	0.67
1:A:2608:THR:HG22	1:A:2615:ILE:HG12	1.75	0.67
1:A:3867:CYS:HB3	1:A:3870:GLY:HA3	1.77	0.66
1:B:1071:ALA:HB1	1:B:1079:CYS:HB3	1.77	0.66
1:B:1125:ASN:HA	1:B:1153:GLN:HE21	1.60	0.66
1:B:2474:ASP:HB2	1:B:2514:LEU:HD13	1.78	0.66
1:B:4022:ARG:HB3	1:B:4029:GLU:HB3	1.75	0.66
1:A:4062:VAL:HG23	1:A:4063:ARG:HG3	1.78	0.66
1:B:1256:CYS:SG	1:B:1260:SER:OG	2.53	0.66
1:A:4311:VAL:HG12	1:A:4312:ASN:H	1.61	0.66
1:B:1058:GLN:HG2	1:B:1059:LEU:HG	1.78	0.66
1:B:1365:VAL:H	1:B:1373:CYS:H	1.43	0.66
1:A:493:MET:HE1	1:A:673:VAL:HG11	1.78	0.66
1:A:3611:TRP:HA	1:A:3614:ASP:HB3	1.77	0.66
1:B:609:LEU:O	1:B:655:ARG:NH1	2.28	0.66
1:A:1256:CYS:SG	1:A:1260:SER:OG	2.54	0.66
1:A:4036:PHE:HB3	1:A:4047:CYS:HB3	1.77	0.66
1:B:1187:CYS:H	1:B:1193:LYS:HE3	1.61	0.66
1:A:229:CYS:HB2	1:A:233:ARG:HG2	1.76	0.66
1:A:2505:ARG:O	1:A:2542:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:991:VAL:HG23	1:B:995:GLN:HG3	1.77	0.65
1:B:3298:ASP:OD1	1:B:3298:ASP:N	2.29	0.65
1:B:4243:ARG:HH21	1:B:4256:THR:HG23	1.59	0.65
1:B:711:LEU:HD11	1:B:960:LEU:HG	1.78	0.65
1:B:2285:VAL:HG22	1:B:2290:ILE:HG22	1.79	0.65
1:A:1156:CYS:HB2	1:A:1160:ARG:H	1.60	0.65
1:A:765:ILE:HD11	1:A:786:VAL:HG21	1.77	0.65
1:B:582:GLU:HG2	1:B:591:ARG:HE	1.61	0.65
1:B:1588:MET:SD	1:B:1718:GLN:NE2	2.69	0.65
1:B:3204:SER:HB3	1:B:3232:LEU:HD23	1.79	0.65
1:B:3836:PHE:CZ	1:B:3840:ALA:HB3	2.32	0.65
1:A:1058:GLN:HG2	1:A:1059:LEU:HG	1.79	0.64
1:A:3578:CYS:HB3	1:A:3583:ASP:HB2	1.78	0.64
1:B:580:TYR:CE2	1:B:582:GLU:HB2	2.33	0.64
1:B:594:VAL:HG12	1:B:595:VAL:HG23	1.80	0.64
1:B:2531:LYS:HB3	1:B:2544:PRO:HB3	1.79	0.64
1:B:4062:VAL:HG23	1:B:4063:ARG:HG3	1.79	0.64
1:A:1367:GLU:HG3	1:A:1370:GLY:H	1.62	0.64
1:A:1187:CYS:H	1:A:1193:LYS:HE3	1.61	0.64
1:A:3142:LYS:N	1:A:3151:VAL:O	2.28	0.64
1:A:3362:THR:O	1:A:3399:ARG:NH1	2.28	0.64
1:B:3856:PRO:HG2	1:B:3859:TRP:HD1	1.62	0.64
1:A:1592:ILE:HG13	1:A:1593:VAL:HG23	1.80	0.64
1:A:3236:ARG:HD3	1:A:3459:PRO:HA	1.80	0.64
1:A:3846:MET:HG2	1:A:3857:PRO:HD3	1.79	0.64
1:B:3835:ARG:HD3	1:B:3841:TYR:HD2	1.61	0.64
1:B:3836:PHE:CD2	1:B:3838:ASP:HB3	2.32	0.64
1:A:1365:VAL:O	1:A:1372:LYS:HB3	1.98	0.64
1:B:3264:ILE:HG22	1:B:3265:ILE:HG13	1.80	0.64
1:A:2479:ARG:HH12	1:A:2499:ASN:HB2	1.63	0.63
1:A:3855:ILE:HD11	1:A:3867:CYS:HB2	1.80	0.63
1:B:1252:GLY:N	1:B:1262:GLU:OE1	2.29	0.63
1:A:1072:PHE:N	1:A:1080:ILE:O	2.31	0.63
1:A:570:ARG:HH11	1:A:583:THR:HG22	1.64	0.63
1:A:1159:HIS:HB2	1:A:1175:VAL:HG22	1.80	0.63
1:A:3298:ASP:N	1:A:3298:ASP:OD1	2.32	0.63
1:A:4204:TRP:HA	1:A:4231:PRO:HD2	1.80	0.63
1:A:602:PRO:HG3	1:A:621:LYS:HE2	1.81	0.63
1:A:620:THR:HA	1:A:1132:ASN:HB2	1.79	0.63
1:A:4279:ILE:HG12	1:A:4284:LEU:HG	1.81	0.63
1:B:366:PRO:HD2	1:B:368:ARG:HH22	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:CYS:SG	1:A:1260:SER:OG	2.57	0.63
1:A:1252:GLY:N	1:A:1262:GLU:OE1	2.30	0.63
1:B:3999:VAL:HG23	1:B:4000:PHE:HD1	1.62	0.63
1:A:2285:VAL:HG22	1:A:2290:ILE:HG22	1.80	0.63
1:B:3073:PRO:HA	1:B:3081:LYS:HD2	1.80	0.63
1:A:2398:LEU:HD22	1:A:2424:LEU:HD21	1.80	0.63
1:A:2759:ARG:NH2	1:A:2761:ASP:OD1	2.32	0.63
1:B:3720:HIS:ND1	1:B:3722:VAL:O	2.32	0.63
1:A:421:GLN:O	1:A:445:GLN:NE2	2.32	0.62
1:A:747:ASP:HA	1:A:961:LYS:HE3	1.81	0.62
1:A:3259:THR:HG21	2:E:1:NAG:C7	2.29	0.62
1:B:3362:THR:O	1:B:3399:ARG:NH1	2.28	0.62
1:B:4170:LYS:HG2	1:B:4174:ARG:HH21	1.63	0.62
1:A:1114:TYR:N	1:A:1122:ILE:O	2.31	0.62
1:B:1354:SER:HB3	1:B:1366:GLN:HG2	1.81	0.62
1:B:2683:TRP:HB3	1:B:2692:CYS:HB3	1.81	0.62
1:A:2683:TRP:HB3	1:A:2692:CYS:HB3	1.80	0.62
1:B:576:SER:HA	1:B:604:PRO:HD2	1.81	0.62
1:B:1826:LEU:HD22	1:B:1835:LEU:HD21	1.80	0.62
1:A:3720:HIS:ND1	1:A:3722:VAL:O	2.32	0.62
1:B:3834:THR:HB	1:B:3840:ALA:O	2.00	0.62
1:B:4279:ILE:HG12	1:B:4284:LEU:HG	1.82	0.62
1:B:2648:LYS:HB2	1:B:2650:GLN:HE22	1.65	0.61
1:A:423:ARG:HA	1:A:1089:ARG:HE	1.65	0.61
1:B:507:GLU:HB3	1:B:548:ARG:NH1	2.15	0.61
1:B:2182:ARG:NH1	1:B:2409:SER:OG	2.33	0.61
1:B:3259:THR:HG21	2:K:1:NAG:C7	2.30	0.61
1:A:1060:CYS:HA	1:A:1065:ASN:HD22	1.66	0.61
1:A:1381:LEU:HB3	1:A:1385:SER:HA	1.82	0.61
1:A:3872:ASP:HB3	1:A:3874:GLU:HG3	1.82	0.61
1:B:580:TYR:HE2	1:B:582:GLU:HB2	1.65	0.61
1:B:3496:ASP:OD2	1:B:3516:GLN:NE2	2.33	0.61
1:A:1160:ARG:HE	1:A:1162:ILE:HG22	1.66	0.61
1:A:3158:GLU:HG2	1:A:3159:MET:HG3	1.82	0.61
1:A:2756:TYR:HA	1:A:2759:ARG:HB3	1.81	0.61
1:B:365:ARG:HB3	1:B:368:ARG:NH2	2.15	0.61
1:A:609:LEU:O	1:A:655:ARG:NH1	2.34	0.61
1:A:2176:ILE:HB	2:C:1:NAG:H82	1.82	0.61
1:A:4020:HIS:NE2	1:A:4033:ALA:HB2	2.16	0.61
1:B:1405:TYR:HB2	1:B:1412:ARG:HB3	1.83	0.61
1:B:4311:VAL:HG12	1:B:4312:ASN:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:SER:OG	1:A:974:CYS:SG	2.59	0.60
1:B:883:ARG:NH2	1:B:903:ASP:O	2.33	0.60
1:B:4036:PHE:HB3	1:B:4047:CYS:HB3	1.84	0.60
1:A:2394:LEU:HD11	1:A:2633:LEU:HD13	1.83	0.60
1:A:3836:PHE:HD2	1:A:3838:ASP:HB3	1.66	0.60
1:B:421:GLN:O	1:B:445:GLN:NE2	2.33	0.60
1:A:2251:VAL:HG12	1:A:2258:ILE:HG12	1.83	0.60
1:B:1349:ASN:HB3	1:B:1370:GLY:HA3	1.81	0.60
1:B:2709:ASN:HB3	1:B:2727:ASP:CG	2.26	0.60
1:A:801:THR:HG22	1:A:808:ILE:HG12	1.83	0.60
1:B:2505:ARG:O	1:B:2542:ARG:NH1	2.34	0.60
1:A:523:TYR:CD2	1:A:540:ARG:HD2	2.36	0.60
1:A:2531:LYS:HB3	1:A:2544:PRO:HB3	1.83	0.60
1:A:3073:PRO:HA	1:A:3081:LYS:HD2	1.82	0.60
1:A:4067:TYR:CD2	1:A:4309:LEU:HD11	2.36	0.60
1:B:747:ASP:HA	1:B:961:LYS:HE3	1.83	0.60
1:A:352:CYS:HA	1:A:357:ILE:HD13	1.84	0.60
1:A:3094:CYS:H	1:A:3105:ASP:HB2	1.66	0.60
1:A:3204:SER:HB3	1:A:3232:LEU:HD23	1.84	0.60
1:B:1356:PHE:C	1:B:1358:GLY:H	2.08	0.60
1:A:527:SER:HB2	1:A:559:PRO:HB2	1.83	0.60
1:A:822:VAL:HG12	1:A:825:LEU:HD21	1.84	0.60
1:A:3496:ASP:OD2	1:A:3516:GLN:NE2	2.35	0.60
1:B:415:ARG:NH2	1:B:453:ILE:O	2.34	0.60
1:B:2251:VAL:HG12	1:B:2258:ILE:HG12	1.84	0.60
1:B:2390:LEU:HD13	1:B:2640:ILE:HD11	1.84	0.60
1:B:3025:ARG:NH1	1:B:3040:GLN:O	2.35	0.60
1:B:4178:TRP:HB3	1:B:4181:SER:HB3	1.82	0.60
1:A:3780:HIS:HE2	1:A:3824:LEU:HB2	1.66	0.60
1:B:1352:SER:HA	1:B:1355:ASP:CB	2.31	0.60
1:B:1510:LEU:HB3	1:B:1528:TYR:HB3	1.83	0.60
1:A:3454:ILE:O	1:A:3455:HIS:ND1	2.34	0.59
1:B:3176:CYS:O	1:B:3184:ARG:NH1	2.35	0.59
1:B:555:LYS:HE3	1:B:1175:VAL:HB	1.84	0.59
1:B:1358:GLY:O	1:B:1386:LYS:HD3	2.01	0.59
1:A:239:TRP:HA	1:A:242:ASP:HB3	1.84	0.59
1:A:1205:ASN:ND2	1:A:1212:ASP:OD2	2.36	0.59
1:A:2532:ILE:HG21	1:A:2565:LEU:HD21	1.85	0.59
1:B:1381:LEU:HB3	1:B:1385:SER:HA	1.84	0.59
1:A:1095:GLY:O	1:A:1099:HIS:N	2.34	0.59
1:A:1250:CYS:HB3	1:A:1268:PRO:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4006:LEU:O	1:A:4008:ILE:HG13	2.01	0.59
1:B:3454:ILE:O	1:B:3455:HIS:ND1	2.35	0.59
1:A:347:VAL:HG22	1:A:349:PHE:H	1.66	0.59
1:A:847:ARG:NH2	1:A:1251:ASP:OD2	2.36	0.59
1:A:1060:CYS:SG	1:A:1061:GLY:N	2.73	0.59
1:A:1510:LEU:HB3	1:A:1528:TYR:HB3	1.85	0.59
1:B:661:ASN:HB3	1:B:664:LYS:HG3	1.84	0.59
1:B:2394:LEU:HD11	1:B:2633:LEU:HD13	1.84	0.59
1:A:3112:ASN:HB3	1:A:3115:HIS:HB2	1.84	0.59
1:B:423:ARG:NH1	1:B:1091:ASP:OD1	2.36	0.59
1:A:2474:ASP:HB2	1:A:2514:LEU:HD13	1.85	0.59
1:A:4280:PHE:HB2	1:A:4320:ILE:HD13	1.84	0.59
1:A:1871:GLY:N	1:A:1889:ASP:OD2	2.35	0.59
1:B:801:THR:HG22	1:B:808:ILE:HG12	1.85	0.59
1:B:558:TRP:HB2	1:B:577:ARG:HB2	1.83	0.59
1:B:602:PRO:HG3	1:B:621:LYS:HE2	1.83	0.59
1:B:1622:MET:HE3	1:B:1642:ILE:HD11	1.85	0.59
1:A:1356:PHE:C	1:A:1358:GLY:H	2.10	0.58
1:A:2648:LYS:HB2	1:A:2650:GLN:HE22	1.68	0.58
1:A:3200:TYR:CE1	2:D:1:NAG:H3	2.38	0.58
1:B:3226:LEU:HD13	1:B:3229:VAL:HG21	1.85	0.58
1:A:1062:THR:H	1:A:1065:ASN:HB2	1.68	0.58
1:A:1351:ASN:HA	1:A:1370:GLY:C	2.28	0.58
1:B:2739:HIS:O	1:B:2740:THR:C	2.46	0.58
1:B:3183:LEU:N	1:B:3192:ARG:O	2.35	0.58
3:G:1:NAG:H61	3:G:2:NAG:C7	2.33	0.58
1:A:817:THR:HG23	1:A:1001:PRO:HB3	1.85	0.58
1:A:1357:ASN:HA	1:A:1364:CYS:SG	2.43	0.58
1:A:2182:ARG:NH1	1:A:2409:SER:OG	2.36	0.58
1:A:2759:ARG:HD2	1:B:979:HIS:CG	2.38	0.58
1:B:887:VAL:HG22	1:B:894:ILE:HG12	1.85	0.58
1:B:2426:TYR:CD2	1:B:2643:VAL:HG13	2.39	0.58
1:B:2711:ARG:NH1	1:B:2724:ASP:O	2.36	0.58
1:A:1206:ARG:HA	1:A:1218:ASP:HB2	1.85	0.58
1:A:1351:ASN:HA	1:A:1370:GLY:CA	2.33	0.58
1:A:1358:GLY:O	1:A:1386:LYS:HD3	2.03	0.58
1:A:2533:GLU:HA	1:A:2544:PRO:HA	1.86	0.58
1:A:2686:ALA:N	1:A:2691:HIS:O	2.35	0.58
1:A:4313:PRO:HD3	1:B:4314:TRP:CE2	2.38	0.58
1:B:1871:GLY:N	1:B:1889:ASP:OD2	2.34	0.58
1:B:2739:HIS:CD2	1:B:2747:THR:HG21	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:HG12	1:A:581:ILE:HB	1.86	0.58
1:A:1405:TYR:HB2	1:A:1412:ARG:HB3	1.84	0.58
1:A:1658:THR:HG22	1:A:1665:VAL:HG22	1.86	0.58
1:B:1592:ILE:HG13	1:B:1593:VAL:HG23	1.84	0.58
1:B:2067:VAL:HG21	1:B:2300:ILE:HD13	1.86	0.58
1:B:2533:GLU:HA	1:B:2544:PRO:HA	1.85	0.58
1:B:3328:LEU:HG	1:B:3335:LEU:HD13	1.85	0.58
1:A:1046:ASP:HA	1:A:1068:SER:HB3	1.86	0.58
1:B:3200:TYR:CE1	2:J:1:NAG:H3	2.38	0.58
1:B:3599:TRP:N	1:B:3607:ILE:O	2.36	0.58
1:A:523:TYR:CE2	1:A:540:ARG:HD2	2.38	0.58
1:A:1945:ARG:NH2	1:A:1954:MET:SD	2.71	0.58
1:A:4293:GLU:HG2	1:A:4310:VAL:HG22	1.85	0.58
1:B:397:ILE:HG12	1:B:406:ILE:HG12	1.86	0.58
1:B:420:SER:O	1:B:1089:ARG:NH2	2.36	0.58
1:B:4101:VAL:HG21	1:B:4120:ILE:HD12	1.86	0.58
1:A:1617:SER:HA	1:A:1645:PRO:HD2	1.86	0.58
1:B:819:ARG:NH2	1:B:1001:PRO:O	2.37	0.58
1:B:1004:MET:HA	1:B:1015:GLY:HA2	1.86	0.58
1:B:3467:ASN:HD21	1:B:3469:CYS:HB2	1.68	0.58
1:A:1361:THR:HB	1:A:1388:CYS:H	1.69	0.58
1:A:3208:TYR:HH	1:A:3760:THR:HG1	1.50	0.57
1:B:402:ARG:HD3	1:B:1089:ARG:HH11	1.68	0.57
1:B:794:ILE:HG21	1:B:972:ASN:HB3	1.86	0.57
1:B:2598:LEU:HD11	1:B:2605:ILE:HD11	1.86	0.57
1:B:3142:LYS:N	1:B:3151:VAL:O	2.28	0.57
1:A:855:TRP:HB3	1:A:991:VAL:HG12	1.86	0.57
1:A:3423:THR:HG22	1:A:3430:VAL:HG22	1.86	0.57
1:A:3467:ASN:HD21	1:A:3469:CYS:HB2	1.69	0.57
1:A:4243:ARG:HH21	1:A:4256:THR:HG23	1.69	0.57
1:B:622:MET:HA	1:B:645:PRO:HD3	1.85	0.57
1:B:883:ARG:HH12	1:B:903:ASP:HB3	1.69	0.57
1:B:1172:LYS:HG2	1:B:1180:GLU:HB2	1.87	0.57
1:B:2704:SER:HA	1:B:2714:SER:HA	1.85	0.57
1:A:3176:CYS:O	1:A:3184:ARG:NH1	2.37	0.57
1:B:1617:SER:HA	1:B:1645:PRO:HD2	1.87	0.57
1:B:2491:ASN:HA	1:B:2502:VAL:HA	1.85	0.57
1:A:2683:TRP:HA	1:A:2693:ILE:O	2.05	0.57
1:A:3657:ASP:OD2	1:A:3706:ARG:NH2	2.35	0.57
1:B:746:ILE:HG13	1:B:961:LYS:HB3	1.86	0.57
1:A:1351:ASN:CG	1:A:1370:GLY:HA2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3599:TRP:N	1:A:3607:ILE:O	2.36	0.57
1:B:4058:LEU:HD13	1:B:4311:VAL:HG21	1.86	0.57
1:B:754:THR:HA	1:B:769:LYS:HA	1.86	0.57
1:B:2399:ARG:HG2	1:B:2414:THR:HG23	1.87	0.57
1:B:3112:ASN:HB3	1:B:3115:HIS:HB2	1.86	0.57
1:B:3360:ILE:HD12	1:B:3399:ARG:HD2	1.86	0.57
1:B:3691:ARG:HG2	1:B:3693:ILE:HG23	1.85	0.57
1:A:4202:THR:HG22	1:A:4210:ILE:HG12	1.86	0.57
1:B:247:CYS:HB3	1:B:252:ASP:H	1.70	0.57
1:B:4007:ASP:HA	1:B:4025:LYS:HA	1.86	0.57
1:A:2711:ARG:HH11	1:A:2725:CYS:HA	1.69	0.57
1:B:1365:VAL:HG21	1:B:1374:LEU:HG	1.87	0.57
1:B:3657:ASP:OD2	1:B:3706:ARG:NH2	2.37	0.57
1:A:3203:PHE:HB3	1:A:3454:ILE:HG13	1.86	0.56
1:A:3691:ARG:HG2	1:A:3693:ILE:HG23	1.87	0.56
1:B:2510:ARG:NH2	1:B:2553:PRO:O	2.38	0.56
1:B:1254:PRO:HG2	4:B:4703:NAG:H83	1.87	0.56
1:A:402:ARG:HG2	1:A:425:VAL:HG12	1.87	0.56
1:A:1156:CYS:HB2	1:A:1159:HIS:HB3	1.87	0.56
1:A:1209:GLY:N	1:A:1219:GLU:OE1	2.37	0.56
1:A:1965:GLY:HA3	1:A:2006:GLY:HA2	1.86	0.56
1:A:3240:ARG:HD3	1:A:3253:ARG:HD2	1.87	0.56
1:A:3025:ARG:NH1	1:A:3040:GLN:O	2.38	0.56
1:B:2247:TYR:OH	1:B:2262:ARG:NH2	2.38	0.56
1:B:2683:TRP:HA	1:B:2693:ILE:O	2.04	0.56
1:B:4174:ARG:HD3	1:B:4374:PRO:HA	1.87	0.56
1:A:794:ILE:HG21	1:A:972:ASN:HB3	1.87	0.56
1:B:619:TRP:CD2	1:B:644:ARG:HD3	2.40	0.56
1:B:1362:HIS:HB3	1:B:1374:LEU:O	2.04	0.56
1:B:1965:GLY:HA3	1:B:2006:GLY:HA2	1.86	0.56
1:B:2432:ARG:HD2	1:B:2448:TYR:CD1	2.41	0.56
1:B:3575:HIS:O	1:B:3577:ASN:ND2	2.39	0.56
1:A:377:TYR:CE1	1:A:654:LEU:HD13	2.40	0.56
1:A:2711:ARG:NH1	1:A:2724:ASP:O	2.37	0.56
1:A:3312:VAL:HG11	1:A:3337:TRP:HZ2	1.70	0.56
1:A:706:ALA:O	1:A:708:GLN:NE2	2.38	0.56
1:A:3531:LYS:HA	1:A:3543:ASP:HB2	1.87	0.56
1:A:4101:VAL:HG21	1:A:4120:ILE:HD12	1.88	0.56
1:B:1846:GLU:HG3	1:B:1859:THR:HA	1.88	0.56
1:A:2426:TYR:CD2	1:A:2643:VAL:HG13	2.40	0.56
1:B:584:VAL:HB	1:B:588:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:LEU:HB2	1:A:1369:PHE:HA	1.87	0.56
1:A:1622:MET:HE3	1:A:1642:ILE:HD11	1.86	0.56
1:A:3359:ILE:HG22	1:A:3360:ILE:HG12	1.88	0.56
1:B:1060:CYS:SG	1:B:1061:GLY:N	2.77	0.56
1:B:2545:ILE:HG22	1:B:2546:VAL:HG23	1.88	0.56
1:B:4202:THR:HG22	1:B:4210:ILE:HG12	1.88	0.56
1:A:2709:ASN:HB3	1:A:2727:ASP:CG	2.31	0.56
1:B:1439:LEU:HD21	1:B:1480:ILE:HD13	1.88	0.56
1:B:4359:PHE:HA	1:B:4367:CYS:HA	1.87	0.56
1:A:1113:GLN:HB3	1:A:1121:CYS:HB3	1.88	0.55
1:A:1136:ASP:OD1	1:A:1136:ASP:N	2.39	0.55
1:A:2510:ARG:NH2	1:A:2553:PRO:O	2.39	0.55
1:A:2644:VAL:HB	1:A:2648:LYS:HG2	1.88	0.55
1:B:1192:PHE:N	1:B:1201:ILE:O	2.38	0.55
1:B:2686:ALA:N	1:B:2691:HIS:O	2.36	0.55
1:B:574:VAL:HG12	1:B:581:ILE:HB	1.88	0.55
1:A:1555:ARG:NH1	1:A:1601:CYS:SG	2.80	0.55
1:A:4089:TYR:HB3	1:A:4101:VAL:HG22	1.89	0.55
1:B:1237:CYS:SG	1:B:1260:SER:OG	2.64	0.55
1:A:2067:VAL:HG21	1:A:2300:ILE:HD13	1.87	0.55
1:A:2432:ARG:HD2	1:A:2448:TYR:CD1	2.41	0.55
1:B:936:ILE:HG12	1:B:957:ILE:HD11	1.88	0.55
1:B:3842:CYS:SG	1:B:3848:GLU:HB3	2.46	0.55
1:B:1060:CYS:HA	1:B:1065:ASN:HD22	1.71	0.55
1:B:2644:VAL:HB	1:B:2648:LYS:HG2	1.88	0.55
1:B:3847:PHE:CE2	1:B:3855:ILE:HD13	2.42	0.55
1:B:1206:ARG:HA	1:B:1218:ASP:HB2	1.89	0.55
1:A:2168:GLU:OE2	1:A:2614:ARG:NH2	2.40	0.55
1:A:2704:SER:HA	1:A:2714:SER:HA	1.88	0.55
1:A:3415:ILE:O	1:A:3461:ARG:NH1	2.39	0.55
1:A:4170:LYS:HG2	1:A:4174:ARG:HH21	1.71	0.55
1:B:1354:SER:N	1:B:1366:GLN:HE21	2.03	0.55
1:A:1868:LEU:HD23	1:A:1910:VAL:HG23	1.89	0.55
1:A:2545:ILE:HG22	1:A:2546:VAL:HG23	1.88	0.55
1:A:4068:ASN:HB3	1:A:4071:SER:OG	2.06	0.55
1:B:366:PRO:HD2	1:B:368:ARG:NH2	2.22	0.55
1:B:1825:ASN:ND2	1:B:1875:GLY:HA2	2.22	0.55
1:B:3199:PRO:HB3	1:B:3458:HIS:HB2	1.89	0.55
1:B:4099:SER:O	1:B:4120:ILE:N	2.37	0.55
1:A:1354:SER:HB3	1:A:1366:GLN:HG2	1.89	0.55
1:B:1559:LEU:HD22	1:B:1584:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2144:GLU:HG3	1:B:2166:VAL:HG23	1.87	0.55
1:A:424:GLY:HA3	1:A:445:GLN:HE21	1.72	0.55
1:A:935:ALA:HB1	1:A:949:VAL:HG13	1.88	0.55
1:A:1191:GLN:HA	1:A:1202:GLY:HA2	1.88	0.55
1:A:1576:HIS:O	1:A:1578:ARG:NH1	2.40	0.55
1:A:1936:ALA:HB2	1:A:1966:ILE:HD11	1.87	0.55
1:A:2099:HIS:CE1	1:A:2194:HIS:HD2	2.25	0.55
1:A:2247:TYR:OH	1:A:2262:ARG:NH2	2.40	0.55
1:B:3311:CYS:HA	1:B:3319:CYS:HA	1.87	0.55
1:B:1354:SER:H	1:B:1366:GLN:NE2	2.03	0.54
1:B:3236:ARG:HD3	1:B:3459:PRO:HA	1.88	0.54
1:B:3284:LEU:N	1:B:3297:SER:O	2.37	0.54
1:B:3415:ILE:O	1:B:3461:ARG:NH1	2.41	0.54
1:A:3332:TYR:O	1:A:3485:GLY:N	2.40	0.54
1:B:2168:GLU:OE2	1:B:2614:ARG:NH2	2.40	0.54
1:B:527:SER:HB2	1:B:559:PRO:HB2	1.89	0.54
2:J:1:NAG:H61	2:J:2:NAG:H82	1.90	0.54
1:A:501:ARG:HG2	1:A:693:PHE:HE2	1.73	0.54
1:A:945:GLY:O	1:A:946:GLU:HG3	2.07	0.54
1:A:1846:GLU:HG3	1:A:1859:THR:HA	1.88	0.54
1:A:3328:LEU:HG	1:A:3335:LEU:HD13	1.90	0.54
1:B:2492:SER:HB3	1:B:2501:THR:HG23	1.89	0.54
1:B:2515:ASP:O	1:B:2519:GLY:N	2.40	0.54
1:B:3872:ASP:HB3	1:B:3874:GLU:HG2	1.89	0.54
1:A:1059:LEU:O	1:A:1065:ASN:ND2	2.40	0.54
1:A:1354:SER:H	1:A:1366:GLN:HE21	1.55	0.54
1:A:2141:GLY:H	1:A:2634:LEU:HD11	1.72	0.54
1:A:2556:LEU:HD23	1:A:2567:TRP:HB3	1.90	0.54
1:A:2709:ASN:HD21	1:A:2725:CYS:HB3	1.72	0.54
1:A:3039:CYS:HB2	1:A:3041:ASN:HD21	1.73	0.54
1:B:237:GLN:HE22	1:B:547:ASN:HB3	1.72	0.54
1:B:2425:ASP:O	1:B:2434:TYR:N	2.38	0.54
1:B:3211:ASN:HB3	1:B:3220:SER:HB3	1.90	0.54
1:B:3819:GLY:N	1:B:3835:ARG:HH21	2.05	0.54
1:A:3311:CYS:HA	1:A:3319:CYS:HA	1.89	0.54
1:A:3819:GLY:H	1:A:3835:ARG:HH21	1.54	0.54
1:B:239:TRP:HA	1:B:242:ASP:HB3	1.90	0.54
1:B:1347:LEU:HB2	1:B:1369:PHE:HA	1.90	0.54
1:B:2141:GLY:H	1:B:2634:LEU:HD11	1.72	0.54
1:B:3849:CYS:SG	1:B:3855:ILE:HD11	2.47	0.54
1:A:368:ARG:HG3	1:A:369:HIS:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ASN:O	1:A:818:ARG:NH1	2.26	0.54
1:A:976:GLN:HB2	1:A:979:HIS:HB3	1.90	0.54
1:A:3861:CYS:SG	1:A:3874:GLU:HB2	2.48	0.54
1:A:4161:VAL:HA	1:A:4187:PRO:HD2	1.89	0.54
1:B:1072:PHE:N	1:B:1080:ILE:O	2.38	0.54
1:B:2711:ARG:HH11	1:B:2725:CYS:HA	1.72	0.54
1:B:3773:PRO:HD2	1:B:3776:TRP:CE3	2.43	0.54
1:B:3835:ARG:HD3	1:B:3841:TYR:CD2	2.43	0.54
1:A:420:SER:O	1:A:1089:ARG:NH2	2.41	0.54
1:A:2390:LEU:HD13	1:A:2640:ILE:HD11	1.88	0.54
1:B:473:ALA:HB3	1:B:482:TYR:HB2	1.89	0.54
1:B:570:ARG:HH11	1:B:583:THR:HG22	1.72	0.54
1:B:1159:HIS:O	1:B:1160:ARG:HB3	2.07	0.54
1:A:661:ASN:HB3	1:A:664:LYS:HG3	1.89	0.54
1:A:1437:LEU:HB2	1:A:1692:VAL:HB	1.90	0.54
1:B:790:ALA:HB3	1:B:799:TYR:HB2	1.89	0.54
1:B:1362:HIS:CG	1:B:1363:GLU:N	2.75	0.54
1:B:4160:ASP:HB3	1:B:4163:ASN:HB2	1.90	0.54
1:A:1559:LEU:HD22	1:A:1584:MET:HE3	1.89	0.54
1:A:3575:HIS:O	1:A:3577:ASN:ND2	2.40	0.54
1:B:365:ARG:HB2	1:B:368:ARG:C	2.33	0.54
1:B:381:ARG:HD3	1:B:384:TYR:HE1	1.73	0.54
1:B:1658:THR:HG22	1:B:1665:VAL:HG22	1.89	0.54
1:B:1906:ASP:HA	1:B:2034:LEU:HD13	1.90	0.54
1:B:3233:ASP:OD2	1:B:3277:VAL:N	2.33	0.54
1:B:4280:PHE:HB2	1:B:4320:ILE:HD13	1.90	0.54
1:B:2325:ASP:OD1	1:B:2326:VAL:N	2.41	0.53
1:A:1362:HIS:HB3	1:A:1374:LEU:O	2.09	0.53
1:A:1487:GLN:OE1	1:A:1491:TRP:NE1	2.36	0.53
1:A:2325:ASP:OD1	1:A:2326:VAL:N	2.40	0.53
1:B:582:GLU:HG3	1:B:583:THR:H	1.73	0.53
1:B:795:SER:OG	1:B:974:CYS:SG	2.65	0.53
1:A:2137:ILE:HG22	1:A:2138:VAL:HG23	1.90	0.53
1:A:4038:SER:OG	1:A:4040:SER:O	2.26	0.53
1:B:1235:PHE:N	1:B:1244:ILE:O	2.41	0.53
1:B:1349:ASN:OD1	1:B:1350:GLY:N	2.34	0.53
1:B:3039:CYS:HB2	1:B:3041:ASN:HD21	1.73	0.53
1:A:1091:ASP:N	1:A:1097:ASP:OD2	2.40	0.53
1:B:3359:ILE:HG22	1:B:3360:ILE:HG12	1.91	0.53
1:A:1235:PHE:N	1:A:1244:ILE:O	2.41	0.53
1:A:2693:ILE:HG22	1:A:2694:VAL:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3626:ASP:HB3	1:A:3629:HIS:HD2	1.74	0.53
1:A:4160:ASP:HB3	1:A:4163:ASN:HB2	1.90	0.53
1:A:4359:PHE:HA	1:A:4367:CYS:HA	1.91	0.53
1:B:1062:THR:H	1:B:1065:ASN:HB2	1.73	0.53
1:B:3823:CYS:HB3	1:B:3825:ASP:OD1	2.08	0.53
1:A:580:TYR:CE2	1:A:582:GLU:HB2	2.43	0.53
1:A:644:ARG:NH2	1:A:1132:ASN:O	2.42	0.53
1:A:2425:ASP:O	1:A:2434:TYR:N	2.39	0.53
1:B:1059:LEU:O	1:B:1065:ASN:ND2	2.42	0.53
1:B:1095:GLY:O	1:B:1099:HIS:N	2.41	0.53
1:B:2520:TYR:HA	1:B:2536:THR:HA	1.90	0.53
1:A:2318:ASP:OD1	1:A:2319:ASN:N	2.42	0.53
1:B:374:GLU:HG3	1:B:567:ILE:HD12	1.90	0.53
1:B:1405:TYR:N	1:B:1412:ARG:O	2.36	0.53
1:B:3094:CYS:H	1:B:3105:ASP:HB2	1.74	0.53
1:A:554:THR:O	1:A:591:ARG:NH1	2.36	0.53
1:A:639:TYR:HE2	1:A:641:ALA:HB2	1.73	0.53
1:A:1439:LEU:HD21	1:A:1480:ILE:HD13	1.89	0.53
1:A:2491:ASN:HA	1:A:2502:VAL:HA	1.91	0.53
1:B:1154:PHE:HE2	1:B:1174:CYS:SG	2.31	0.53
1:A:930:ASP:HB3	1:A:933:LEU:HB2	1.90	0.53
1:A:2775:CYS:HB2	1:B:978:THR:HG21	1.91	0.53
1:A:3509:MET:HB3	1:A:3511:MET:HG2	1.91	0.53
1:B:1156:CYS:HB2	1:B:1160:ARG:H	1.72	0.53
1:B:1825:ASN:HD22	1:B:1875:GLY:HA2	1.74	0.53
1:B:4208:PRO:HB2	1:B:4228:LEU:CB	2.35	0.53
1:A:580:TYR:HE2	1:A:582:GLU:HB2	1.74	0.53
1:A:1004:MET:HA	1:A:1015:GLY:HA2	1.91	0.53
1:A:1906:ASP:HA	1:A:2034:LEU:HD13	1.91	0.53
1:B:842:PHE:CE1	1:B:852:MET:HB2	2.44	0.53
1:A:594:VAL:HG12	1:A:595:VAL:HG23	1.90	0.52
1:A:1351:ASN:HA	1:A:1370:GLY:HA2	1.90	0.52
1:A:1825:ASN:ND2	1:A:1875:GLY:HA2	2.24	0.52
1:A:2598:LEU:HD11	1:A:2605:ILE:HD11	1.91	0.52
1:A:3773:PRO:HD2	1:A:3776:TRP:CE3	2.44	0.52
1:B:768:GLN:HE21	1:B:772:GLY:HA2	1.74	0.52
1:B:1945:ARG:NH2	1:B:1954:MET:SD	2.74	0.52
1:A:1356:PHE:C	1:A:1358:GLY:N	2.65	0.52
1:A:3798:CYS:SG	1:A:3799:HIS:N	2.82	0.52
1:B:460:GLU:CD	1:B:463:ASN:HD22	2.18	0.52
1:B:490:ARG:HA	1:B:506:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:HIS:CD2	1:B:837:ALA:H	2.27	0.52
1:B:1351:ASN:ND2	1:B:1370:GLY:HA2	2.25	0.52
1:B:2532:ILE:HG21	1:B:2565:LEU:HD21	1.91	0.52
1:B:2693:ILE:HG22	1:B:2694:VAL:H	1.73	0.52
1:B:4247:SER:HB3	1:B:4277:LEU:HD21	1.92	0.52
1:A:626:LYS:N	1:A:636:GLN:O	2.41	0.52
1:A:833:VAL:HG22	1:A:840:LEU:HD12	1.91	0.52
1:A:852:MET:HA	1:A:863:PRO:HA	1.92	0.52
1:A:2758:TYR:CD2	1:A:2765:ASP:HB2	2.44	0.52
1:B:1046:ASP:HA	1:B:1068:SER:HB3	1.91	0.52
1:A:3080:PHE:N	1:A:3088:ILE:O	2.37	0.52
1:A:3211:ASN:HB3	1:A:3220:SER:HB3	1.92	0.52
1:B:1225:ARG:O	1:B:1227:PRO:HD3	2.10	0.52
1:B:1484:ASP:HB3	1:B:1487:GLN:HB2	1.92	0.52
1:A:424:GLY:HA2	1:A:444:VAL:HB	1.90	0.52
1:A:576:SER:HA	1:A:604:PRO:HD2	1.91	0.52
1:A:2515:ASP:O	1:A:2519:GLY:N	2.43	0.52
1:A:3111:ILE:N	1:A:3113:GLU:OE2	2.40	0.52
1:B:1206:ARG:NH2	1:B:1217:SER:O	2.42	0.52
1:B:1250:CYS:HB3	1:B:1268:PRO:HG3	1.91	0.52
1:B:2556:LEU:HD23	1:B:2567:TRP:HB3	1.90	0.52
1:B:3047:LYS:HD3	1:B:3054:ASP:HB2	1.91	0.52
1:A:354:ILE:HD13	1:A:357:ILE:HD12	1.91	0.52
1:A:977:PRO:HD2	1:B:2776:LEU:HD22	1.91	0.52
1:B:3203:PHE:HB3	1:B:3454:ILE:HG13	1.92	0.52
1:B:3599:TRP:CE2	1:B:3612:GLN:HG3	2.45	0.52
1:B:3832:CYS:HB2	1:B:3833:PRO:HD2	1.91	0.52
1:A:713:PHE:HB3	1:A:960:LEU:HD12	1.90	0.52
1:A:1353:CYS:SG	1:A:1364:CYS:HB2	2.50	0.52
1:A:2688:ASN:HB2	1:A:2690:LYS:HE3	1.92	0.52
1:A:4060:ASP:HB3	1:A:4312:ASN:HD21	1.74	0.52
1:A:4174:ARG:HD3	1:A:4374:PRO:HA	1.92	0.52
1:A:4280:PHE:HB2	1:A:4320:ILE:HG21	1.92	0.52
1:B:578:PHE:CB	1:B:1175:VAL:HG12	2.39	0.52
1:B:1238:GLN:HE22	1:B:3178:CYS:H	1.57	0.52
1:B:1936:ALA:HB2	1:B:1966:ILE:HD11	1.90	0.52
1:A:1192:PHE:N	1:A:1201:ILE:O	2.43	0.52
1:A:1731:TRP:HB3	1:A:1740:CYS:SG	2.50	0.52
1:A:2432:ARG:NH2	1:A:2495:GLU:O	2.42	0.52
1:B:1205:ASN:ND2	1:B:1212:ASP:OD1	2.43	0.52
1:B:1731:TRP:HB3	1:B:1740:CYS:SG	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2318:ASP:OD1	1:B:2319:ASN:N	2.43	0.52
1:A:368:ARG:CG	1:A:369:HIS:H	2.23	0.51
1:A:1746:PRO:HB3	1:A:2011:HIS:HA	1.92	0.51
1:A:4020:HIS:CD2	1:A:4033:ALA:HB2	2.44	0.51
1:B:3332:TYR:O	1:B:3485:GLY:N	2.40	0.51
1:A:336:TYR:O	1:A:346:CYS:HB2	2.11	0.51
1:A:843:THR:CG2	1:A:872:PRO:HG2	2.39	0.51
1:B:1162:ILE:HG21	1:B:1173:ASP:HB3	1.93	0.51
1:B:1356:PHE:C	1:B:1358:GLY:N	2.65	0.51
1:B:3782:ASN:O	1:B:3782:ASN:ND2	2.43	0.51
1:A:946:GLU:O	1:A:947:MET:C	2.52	0.51
1:A:1073:THR:HA	1:A:1079:CYS:HA	1.92	0.51
1:B:1549:LYS:O	1:B:1589:ARG:NH1	2.34	0.51
1:B:1966:ILE:HG23	1:B:1973:LEU:HD11	1.92	0.51
1:A:2706:THR:HA	1:A:2712:CYS:HA	1.92	0.51
1:B:3245:ASP:O	1:B:3249:GLN:N	2.43	0.51
1:B:3509:MET:HB3	1:B:3511:MET:HG2	1.92	0.51
1:B:3688:THR:HB	1:B:3707:ASP:HB3	1.92	0.51
1:A:719:ILE:HD11	1:A:743:PHE:HB3	1.92	0.51
1:A:1685:TRP:HB3	1:A:1687:LEU:HD13	1.91	0.51
1:A:2523:TRP:NE1	1:A:2533:GLU:HB2	2.26	0.51
1:B:1113:GLN:HB3	1:B:1121:CYS:HB3	1.93	0.51
1:A:711:LEU:HD11	1:A:960:LEU:HG	1.92	0.51
1:A:862:LEU:HD12	1:A:863:PRO:HD2	1.92	0.51
1:A:907:LEU:HD22	1:A:943:ASP:HA	1.92	0.51
1:A:2569:ASP:HB3	1:A:2572:LEU:HB2	1.92	0.51
1:A:4091:TRP:CZ2	1:A:4323:GLN:HB2	2.46	0.51
1:B:441:THR:HG22	1:B:448:VAL:HG22	1.91	0.51
1:B:2242:ASP:OD2	1:B:2305:LYS:NZ	2.41	0.51
1:A:237:GLN:HE22	1:A:547:ASN:HB3	1.76	0.51
1:A:1484:ASP:HB3	1:A:1487:GLN:HB2	1.93	0.51
1:A:1650:LEU:O	1:A:1696:LYS:NZ	2.38	0.51
1:A:4224:VAL:HG23	1:A:4228:LEU:HD11	1.92	0.51
1:A:4232:THR:O	1:A:4247:SER:OG	2.29	0.51
1:B:465:SER:OG	1:B:501:ARG:NH1	2.43	0.51
1:B:1009:ASN:HD21	1:B:1011:LEU:HD12	1.75	0.51
1:B:1576:HIS:O	1:B:1578:ARG:NH1	2.41	0.51
1:B:1746:PRO:HB3	1:B:2011:HIS:HA	1.93	0.51
1:B:3862:ASP:O	1:B:3863:GLY:C	2.54	0.51
1:A:834:HIS:CD2	1:A:879:TRP:HZ3	2.28	0.51
1:A:2141:GLY:O	1:A:2163:ASN:ND2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2534:ARG:HE	1:A:2545:ILE:HD11	1.75	0.51
1:A:3103:ASN:O	1:A:3107:LYS:HB3	2.11	0.51
1:B:1191:GLN:HA	1:B:1202:GLY:HA2	1.93	0.51
1:B:3798:CYS:SG	1:B:3799:HIS:N	2.84	0.51
1:A:1626:ASP:OD1	1:A:1626:ASP:N	2.41	0.51
1:A:4099:SER:O	1:A:4120:ILE:N	2.37	0.51
1:B:847:ARG:HD2	1:B:848:PRO:HA	1.92	0.51
1:B:1838:THR:HG23	1:B:1873:PRO:HG2	1.93	0.51
1:A:995:GLN:HA	1:B:2756:TYR:CE2	2.46	0.51
1:A:3329:HIS:HB2	1:A:3372:ILE:HD13	1.93	0.51
1:A:3479:LEU:HB2	1:A:3492:GLU:HB2	1.92	0.51
1:B:485:GLU:HG2	1:B:490:ARG:CZ	2.41	0.51
1:B:1187:CYS:SG	1:B:1193:LYS:HG2	2.51	0.51
1:B:1353:CYS:SG	1:B:1371:ALA:HA	2.51	0.51
1:B:1650:LEU:O	1:B:1696:LYS:NZ	2.35	0.51
1:B:3371:THR:HG23	1:B:3380:TYR:HB2	1.93	0.51
1:B:3398:HIS:HB2	1:B:3400:HIS:CE1	2.46	0.51
1:A:626:LYS:HB3	1:A:636:GLN:HB2	1.92	0.50
1:B:744:VAL:HG22	1:B:958:LEU:HD13	1.93	0.50
1:B:2523:TRP:NE1	1:B:2533:GLU:HB2	2.26	0.50
1:A:1198:ASP:N	1:A:1198:ASP:OD1	2.43	0.50
1:A:1378:GLY:HA3	1:A:1409:GLY:HA2	1.92	0.50
1:A:2176:ILE:HG22	1:A:2177:ASN:OD1	2.11	0.50
1:A:2653:ASN:HB3	1:A:2656:GLU:HG3	1.92	0.50
1:B:779:ALA:HB2	1:B:811:MET:HE1	1.93	0.50
1:B:1131:ASP:C	1:B:1133:ASP:H	2.19	0.50
1:B:1209:GLY:N	1:B:1219:GLU:OE1	2.41	0.50
1:B:3281:SER:O	1:B:3283:LYS:NZ	2.43	0.50
1:B:4091:TRP:CZ2	1:B:4323:GLN:HB2	2.47	0.50
1:A:3998:ASN:ND2	1:A:4000:PHE:H	2.09	0.50
1:B:3644:ASN:ND2	1:B:3662:ASP:OD2	2.45	0.50
1:B:4089:TYR:HB3	1:B:4101:VAL:HG22	1.92	0.50
1:A:1170:GLY:N	1:A:1180:GLU:OE2	2.45	0.50
1:A:3284:LEU:N	1:A:3297:SER:O	2.39	0.50
1:A:3782:ASN:O	1:A:3782:ASN:ND2	2.44	0.50
1:B:488:VAL:HG11	1:B:720:ARG:HD2	1.94	0.50
1:B:897:SER:HA	1:B:903:ASP:O	2.11	0.50
1:B:2603:GLN:HA	1:B:2620:LYS:HE3	1.93	0.50
1:B:2608:THR:HB	1:B:2637:PRO:HG2	1.93	0.50
1:B:2686:ALA:O	1:B:2690:LYS:N	2.34	0.50
1:A:3371:THR:HG23	1:A:3380:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ASP:OD1	1:B:892:ASP:N	2.44	0.50
1:B:1198:ASP:OD1	1:B:1198:ASP:N	2.42	0.50
1:B:1967:ALA:HB1	1:B:2009:VAL:HG23	1.94	0.50
1:B:2137:ILE:HG22	1:B:2138:VAL:HG23	1.92	0.50
1:B:3208:TYR:HB3	1:B:3221:LEU:HD21	1.93	0.50
1:B:3799:HIS:HB2	1:B:3802:TYR:HD2	1.76	0.50
1:A:2492:SER:HB3	1:A:2501:THR:HG23	1.93	0.50
1:B:339:ASN:HB2	1:B:342:ASP:O	2.11	0.50
1:B:3531:LYS:HA	1:B:3543:ASP:HB2	1.93	0.50
1:A:1071:ALA:HB1	1:A:1079:CYS:HB3	1.93	0.50
1:A:3047:LYS:HD3	1:A:3054:ASP:HB2	1.93	0.50
1:A:3129:THR:OG1	1:A:3130:LEU:N	2.44	0.50
1:A:3183:LEU:N	1:A:3192:ARG:O	2.43	0.50
1:B:747:ASP:OD1	1:B:748:PHE:N	2.42	0.50
1:B:1367:GLU:HG3	1:B:1370:GLY:H	1.77	0.50
1:B:2476:ILE:HG13	1:B:2516:PRO:HB2	1.94	0.50
1:B:2758:TYR:HB2	1:B:2766:CYS:HB3	1.94	0.50
1:A:1518:TRP:HA	1:A:1521:ARG:HH21	1.77	0.50
1:A:4178:TRP:HB3	1:A:4181:SER:HB3	1.92	0.50
1:B:2257:ILE:HG13	1:B:2270:VAL:HG13	1.94	0.50
1:B:2432:ARG:NH2	1:B:2495:GLU:O	2.45	0.50
1:B:3626:ASP:HB3	1:B:3629:HIS:HD2	1.77	0.50
1:A:539:GLU:OE2	1:A:548:ARG:NE	2.45	0.50
1:A:892:ASP:OD1	1:A:892:ASP:N	2.44	0.50
1:B:336:TYR:O	1:B:346:CYS:HB2	2.11	0.50
1:B:556:LEU:HD11	1:B:559:PRO:HB3	1.93	0.50
1:B:940:ARG:NE	1:B:944:GLY:O	2.32	0.50
1:B:1685:TRP:HB3	1:B:1687:LEU:HD13	1.93	0.50
1:B:3608:PRO:HD2	1:B:3611:TRP:CE3	2.47	0.50
1:A:1549:LYS:O	1:A:1589:ARG:NH1	2.33	0.49
1:A:1822:PRO:HG3	1:A:1841:ARG:HH11	1.77	0.49
1:A:3599:TRP:CE2	1:A:3612:GLN:HG3	2.47	0.49
1:B:3111:ILE:N	1:B:3113:GLU:OE2	2.41	0.49
1:B:3855:ILE:HD12	1:B:3855:ILE:H	1.76	0.49
1:A:2167:SER:O	1:B:1618:TYR:OH	2.27	0.49
1:A:2449:ALA:HA	1:A:2456:HIS:CD2	2.47	0.49
1:B:1365:VAL:HG11	1:B:1372:LYS:HD3	1.94	0.49
1:B:2774:GLY:HA3	1:B:2777:PHE:HD2	1.77	0.49
1:B:3345:TYR:HD2	1:B:3347:GLY:H	1.60	0.49
1:B:3612:GLN:HG2	1:B:3629:HIS:HE1	1.75	0.49
1:B:3811:VAL:HG21	1:B:3822:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3829:GLU:HB3	1:B:3835:ARG:HH22	1.76	0.49
1:A:750:ALA:N	1:A:968:GLN:OE1	2.38	0.49
1:A:1225:ARG:O	1:A:1227:PRO:HD3	2.12	0.49
1:A:2426:TYR:CZ	1:A:2428:SER:HA	2.47	0.49
1:A:3398:HIS:HB2	1:A:3400:HIS:CE1	2.47	0.49
1:B:501:ARG:HG2	1:B:693:PHE:HE2	1.77	0.49
1:B:3312:VAL:HA	1:B:3356:LYS:HD3	1.94	0.49
1:B:3423:THR:HG22	1:B:3430:VAL:HG22	1.94	0.49
1:B:3804:GLN:HE21	1:B:3808:GLY:HA2	1.77	0.49
1:A:337:ILE:HA	1:A:346:CYS:HB2	1.94	0.49
1:A:3124:HIS:HE1	1:A:3141:TYR:CG	2.30	0.49
1:A:4008:ILE:N	1:A:4026:GLY:H	2.09	0.49
1:B:2345:PRO:HB2	1:B:2366:PRO:HB3	1.94	0.49
1:B:2548:SER:O	1:B:2585:ARG:NH1	2.38	0.49
1:B:4038:SER:OG	1:B:4040:SER:O	2.30	0.49
1:A:2393:ALA:HB2	1:A:2424:LEU:HG	1.93	0.49
1:A:2758:TYR:HB3	1:A:2763:TYR:HB2	1.94	0.49
1:A:2759:ARG:NE	1:A:2759:ARG:O	2.45	0.49
1:A:3199:PRO:HB3	1:A:3458:HIS:HB2	1.94	0.49
1:B:4116:LYS:HG2	1:B:4135:ASP:HA	1.94	0.49
1:A:768:GLN:HE21	1:A:772:GLY:HA2	1.77	0.49
1:A:1403:HIS:CD2	1:A:1403:HIS:H	2.29	0.49
1:A:1966:ILE:HG23	1:A:1973:LEU:HD11	1.94	0.49
1:A:1986:VAL:HB	1:A:1991:GLY:HA2	1.94	0.49
1:A:3513:SER:HB3	1:A:3593:HIS:CG	2.48	0.49
1:B:493:MET:HE1	1:B:673:VAL:HG11	1.94	0.49
1:B:744:VAL:HG13	1:B:959:HIS:HE1	1.78	0.49
1:B:3560:CYS:SG	1:B:3582:SER:HB3	2.53	0.49
1:A:754:THR:HG21	1:A:767:LYS:HE3	1.93	0.49
1:A:1416:ASP:OD1	1:A:1417:THR:N	2.45	0.49
1:A:1615:MET:HG3	1:A:1648:LEU:HD12	1.94	0.49
1:A:3268:ARG:HB2	1:A:3304:ARG:HH12	1.78	0.49
1:B:1822:PRO:HG3	1:B:1841:ARG:HH11	1.77	0.49
1:B:2706:THR:HA	1:B:2712:CYS:HA	1.94	0.49
1:B:3312:VAL:HG11	1:B:3337:TRP:HZ2	1.77	0.49
1:B:3821:ALA:HA	1:B:3829:GLU:HG2	1.94	0.49
1:A:359:ASP:O	1:A:629:LYS:NZ	2.40	0.49
1:A:894:ILE:HG13	1:A:913:MET:HE1	1.94	0.49
1:A:3081:LYS:HA	1:A:3087:CYS:HA	1.95	0.49
1:A:3360:ILE:HD12	1:A:3399:ARG:HD2	1.93	0.49
1:A:3608:PRO:HD2	1:A:3611:TRP:CE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3644:ASN:ND2	1:A:3662:ASP:OD2	2.46	0.49
1:B:3780:HIS:N	1:B:3790:GLU:OE1	2.40	0.49
1:B:4230:TRP:CG	1:B:4250:LYS:HB2	2.48	0.49
1:A:338:ILE:HG23	1:A:347:VAL:HG12	1.95	0.49
1:A:1967:ALA:HB1	1:A:2009:VAL:HG23	1.95	0.49
1:A:2242:ASP:OD2	1:A:2305:LYS:NZ	2.42	0.49
1:A:2420:THR:O	1:A:2438:ASN:N	2.46	0.49
1:A:2557:THR:HG21	1:A:2599:THR:HA	1.94	0.49
1:A:3259:THR:HG21	2:E:1:NAG:N2	2.28	0.49
1:A:3835:ARG:HH11	1:A:3841:TYR:HD2	1.60	0.49
1:B:1437:LEU:HB2	1:B:1692:VAL:HB	1.93	0.49
1:B:2176:ILE:HG22	1:B:2177:ASN:OD1	2.13	0.49
1:B:3657:ASP:OD1	1:B:3706:ARG:NE	2.46	0.49
1:A:2513:VAL:HB	1:A:2522:TYR:HB2	1.94	0.49
1:A:3657:ASP:OD1	1:A:3706:ARG:NE	2.45	0.49
1:A:3688:THR:HB	1:A:3707:ASP:HB3	1.94	0.49
1:B:1986:VAL:HB	1:B:1991:GLY:HA2	1.94	0.49
1:B:2475:TRP:CZ2	1:B:2649:GLN:HB2	2.39	0.49
1:A:865:ILE:HG22	1:A:869:LEU:HD11	1.94	0.48
1:A:1357:ASN:O	1:A:1364:CYS:HB3	2.13	0.48
1:A:2144:GLU:HG3	1:A:2166:VAL:HG23	1.94	0.48
1:B:390:SER:HB2	4:B:4701:NAG:O5	2.13	0.48
1:B:1170:GLY:N	1:B:1180:GLU:OE2	2.44	0.48
1:B:1856:TYR:HB3	1:B:2046:ALA:HB2	1.94	0.48
1:B:2601:TYR:HB2	1:B:2642:THR:HG21	1.95	0.48
1:A:887:VAL:HG22	1:A:894:ILE:HG12	1.94	0.48
1:A:924:GLU:HA	1:A:941:LYS:HE3	1.94	0.48
1:A:1362:HIS:CG	1:A:1363:GLU:N	2.80	0.48
1:A:1519:VAL:HB	1:A:1561:PRO:HB2	1.95	0.48
1:A:2493:MET:HG2	1:A:2497:GLY:HA2	1.95	0.48
1:A:2550:LEU:HD11	1:A:2553:PRO:HB3	1.94	0.48
1:A:2603:GLN:HA	1:A:2620:LYS:HE3	1.94	0.48
1:A:3518:LEU:HD11	1:A:3522:ASN:HD22	1.78	0.48
1:B:2466:GLY:HA3	1:B:2486:LEU:HD22	1.94	0.48
1:B:3129:THR:OG1	1:B:3130:LEU:N	2.46	0.48
1:A:1848:LEU:HD11	1:A:1855:ARG:HB3	1.95	0.48
1:A:3245:ASP:O	1:A:3249:GLN:N	2.45	0.48
1:A:4102:TYR:OH	1:A:4171:LEU:HG	2.14	0.48
1:B:1378:GLY:HA3	1:B:1409:GLY:HA2	1.95	0.48
1:B:1518:TRP:HA	1:B:1521:ARG:HH21	1.78	0.48
1:B:2428:SER:O	1:B:2429:VAL:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2449:ALA:HA	1:B:2456:HIS:CD2	2.48	0.48
1:B:3081:LYS:HA	1:B:3087:CYS:HA	1.94	0.48
1:B:3259:THR:HG21	2:K:1:NAG:N2	2.28	0.48
1:B:3582:SER:HA	1:B:3585:ASP:HB2	1.95	0.48
1:B:3849:CYS:SG	1:B:3853:VAL:HB	2.53	0.48
1:A:582:GLU:HG3	1:A:583:THR:H	1.78	0.48
1:A:748:PHE:O	1:A:968:GLN:NE2	2.46	0.48
1:A:1844:SER:OG	1:A:1846:GLU:OE2	2.24	0.48
1:A:2475:TRP:CZ2	1:A:2649:GLN:HB2	2.44	0.48
1:A:3056:ASP:OD1	1:A:3056:ASP:N	2.44	0.48
1:B:639:TYR:HE1	1:B:641:ALA:HB2	1.79	0.48
1:B:2450:THR:H	1:B:2456:HIS:CE1	2.31	0.48
1:B:2569:ASP:HB3	1:B:2572:LEU:HB2	1.95	0.48
1:B:2654:PRO:HB2	1:B:2673:ALA:HB2	1.95	0.48
1:A:1551:LEU:HD11	1:A:1554:PRO:HB3	1.95	0.48
1:A:3103:ASN:HD21	1:A:3106:GLU:HG2	1.78	0.48
1:B:424:GLY:HA2	1:B:444:VAL:HB	1.95	0.48
1:B:494:VAL:HG12	1:B:501:ARG:HA	1.95	0.48
1:B:2393:ALA:HB2	1:B:2424:LEU:HG	1.93	0.48
1:B:2394:LEU:HD22	1:B:2399:ARG:CZ	2.43	0.48
1:A:484:VAL:HG22	1:A:491:ILE:HG12	1.95	0.48
1:A:940:ARG:HG3	1:A:946:GLU:HG3	1.95	0.48
1:A:945:GLY:C	1:A:946:GLU:HG3	2.39	0.48
1:B:1868:LEU:HD23	1:B:1910:VAL:HG23	1.94	0.48
1:B:3103:ASN:ND2	1:B:3105:ASP:OD1	2.47	0.48
1:A:563:THR:HG23	1:A:572:TYR:HB2	1.96	0.48
1:A:842:PHE:CE1	1:A:852:MET:HB2	2.49	0.48
1:A:974:CYS:HB3	1:A:981:ASN:HA	1.95	0.48
1:A:1903:ALA:HB2	1:A:1910:VAL:HG12	1.94	0.48
1:A:1927:ASP:OD2	1:A:1988:LYS:NZ	2.46	0.48
1:A:2036:VAL:HG12	1:A:2040:LEU:HB2	1.96	0.48
1:A:2686:ALA:HB3	1:A:2691:HIS:HB2	1.96	0.48
1:B:555:LYS:HB3	1:B:591:ARG:HH22	1.79	0.48
1:B:685:LEU:HB3	1:B:687:PHE:CE2	2.49	0.48
1:B:1580:GLU:HG2	1:B:1591:VAL:HG22	1.96	0.48
1:B:4208:PRO:O	1:B:4228:LEU:HD12	2.13	0.48
1:A:1074:CYS:N	1:A:1078:GLU:O	2.44	0.48
1:A:1154:PHE:CG	1:A:1155:ASN:N	2.82	0.48
1:A:1469:VAL:HG13	1:A:1687:LEU:HD23	1.96	0.48
1:A:3244:ILE:HD13	1:A:3272:ALA:HB1	1.96	0.48
1:B:1136:ASP:OD1	1:B:1136:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:CYS:CB	1:A:1159:HIS:HB3	2.43	0.48
1:A:2608:THR:HB	1:A:2637:PRO:HG2	1.95	0.48
1:B:1160:ARG:NE	1:B:1162:ILE:HG22	2.28	0.48
1:B:1362:HIS:O	1:B:1363:GLU:C	2.57	0.48
1:B:1755:ILE:HD12	1:B:1757:PHE:HE2	1.79	0.48
1:B:3329:HIS:HB2	1:B:3372:ILE:HD13	1.96	0.48
1:B:3859:TRP:HA	1:B:3862:ASP:HB3	1.96	0.48
1:A:788:SER:HB2	1:A:830:SER:HA	1.96	0.48
1:B:981:ASN:HA	1:B:988:CYS:HB2	1.96	0.48
1:B:1483:SER:HB2	1:B:1514:ILE:HD11	1.96	0.48
1:B:1487:GLN:OE1	1:B:1491:TRP:NE1	2.36	0.48
1:B:2502:VAL:H	1:B:2679:HIS:HB3	1.79	0.48
1:B:4000:PHE:HA	1:B:4004:SER:HB3	1.96	0.48
1:B:4175:TYR:HB3	1:B:4354:PRO:HB3	1.96	0.48
1:A:354:ILE:HB	1:A:357:ILE:HB	1.95	0.47
1:A:584:VAL:HB	1:A:588:GLY:HA2	1.96	0.47
1:A:883:ARG:HH12	1:A:903:ASP:HB3	1.79	0.47
1:A:2020:ASN:N	1:A:2023:SER:OG	2.38	0.47
1:A:3836:PHE:CD2	1:A:3838:ASP:HB3	2.47	0.47
1:B:3834:THR:HA	1:B:3841:TYR:CE2	2.49	0.47
1:A:867:THR:O	1:A:904:ARG:NH1	2.37	0.47
1:B:1465:GLY:HA3	1:B:1468:ILE:HD11	1.95	0.47
1:B:1510:LEU:HD23	1:B:1528:TYR:HB3	1.96	0.47
1:B:1903:ALA:HB2	1:B:1910:VAL:HG12	1.95	0.47
1:B:3220:SER:OG	1:B:3221:LEU:N	2.47	0.47
1:A:397:ILE:HG12	1:A:406:ILE:HG12	1.95	0.47
1:A:520:THR:HA	1:A:679:ARG:HH21	1.79	0.47
1:A:3103:ASN:ND2	1:A:3105:ASP:OD1	2.47	0.47
1:A:3801:GLU:N	1:A:3801:GLU:OE1	2.42	0.47
1:A:3819:GLY:N	1:A:3829:GLU:OE1	2.47	0.47
1:B:479:ASN:N	1:B:479:ASN:OD1	2.48	0.47
1:B:3244:ILE:HG21	1:B:3272:ALA:HB3	1.96	0.47
1:B:3294:LEU:HD21	1:B:3335:LEU:HD23	1.97	0.47
1:B:3533:ASP:HA	1:B:3551:ARG:NE	2.29	0.47
1:A:1175:VAL:HG23	1:A:1176:ASP:N	2.30	0.47
1:A:2548:SER:O	1:A:2585:ARG:NH1	2.39	0.47
1:A:3560:CYS:SG	1:A:3582:SER:HB3	2.54	0.47
1:A:4182:THR:O	1:A:4184:LEU:HG	2.14	0.47
1:A:4255:GLU:HG2	1:A:4266:VAL:HG22	1.96	0.47
1:B:972:ASN:OD1	1:B:973:ALA:N	2.43	0.47
1:B:1522:ASN:HD22	1:B:1537:LYS:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1567:LEU:HD13	1:B:1581:ARG:HD2	1.96	0.47
2:I:1:NAG:H61	2:I:2:NAG:H82	1.95	0.47
1:A:395:SER:HB2	1:A:651:TYR:HB3	1.96	0.47
1:A:843:THR:HG21	1:A:872:PRO:O	2.15	0.47
1:A:883:ARG:HH21	1:A:896:HIS:CD2	2.32	0.47
1:A:2000:ASN:ND2	1:B:2254:SER:O	2.47	0.47
1:B:224:GLY:O	1:B:523:TYR:OH	2.32	0.47
1:B:781:ASN:O	1:B:818:ARG:NH1	2.25	0.47
1:B:1416:ASP:OD1	1:B:1417:THR:N	2.47	0.47
1:B:3513:SER:HB3	1:B:3593:HIS:CG	2.48	0.47
1:A:1354:SER:H	1:A:1366:GLN:NE2	2.13	0.47
1:A:1825:ASN:HD22	1:A:1875:GLY:HA2	1.80	0.47
1:A:1838:THR:HG23	1:A:1873:PRO:HG2	1.95	0.47
1:A:1937:VAL:HG12	1:A:1940:ARG:H	1.80	0.47
1:A:3110:GLY:C	1:A:3111:ILE:HD12	2.40	0.47
1:A:4247:SER:HB3	1:A:4277:LEU:HD21	1.96	0.47
1:B:2707:CYS:CB	1:B:2729:SER:HB3	2.42	0.47
1:A:446:ASN:HB3	1:A:467:GLU:HA	1.96	0.47
1:A:1154:PHE:N	1:A:1162:ILE:O	2.48	0.47
1:A:2345:PRO:HB2	1:A:2366:PRO:HB3	1.96	0.47
1:A:3078:HIS:C	1:A:3090:MET:HG2	2.40	0.47
1:A:3633:ARG:HB3	1:A:3641:ARG:HH12	1.79	0.47
1:B:347:VAL:HG22	1:B:349:PHE:H	1.80	0.47
1:B:351:ASP:OD1	1:B:351:ASP:N	2.47	0.47
1:B:467:GLU:N	1:B:485:GLU:OE2	2.46	0.47
1:B:513:ARG:HD2	1:B:605:PHE:HE1	1.79	0.47
1:B:1519:VAL:HB	1:B:1561:PRO:HB2	1.96	0.47
1:B:1937:VAL:HG12	1:B:1940:ARG:H	1.79	0.47
1:B:2568:VAL:HG12	1:B:2575:ILE:HG23	1.95	0.47
1:B:2653:ASN:HB3	1:B:2656:GLU:HG3	1.96	0.47
1:B:3390:GLU:HG2	1:B:3401:THR:HA	1.96	0.47
1:B:4312:ASN:N	1:B:4312:ASN:HD22	2.12	0.47
1:A:248:LYS:C	1:A:250:ASN:H	2.23	0.47
1:B:617:THR:HG22	1:B:624:VAL:HG22	1.97	0.47
1:B:852:MET:HE3	1:B:863:PRO:HB3	1.96	0.47
1:B:1141:LYS:O	1:B:1142:ASN:C	2.57	0.47
1:B:1551:LEU:HD11	1:B:1554:PRO:HB3	1.97	0.47
1:B:3599:TRP:HB2	1:B:3609:GLU:HA	1.96	0.47
1:B:4293:GLU:OE1	1:B:4307:LYS:HE2	2.15	0.47
1:A:1163:ASP:OD1	1:A:1164:LEU:N	2.47	0.47
1:A:2686:ALA:O	1:A:2690:LYS:N	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1615:MET:HG3	1:B:1648:LEU:HD12	1.97	0.47
1:B:1626:ASP:OD1	1:B:1626:ASP:N	2.45	0.47
1:B:1848:LEU:HD11	1:B:1855:ARG:HB3	1.97	0.47
1:B:1975:TYR:OH	1:B:1984:GLU:OE1	2.21	0.47
1:B:2490:ILE:N	1:B:2504:ALA:O	2.47	0.47
1:B:2599:THR:HG22	1:B:2606:TYR:HB2	1.97	0.47
1:B:3195:SER:HB2	1:B:3460:TYR:CZ	2.50	0.47
1:B:3633:ARG:HB3	1:B:3641:ARG:HH12	1.80	0.47
1:B:3875:LEU:HD22	1:B:3880:ASP:H	1.80	0.47
1:B:4067:TYR:CD2	1:B:4309:LEU:HD11	2.49	0.47
1:B:4255:GLU:HG2	1:B:4266:VAL:HG22	1.96	0.47
1:A:989:PHE:HB2	1:A:997:VAL:O	2.15	0.47
1:A:1031:PHE:N	1:A:1039:VAL:O	2.40	0.47
1:A:1405:TYR:N	1:A:1412:ARG:O	2.36	0.47
1:A:2124:ILE:HD11	1:A:2147:VAL:HG11	1.97	0.47
1:A:3312:VAL:HA	1:A:3356:LYS:HD3	1.96	0.47
1:B:2127:ILE:HA	1:B:2133:SER:O	2.14	0.47
1:B:2435:PHE:HZ	1:B:2458:PRO:HB3	1.80	0.47
1:B:3518:LEU:HD11	1:B:3522:ASN:HD22	1.80	0.47
1:A:539:GLU:CD	1:A:548:ARG:HE	2.23	0.46
1:A:1187:CYS:SG	1:A:1193:LYS:HG2	2.55	0.46
1:A:1618:TYR:OH	1:B:2167:SER:O	2.25	0.46
1:A:1667:ARG:NH2	1:A:1677:SER:OG	2.47	0.46
1:A:3533:ASP:HA	1:A:3551:ARG:NE	2.30	0.46
1:A:3775:ARG:HD2	1:A:3802:TYR:HE2	1.80	0.46
1:B:867:THR:O	1:B:904:ARG:NH1	2.34	0.46
1:A:465:SER:OG	1:A:501:ARG:NH1	2.48	0.46
1:A:490:ARG:HH21	1:A:501:ARG:NH2	2.13	0.46
1:A:829:ARG:HB2	1:A:845:TRP:CD1	2.50	0.46
1:A:1825:ASN:OD1	1:A:1826:LEU:N	2.48	0.46
1:A:2428:SER:O	1:A:2429:VAL:C	2.58	0.46
1:A:3047:LYS:HA	1:A:3052:ASP:HB2	1.98	0.46
1:A:3103:ASN:O	1:A:3107:LYS:N	2.41	0.46
1:A:3502:LEU:HD11	1:A:3507:TYR:HB2	1.96	0.46
1:B:400:ASN:OD1	1:B:401:GLY:N	2.47	0.46
1:B:490:ARG:HH21	1:B:501:ARG:NH2	2.12	0.46
1:B:518:ASP:OD1	1:B:520:THR:OG1	2.30	0.46
1:B:552:VAL:HG21	1:B:573:TRP:CH2	2.51	0.46
1:B:3376:ASN:ND2	1:B:3436:TYR:OH	2.48	0.46
1:A:910:ILE:HG21	1:A:913:MET:HB2	1.97	0.46
1:A:3640:PHE:HE2	1:A:3665:ASP:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ARG:HD2	1:B:605:PHE:CE1	2.51	0.46
1:B:677:SER:OG	1:B:678:HIS:N	2.48	0.46
1:B:2426:TYR:CZ	1:B:2428:SER:HA	2.51	0.46
1:A:1081:PRO:HD2	1:A:1084:TRP:CE3	2.50	0.46
1:A:2576:GLU:HG2	1:A:2587:VAL:HG22	1.98	0.46
1:A:4058:LEU:HD13	1:A:4311:VAL:HG21	1.97	0.46
1:B:1084:TRP:HB3	1:B:1091:ASP:OD2	2.16	0.46
1:B:1156:CYS:HB3	1:B:1159:HIS:HB3	1.98	0.46
1:B:1606:ASP:N	1:B:1606:ASP:OD1	2.48	0.46
1:B:4224:VAL:HG23	1:B:4228:LEU:HD11	1.97	0.46
1:B:4277:LEU:HB3	1:B:4284:LEU:HD21	1.96	0.46
1:A:949:VAL:HG11	1:A:952:SER:HB3	1.97	0.46
1:A:2192:PRO:HB3	1:A:2206:TRP:CD1	2.50	0.46
1:A:4312:ASN:ND2	1:A:4314:TRP:HB2	2.30	0.46
1:A:685:LEU:HB3	1:A:687:PHE:CE2	2.49	0.46
1:A:2254:SER:O	1:B:2000:ASN:ND2	2.48	0.46
1:A:3092:LYS:HB3	1:A:3099:ASP:OD2	2.15	0.46
1:A:3204:SER:O	1:A:3452:PHE:HB2	2.16	0.46
1:A:3220:SER:OG	1:A:3221:LEU:N	2.48	0.46
1:A:3458:HIS:CD2	1:A:3460:TYR:H	2.34	0.46
1:B:248:LYS:C	1:B:250:ASN:H	2.24	0.46
1:B:2523:TRP:NE1	1:B:2533:GLU:OE1	2.38	0.46
1:B:2550:LEU:HD11	1:B:2553:PRO:HB3	1.97	0.46
1:B:4057:LEU:HG	1:B:4321:PHE:HB2	1.98	0.46
1:B:4098:LEU:HD13	1:B:4380:PRO:HG2	1.97	0.46
1:A:847:ARG:HH11	1:A:848:PRO:HA	1.81	0.46
1:A:1097:ASP:OD1	1:A:1097:ASP:N	2.49	0.46
1:A:2568:VAL:HG13	1:A:2598:LEU:HD22	1.97	0.46
1:A:3270:PRO:HB2	1:A:3290:ARG:HB3	1.98	0.46
1:B:508:ASN:O	1:B:532:LEU:HG	2.16	0.46
1:B:862:LEU:HD12	1:B:863:PRO:HD2	1.98	0.46
1:B:2450:THR:O	1:B:2453:SER:OG	2.33	0.46
1:B:3103:ASN:O	1:B:3107:LYS:N	2.48	0.46
1:B:3573:ASN:OD1	1:B:3577:ASN:ND2	2.40	0.46
1:B:3626:ASP:HB3	1:B:3629:HIS:CD2	2.51	0.46
1:B:4186:GLN:HB3	1:B:4204:TRP:CZ3	2.51	0.46
1:B:4272:MET:HE1	1:B:4295:TRP:CE2	2.51	0.46
1:A:1422:GLU:HG2	1:A:1423:SER:H	1.80	0.46
1:A:4203:ASP:O	1:A:4208:PRO:HA	2.16	0.46
1:A:4329:SER:HB3	3:G:1:NAG:H5	1.97	0.46
1:B:1249:GLU:HA	1:B:1261:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1403:HIS:CD2	1:B:1403:HIS:H	2.31	0.46
1:B:2576:GLU:HG2	1:B:2587:VAL:HG22	1.97	0.46
1:B:3103:ASN:HD21	1:B:3106:GLU:HG2	1.81	0.46
1:B:4087:VAL:HG12	1:B:4103:TYR:HB3	1.97	0.46
1:A:406:ILE:HD11	1:A:417:LEU:HD22	1.98	0.46
1:A:1352:SER:HA	1:A:1355:ASP:CB	2.43	0.46
1:A:1856:TYR:HB3	1:A:2046:ALA:HB2	1.98	0.46
1:A:3238:GLU:HG3	1:A:3282:ARG:HH22	1.81	0.46
1:B:1825:ASN:OD1	1:B:1826:LEU:N	2.48	0.46
1:B:3273:GLU:OE2	1:B:3324:ARG:NH2	2.48	0.46
1:B:3458:HIS:CD2	1:B:3460:TYR:H	2.34	0.46
1:B:4092:ASP:OD1	1:B:4092:ASP:N	2.48	0.46
1:A:771:ASP:OD1	1:A:771:ASP:N	2.38	0.46
1:A:1580:GLU:HG2	1:A:1591:VAL:HG22	1.98	0.46
1:A:3345:TYR:HD2	1:A:3347:GLY:H	1.64	0.46
1:A:4068:ASN:ND2	3:H:1:NAG:O7	2.49	0.46
1:B:1154:PHE:CD1	1:B:1167:VAL:HG22	2.51	0.46
1:B:1828:LEU:HD12	1:B:1835:LEU:HD12	1.98	0.46
1:B:2725:CYS:HB2	1:B:2727:ASP:O	2.15	0.46
1:B:3729:ASN:N	1:B:3747:ASP:OD2	2.47	0.46
1:A:513:ARG:HD2	1:A:605:PHE:HE1	1.81	0.45
1:A:1606:ASP:OD1	1:A:1606:ASP:N	2.49	0.45
1:A:2572:LEU:HD13	1:A:2574:ARG:HH21	1.81	0.45
1:A:3294:LEU:HD21	1:A:3335:LEU:HD23	1.97	0.45
1:A:4252:ASP:OD1	1:A:4272:MET:N	2.49	0.45
1:B:1960:LEU:HD13	1:B:1963:PRO:HB3	1.98	0.45
1:B:3047:LYS:HA	1:B:3052:ASP:HB2	1.98	0.45
1:B:3453:ASP:OD1	1:B:3454:ILE:N	2.48	0.45
1:A:3233:ASP:OD2	1:A:3277:VAL:N	2.36	0.45
1:B:1251:ASP:N	1:B:1262:GLU:OE1	2.49	0.45
1:B:1365:VAL:H	1:B:1373:CYS:N	2.12	0.45
1:B:1956:LEU:HD23	1:B:1973:LEU:HD22	1.97	0.45
1:B:2557:THR:HG21	1:B:2599:THR:HA	1.99	0.45
1:A:518:ASP:OD1	1:A:521:VAL:HG22	2.17	0.45
1:A:1440:VAL:HG21	1:A:1665:VAL:HG21	1.97	0.45
1:A:2140:HIS:O	1:A:2181:ARG:NH1	2.35	0.45
1:A:2450:THR:H	1:A:2456:HIS:CE1	2.34	0.45
1:B:558:TRP:H	1:B:575:ASP:CG	2.24	0.45
1:B:1109:CYS:HB3	1:B:1113:GLN:HB2	1.99	0.45
1:B:2618:ALA:HB1	1:B:2623:GLY:HA2	1.98	0.45
1:B:3124:HIS:HE1	1:B:3141:TYR:CG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4007:ASP:HA	1:B:4026:GLY:H	1.80	0.45
1:A:578:PHE:CG	1:A:1175:VAL:HG12	2.52	0.45
1:A:754:THR:HA	1:A:769:LYS:HA	1.97	0.45
1:A:1721:HIS:HB3	1:A:1723:TYR:CE2	2.52	0.45
1:A:2601:TYR:HB2	1:A:2642:THR:HG21	1.99	0.45
1:A:3226:LEU:HD13	1:A:3229:VAL:HG21	1.99	0.45
1:A:3533:ASP:HA	1:A:3551:ARG:HE	1.82	0.45
1:B:754:THR:HG21	1:B:767:LYS:HE3	1.97	0.45
1:B:1644:HIS:CE1	1:B:1660:ARG:HD3	2.52	0.45
1:A:978:THR:C	1:A:980:PRO:HD3	2.41	0.45
1:A:1158:ASN:HB3	1:A:1175:VAL:CG2	2.46	0.45
1:A:3517:PHE:N	1:A:3526:ILE:O	2.49	0.45
1:A:4312:ASN:HB3	1:B:4312:ASN:HB3	1.98	0.45
1:B:369:HIS:HE1	1:B:371:CYS:HB2	1.82	0.45
1:B:2124:ILE:HD11	1:B:2147:VAL:HG11	1.99	0.45
1:B:2572:LEU:HD13	1:B:2574:ARG:HE	1.81	0.45
1:B:3479:LEU:HB2	1:B:3492:GLU:HB2	1.99	0.45
1:A:381:ARG:HD3	1:A:384:TYR:HE1	1.81	0.45
1:A:2102:VAL:O	1:A:2334:GLN:NE2	2.40	0.45
1:A:4006:LEU:O	1:A:4007:ASP:C	2.59	0.45
1:B:622:MET:HE3	1:B:622:MET:HB2	1.63	0.45
1:B:1203:VAL:HA	1:B:1206:ARG:HB2	1.99	0.45
1:A:1203:VAL:HA	1:A:1206:ARG:HB2	1.99	0.45
1:A:1483:SER:HB2	1:A:1514:ILE:HD11	1.98	0.45
1:A:2127:ILE:HA	1:A:2133:SER:O	2.17	0.45
1:A:2155:VAL:HG21	1:A:2341:VAL:HG11	1.98	0.45
1:A:2450:THR:O	1:A:2453:SER:OG	2.29	0.45
1:A:3706:ARG:H	1:A:3706:ARG:HD2	1.81	0.45
1:A:4077:TYR:CE1	1:A:4120:ILE:HG12	2.51	0.45
1:A:4087:VAL:HG12	1:A:4103:TYR:HB3	1.98	0.45
1:B:597:GLY:N	1:B:1158:ASN:HD21	2.15	0.45
1:B:765:ILE:HD11	1:B:786:VAL:HG21	1.97	0.45
1:B:1949:ASP:OD1	1:B:1951:THR:OG1	2.28	0.45
1:B:3078:HIS:C	1:B:3090:MET:HG2	2.42	0.45
1:B:3801:GLU:OE1	1:B:3801:GLU:N	2.49	0.45
1:B:4280:PHE:HB2	1:B:4320:ILE:HG21	1.98	0.45
2:C:1:NAG:H61	2:C:2:NAG:H82	1.98	0.45
1:A:3660:CYS:HB3	1:A:3665:ASP:HB3	1.99	0.45
1:A:4285:TYR:HD2	1:A:4320:ILE:HD11	1.82	0.45
1:B:883:ARG:HH21	1:B:896:HIS:HD2	1.65	0.45
1:B:1747:PHE:HA	1:B:1761:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2374:THR:HG23	1:B:2376:GLN:HE22	1.82	0.45
1:B:2426:TYR:HA	1:B:2433:ILE:HA	1.99	0.45
1:B:2738:LEU:HB3	1:B:2740:THR:HG23	1.99	0.45
1:B:2774:GLY:HA3	1:B:2777:PHE:CD2	2.51	0.45
1:B:3158:GLU:HG2	1:B:3159:MET:HG3	1.99	0.45
1:B:3533:ASP:HA	1:B:3551:ARG:HE	1.82	0.45
1:B:3775:ARG:HD2	1:B:3802:TYR:HE2	1.82	0.45
1:B:4006:LEU:O	1:B:4008:ILE:HG13	2.16	0.45
1:B:1087:ASP:OD1	1:B:1087:ASP:N	2.46	0.45
1:B:3204:SER:O	1:B:3452:PHE:HB2	2.17	0.45
1:A:558:TRP:HB2	1:A:577:ARG:HB2	1.99	0.45
1:A:1049:ASP:HB2	1:A:1054:ASN:HA	1.99	0.45
1:A:1494:PHE:HB2	1:A:1496:ASN:OD1	2.17	0.45
1:A:1567:LEU:HD13	1:A:1581:ARG:HD2	1.99	0.45
1:A:2520:TYR:HA	1:A:2536:THR:HA	1.98	0.45
1:A:3208:TYR:HB3	1:A:3221:LEU:HD21	1.98	0.45
1:B:910:ILE:HD12	1:B:939:VAL:HG11	1.99	0.45
1:B:1422:GLU:HG2	1:B:1423:SER:H	1.80	0.45
1:B:2709:ASN:HD21	1:B:2725:CYS:HB3	1.82	0.45
1:B:4059:PRO:HD2	1:B:4317:GLN:O	2.17	0.45
2:D:1:NAG:H61	2:D:2:NAG:H82	1.99	0.45
1:A:1109:CYS:HB3	1:A:1113:GLN:HB2	1.99	0.44
1:A:2725:CYS:HB2	1:A:2727:ASP:O	2.18	0.44
1:A:3236:ARG:NH2	1:A:3462:GLN:O	2.50	0.44
1:A:3567:SER:O	1:A:3570:THR:OG1	2.33	0.44
1:A:4008:ILE:H	1:A:4026:GLY:H	1.65	0.44
1:A:4171:LEU:HD12	1:A:4171:LEU:HA	1.77	0.44
1:B:695:PHE:HB3	1:B:704:CYS:HB3	1.99	0.44
1:B:830:SER:H	1:B:843:THR:HG23	1.81	0.44
1:B:3244:ILE:HD13	1:B:3272:ALA:HB1	1.99	0.44
1:B:4390:TYR:CD1	1:B:4400:LYS:HG2	2.52	0.44
1:A:1360:CYS:HB3	1:A:1373:CYS:HB3	1.74	0.44
1:A:1522:ASN:HD22	1:A:1537:LYS:HA	1.82	0.44
1:A:1883:GLY:C	1:A:1905:MET:HG3	2.42	0.44
1:A:4004:SER:O	1:A:4006:LEU:HG	2.18	0.44
1:A:4091:TRP:O	1:A:4093:PRO:HD3	2.17	0.44
1:B:1563:MET:HA	1:B:1566:HIS:CE1	2.51	0.44
1:B:1844:SER:OG	1:B:1846:GLU:OE2	2.25	0.44
1:B:3567:SER:O	1:B:3570:THR:OG1	2.33	0.44
1:A:2304:SER:HB3	1:A:2309:ASN:HD22	1.82	0.44
1:A:3799:HIS:HB2	1:A:3802:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:LYS:N	1:B:636:GLN:O	2.47	0.44
1:B:2209:TYR:HB3	1:B:2236:PRO:HD2	2.00	0.44
1:B:2233:ILE:HD11	1:B:2236:PRO:HG3	1.98	0.44
1:B:2475:TRP:H	1:B:2475:TRP:HE3	1.64	0.44
1:B:4091:TRP:O	1:B:4093:PRO:HD3	2.17	0.44
1:A:584:VAL:HG12	1:A:591:ARG:HA	1.98	0.44
1:A:628:ASN:H	1:A:632:GLU:HB2	1.83	0.44
1:A:897:SER:HA	1:A:903:ASP:O	2.18	0.44
1:A:938:ARG:HB3	1:A:948:THR:HB	1.99	0.44
1:A:2653:ASN:HD21	1:A:2655:CYS:HB2	1.81	0.44
1:A:3110:GLY:N	1:A:3130:LEU:O	2.44	0.44
1:A:3110:GLY:H	1:A:3131:THR:HA	1.82	0.44
1:A:3615:THR:HA	1:A:3625:GLU:OE1	2.18	0.44
1:A:3682:THR:O	1:A:3695:LYS:N	2.51	0.44
1:A:3684:PHE:N	1:A:3693:ILE:O	2.41	0.44
1:A:3806:THR:OG1	1:A:3825:ASP:OD2	2.27	0.44
1:B:1044:LEU:HA	1:B:1056:ASP:HB2	2.00	0.44
1:B:1130:THR:HG1	1:B:1160:ARG:HH11	1.65	0.44
1:B:1154:PHE:CD2	1:B:1162:ILE:HD11	2.53	0.44
1:B:1830:TRP:HA	1:B:1833:ARG:HH21	1.83	0.44
1:B:1883:GLY:C	1:B:1905:MET:HG3	2.42	0.44
1:B:2140:HIS:O	1:B:2181:ARG:NH1	2.34	0.44
1:B:3298:ASP:OD1	1:B:3302:GLY:N	2.51	0.44
1:A:2490:ILE:N	1:A:2504:ALA:O	2.46	0.44
1:A:3278:ASP:OD2	1:A:3283:LYS:N	2.42	0.44
1:A:3599:TRP:HB2	1:A:3609:GLU:HA	2.00	0.44
1:B:350:ASP:HB3	1:B:353:GLN:HB2	1.99	0.44
1:B:865:ILE:HG22	1:B:869:LEU:HD11	1.98	0.44
1:B:935:ALA:HB1	1:B:949:VAL:HG13	1.99	0.44
1:B:1226:PRO:O	1:B:1228:GLY:N	2.44	0.44
1:B:1402:GLN:OE1	1:B:1416:ASP:N	2.50	0.44
1:B:1440:VAL:HG21	1:B:1665:VAL:HG21	1.99	0.44
1:B:1721:HIS:HB3	1:B:1723:TYR:CE2	2.52	0.44
1:B:2572:LEU:HD13	1:B:2574:ARG:HH21	1.81	0.44
1:B:3706:ARG:H	1:B:3706:ARG:HD2	1.81	0.44
1:B:3836:PHE:HD1	1:B:3843:GLN:HG3	1.83	0.44
1:B:4034:ASP:HB2	2:N:1:NAG:H5	1.98	0.44
1:A:3078:HIS:N	1:B:3078:HIS:HB3	2.33	0.44
1:A:3516:GLN:HA	1:A:3527:PRO:HA	1.99	0.44
1:A:4230:TRP:CG	1:A:4250:LYS:HB2	2.52	0.44
1:B:1347:LEU:N	1:B:1369:PHE:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2534:ARG:HE	1:B:2545:ILE:HD11	1.83	0.44
1:B:4212:SER:HB2	1:B:4223:LEU:HD11	2.00	0.44
1:A:612:GLY:HA2	1:A:629:LYS:HE2	1.98	0.44
1:A:683:ASP:OD1	1:A:683:ASP:N	2.50	0.44
1:A:714:SER:HA	1:A:719:ILE:HG12	1.98	0.44
1:A:1747:PHE:HA	1:A:1761:LEU:HG	1.99	0.44
1:A:2093:GLN:HE21	1:A:2093:GLN:HB3	1.63	0.44
1:A:3846:MET:HB3	1:A:3855:ILE:O	2.18	0.44
1:A:4098:LEU:HD13	1:A:4380:PRO:HG2	1.98	0.44
1:B:437:ARG:NH2	1:B:450:SER:OG	2.51	0.44
1:B:520:THR:HG22	1:B:659:ALA:HB2	2.00	0.44
1:B:2069:MET:HG2	1:B:2072:ALA:O	2.17	0.44
1:B:3789:ASP:OD1	1:B:3789:ASP:N	2.50	0.44
3:G:1:NAG:H61	3:G:2:NAG:N2	2.33	0.44
1:A:351:ASP:OD1	1:A:351:ASP:N	2.51	0.44
1:A:981:ASN:HA	1:A:988:CYS:HB2	2.00	0.44
1:A:1373:CYS:SG	1:A:1386:LYS:HG2	2.58	0.44
1:A:1834:ASN:ND2	1:A:2033:CYS:O	2.50	0.44
1:A:3612:GLN:HG2	1:A:3629:HIS:HE1	1.82	0.44
1:B:1751:VAL:HG21	1:B:1783:VAL:HB	2.00	0.44
1:B:2421:VAL:HG21	1:B:2435:PHE:HB2	2.00	0.44
1:B:4017:CYS:HB3	1:B:4021:CYS:HB2	1.99	0.44
1:B:4031:VAL:HA	1:B:4045:LYS:HD2	2.00	0.44
1:B:4083:TYR:HB3	1:B:4106:ARG:HG3	1.99	0.44
1:B:4396:LEU:HD12	1:B:4397:PRO:HD2	1.99	0.44
1:A:558:TRP:H	1:A:575:ASP:CG	2.26	0.44
1:A:847:ARG:HH21	1:A:1248:TRP:CD1	2.36	0.44
1:A:1206:ARG:NH1	1:A:1221:GLY:O	2.48	0.44
1:A:1675:ASN:N	1:A:1675:ASN:HD22	2.15	0.44
1:A:2209:TYR:HB3	1:A:2236:PRO:HD2	1.99	0.44
1:A:2466:GLY:HA3	1:A:2486:LEU:HD22	2.00	0.44
1:A:2502:VAL:HG23	1:A:2679:HIS:CD2	2.53	0.44
1:A:4273:ASN:OD1	1:A:4273:ASN:N	2.51	0.44
1:A:4327:ASN:ND2	3:G:1:NAG:O7	2.51	0.44
1:B:762:LYS:HA	1:B:1052:HIS:CE1	2.53	0.44
1:B:1467:TYR:H	1:B:1484:ASP:CG	2.26	0.44
1:B:1622:MET:HE1	1:B:1657:TRP:CE3	2.53	0.44
1:A:1173:ASP:N	1:A:1179:ASP:OD2	2.50	0.43
1:A:1266:CYS:HB3	1:A:1268:PRO:HD3	2.00	0.43
1:A:4000:PHE:HA	1:A:4004:SER:HB3	1.98	0.43
1:A:4390:TYR:CD1	1:A:4400:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:TRP:CE2	1:B:630:PHE:HD1	2.36	0.43
1:B:480:LYS:NZ	1:B:495:ASN:OD1	2.31	0.43
1:B:875:LEU:HB3	1:B:884:LEU:HD11	2.00	0.43
1:B:3388:TYR:CD1	1:B:3390:GLU:HG3	2.53	0.43
1:B:3517:PHE:N	1:B:3526:ILE:O	2.51	0.43
1:A:473:ALA:HB1	1:A:517:VAL:HG22	1.99	0.43
1:A:661:ASN:HB3	1:A:664:LYS:HE3	2.00	0.43
1:A:1436:LEU:HD23	1:A:1436:LEU:H	1.82	0.43
1:A:1510:LEU:HD23	1:A:1528:TYR:HB3	1.99	0.43
1:A:2654:PRO:HB2	1:A:2673:ALA:HB2	1.99	0.43
1:B:1469:VAL:HG13	1:B:1687:LEU:HD23	1.99	0.43
1:B:2049:PHE:HA	1:B:2060:PRO:HA	2.01	0.43
1:B:2151:ALA:HB1	1:B:2197:VAL:HG12	2.00	0.43
1:B:3818:ASP:N	1:B:3829:GLU:OE1	2.52	0.43
1:B:3849:CYS:HB3	1:B:3870:GLY:CA	2.48	0.43
1:A:242:ASP:N	1:A:242:ASP:OD1	2.51	0.43
1:A:1216:ASN:O	1:A:1220:ALA:N	2.50	0.43
1:A:1960:LEU:HD13	1:A:1963:PRO:HB3	2.00	0.43
1:A:3434:ASN:HB3	1:A:3439:SER:H	1.84	0.43
1:A:4116:LYS:HG2	1:A:4135:ASP:HA	2.01	0.43
1:B:767:LYS:HB3	1:B:778:LEU:HD11	2.00	0.43
1:B:937:ILE:HG21	1:B:947:MET:HE2	2.00	0.43
1:B:1016:ASP:O	1:B:1020:GLU:N	2.46	0.43
1:B:1097:ASP:N	1:B:1097:ASP:OD1	2.52	0.43
1:B:1352:SER:CB	1:B:1358:GLY:HA2	2.48	0.43
1:B:4085:GLN:HG2	1:B:4145:ASP:HA	2.00	0.43
1:A:991:VAL:HB	1:A:992:PRO:HD2	2.00	0.43
1:A:1550:ASN:O	1:A:1589:ARG:NH2	2.52	0.43
1:A:2233:ILE:HD11	1:A:2236:PRO:HG3	1.99	0.43
1:A:2618:ALA:HB1	1:A:2623:GLY:HA2	2.01	0.43
1:A:3729:ASN:N	1:A:3747:ASP:OD2	2.48	0.43
1:A:3780:HIS:N	1:A:3790:GLU:OE1	2.43	0.43
1:A:4298:ASN:HB3	1:A:4302:GLN:O	2.18	0.43
1:B:402:ARG:CZ	1:B:1089:ARG:HD3	2.48	0.43
1:B:619:TRP:HB3	1:B:644:ARG:NH1	2.33	0.43
1:B:799:TYR:CD1	1:B:833:VAL:HG21	2.54	0.43
1:B:1555:ARG:NH1	1:B:1601:CYS:SG	2.90	0.43
1:B:1648:LEU:HD23	1:B:1649:THR:N	2.33	0.43
1:B:2401:LEU:HD21	1:B:2629:MET:HB3	2.00	0.43
1:B:3240:ARG:HD3	1:B:3253:ARG:HD2	1.99	0.43
1:B:3467:ASN:ND2	1:B:3469:CYS:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3858:TYR:CE1	1:B:3859:TRP:CD1	3.06	0.43
1:A:493:MET:HE3	1:A:493:MET:HB3	1.87	0.43
1:A:524:LEU:N	1:A:541:ALA:O	2.51	0.43
1:A:543:MET:HB2	1:A:676:LEU:O	2.19	0.43
1:A:889:ALA:HA	1:A:916:PRO:HD2	1.99	0.43
1:A:3708:ASN:O	1:A:3712:GLN:HG3	2.19	0.43
1:B:1534:GLU:OE1	1:B:1543:ARG:NH2	2.49	0.43
1:B:1927:ASP:OD2	1:B:1988:LYS:NZ	2.41	0.43
1:B:2124:ILE:HB	1:B:2138:VAL:HB	2.00	0.43
1:B:4272:MET:HE2	1:B:4272:MET:HB2	1.86	0.43
1:A:682:ASN:ND2	1:A:687:PHE:O	2.43	0.43
1:A:2572:LEU:HD13	1:A:2574:ARG:HE	1.83	0.43
1:A:3275:LEU:HD21	1:A:3277:VAL:HG23	2.00	0.43
1:A:3365:GLU:HB2	1:A:3682:THR:HG21	2.00	0.43
1:A:4009:ASN:C	1:A:4011:CYS:N	2.77	0.43
1:B:643:LEU:H	1:B:643:LEU:HD12	1.83	0.43
1:B:2523:TRP:CE2	1:B:2533:GLU:HB2	2.54	0.43
1:B:2758:TYR:CD2	1:B:2765:ASP:HB2	2.53	0.43
1:B:3080:PHE:N	1:B:3088:ILE:O	2.43	0.43
1:B:3850:LYS:C	1:B:3852:HIS:H	2.25	0.43
1:A:1117:ASP:N	1:A:1136:ASP:OD2	2.52	0.43
1:A:1977:ASP:HB3	1:A:1980:TYR:HB2	2.00	0.43
1:A:2074:ARG:NH1	1:A:2085:GLU:OE2	2.51	0.43
1:A:2483:SER:HB2	1:A:2512:ILE:HD11	2.01	0.43
1:A:3458:HIS:HD2	1:A:3460:TYR:H	1.67	0.43
1:A:3873:GLU:H	1:A:3873:GLU:CD	2.27	0.43
1:A:4042:ARG:HA	1:A:4045:LYS:NZ	2.34	0.43
1:B:1357:ASN:HA	1:B:1364:CYS:SG	2.58	0.43
1:B:1820:VAL:HG13	1:B:1857:ARG:HD3	2.01	0.43
1:B:2141:GLY:O	1:B:2163:ASN:ND2	2.45	0.43
1:B:3846:MET:HB3	1:B:3857:PRO:HD3	2.01	0.43
1:A:368:ARG:NH1	1:A:369:HIS:CD2	2.87	0.43
1:A:1352:SER:HB2	1:A:1356:PHE:CZ	2.54	0.43
1:A:1622:MET:HE1	1:A:1657:TRP:CE3	2.53	0.43
1:A:1961:SER:OG	1:A:1979:GLN:HB2	2.18	0.43
1:A:4175:TYR:HB3	1:A:4354:PRO:HB3	2.01	0.43
1:B:488:VAL:CG1	1:B:720:ARG:HD2	2.49	0.43
1:B:3056:ASP:OD1	1:B:3056:ASP:N	2.51	0.43
1:B:3532:CYS:N	1:B:3543:ASP:O	2.52	0.43
1:B:3774:SER:O	1:B:3777:ILE:HG22	2.18	0.43
1:B:4158:TRP:CZ2	1:B:4167:GLU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLY:HA3	1:A:890:TYR:HB3	2.01	0.43
1:A:1402:GLN:OE1	1:A:1416:ASP:N	2.51	0.43
1:A:1648:LEU:HD23	1:A:1649:THR:N	2.34	0.43
1:A:1830:TRP:HA	1:A:1833:ARG:HH21	1.84	0.43
1:A:2619:ASN:OD1	1:A:2622:ASP:N	2.40	0.43
1:A:4103:TYR:CZ	1:A:4116:LYS:HB2	2.54	0.43
1:B:1129:ASP:O	1:B:1160:ARG:NH1	2.52	0.43
1:B:1149:CYS:O	1:B:1150:GLN:C	2.62	0.43
1:B:2397:SER:HA	1:B:2417:VAL:HG22	2.00	0.43
1:B:3834:THR:HB	1:B:3840:ALA:C	2.44	0.43
1:B:3835:ARG:HB2	1:B:3841:TYR:HA	2.00	0.43
1:B:4382:ARG:HB3	1:B:4409:TYR:CD1	2.54	0.43
1:A:446:ASN:N	1:A:446:ASN:OD1	2.51	0.43
1:A:1367:GLU:O	1:A:1368:PRO:C	2.60	0.43
1:A:2124:ILE:HB	1:A:2138:VAL:HB	1.99	0.43
1:A:2599:THR:HG22	1:A:2606:TYR:HB2	2.00	0.43
1:A:3089:GLU:HG2	1:A:3091:MET:H	1.83	0.43
1:A:3573:ASN:O	1:A:3605:ARG:NH2	2.50	0.43
1:B:1238:GLN:NE2	1:B:3178:CYS:H	2.17	0.43
1:B:1535:VAL:HG11	1:B:1714:LEU:HD11	2.01	0.43
1:B:2036:VAL:HG12	1:B:2040:LEU:HB2	1.99	0.43
1:B:3450:ARG:HB2	1:B:3452:PHE:CE2	2.53	0.43
1:A:521:VAL:HG23	1:A:523:TYR:CD1	2.54	0.42
1:A:937:ILE:HD12	1:A:937:ILE:N	2.34	0.42
1:A:977:PRO:HB2	1:B:2776:LEU:CB	2.48	0.42
1:A:2330:ASP:OD1	1:A:2331:LYS:N	2.51	0.42
1:A:3996:GLU:OE2	1:A:3998:ASN:HB3	2.19	0.42
1:A:4216:ASN:ND2	1:A:4345:ARG:HB3	2.34	0.42
1:A:4396:LEU:HD12	1:A:4397:PRO:HD2	2.01	0.42
1:B:452:ASP:OD2	1:B:457:ASN:ND2	2.51	0.42
1:B:539:GLU:CD	1:B:548:ARG:HE	2.27	0.42
1:B:579:ASP:HB3	1:B:601:ILE:O	2.19	0.42
1:B:1360:CYS:HB3	1:B:1373:CYS:HB3	1.65	0.42
1:B:1558:ALA:HB1	1:B:1605:ILE:HG13	2.00	0.42
1:B:2095:ARG:HD3	1:B:2095:ARG:HA	1.85	0.42
1:B:2550:LEU:HD21	1:B:2553:PRO:HB3	2.01	0.42
1:B:3135:CYS:SG	1:B:3136:SER:N	2.92	0.42
1:B:4311:VAL:HG12	1:B:4312:ASN:N	2.31	0.42
1:A:513:ARG:HD2	1:A:605:PHE:CE1	2.54	0.42
1:A:1084:TRP:HB3	1:A:1091:ASP:OD2	2.18	0.42
1:A:1578:ARG:NE	1:A:1580:GLU:OE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:HIS:CE1	1:A:1660:ARG:HD3	2.55	0.42
1:A:3298:ASP:OD1	1:A:3302:GLY:N	2.52	0.42
1:A:4059:PRO:HD2	1:A:4317:GLN:O	2.19	0.42
1:B:2106:SER:HA	2:I:2:NAG:O6	2.19	0.42
1:B:3093:LEU:HA	1:B:3105:ASP:HB2	2.02	0.42
1:B:4103:TYR:CZ	1:B:4116:LYS:HB2	2.54	0.42
1:B:4243:ARG:NE	1:B:4256:THR:OG1	2.52	0.42
1:A:1822:PRO:HG3	1:A:1841:ARG:NH1	2.34	0.42
1:A:2482:TYR:CZ	1:A:2491:ASN:HB2	2.55	0.42
1:A:3698:VAL:HA	1:A:3710:ASP:HB2	2.00	0.42
1:A:3819:GLY:N	1:A:3835:ARG:HH21	2.17	0.42
1:A:3843:GLN:HE21	1:A:3843:GLN:HB2	1.65	0.42
1:A:4031:VAL:HA	1:A:4045:LYS:HD2	2.00	0.42
1:B:733:MET:HE1	1:B:755:ILE:HD13	2.01	0.42
1:B:829:ARG:HD2	1:B:873:ASN:HA	2.01	0.42
1:B:830:SER:HB3	1:B:843:THR:HG22	2.01	0.42
1:B:1436:LEU:H	1:B:1436:LEU:HD23	1.85	0.42
1:B:3146:ASP:O	1:B:3148:ARG:NH1	2.52	0.42
1:B:3821:ALA:HA	1:B:3829:GLU:CG	2.49	0.42
1:B:4067:TYR:CZ	1:B:4072:GLU:HA	2.55	0.42
3:G:1:NAG:H61	3:G:2:NAG:H82	2.00	0.42
1:A:978:THR:OG1	1:B:2776:LEU:N	2.52	0.42
1:A:1175:VAL:HG23	1:A:1176:ASP:H	1.83	0.42
1:A:1558:ALA:HB1	1:A:1605:ILE:HG13	2.01	0.42
1:A:1878:VAL:HB	1:A:1905:MET:HE3	2.02	0.42
1:A:3774:SER:O	1:A:3777:ILE:HG22	2.19	0.42
1:A:4067:TYR:CG	1:A:4309:LEU:HD11	2.54	0.42
1:B:339:ASN:HD22	1:B:346:CYS:HA	1.84	0.42
1:B:1025:GLN:HG2	1:B:1026:CYS:SG	2.59	0.42
1:B:1263:HIS:CD2	1:B:1263:HIS:H	2.35	0.42
1:B:2653:ASN:HD21	1:B:2655:CYS:HB2	1.85	0.42
1:B:3270:PRO:HB2	1:B:3290:ARG:HB3	2.01	0.42
1:A:558:TRP:HB2	1:A:577:ARG:H	1.85	0.42
1:A:851:ILE:HB	1:A:865:ILE:HB	2.00	0.42
1:A:1571:SER:HB3	1:A:1600:PRO:HB2	2.01	0.42
1:A:1609:ASN:HB3	1:A:1611:LEU:HD23	2.01	0.42
1:A:2102:VAL:HG12	1:A:2109:ILE:HG12	2.01	0.42
1:A:2568:VAL:HG12	1:A:2575:ILE:HG23	2.00	0.42
1:A:2684:TYR:O	1:A:2693:ILE:HG13	2.20	0.42
1:A:3082:CYS:N	1:A:3086:ARG:O	2.37	0.42
1:A:3199:PRO:HG3	1:A:3416:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:PHE:O	1:B:656:GLN:NE2	2.47	0.42
1:B:1834:ASN:ND2	1:B:2033:CYS:O	2.51	0.42
1:B:2330:ASP:OD1	1:B:2331:LYS:N	2.53	0.42
1:B:3698:VAL:HA	1:B:3710:ASP:HB2	2.00	0.42
1:A:470:GLU:OE1	1:A:513:ARG:HD3	2.19	0.42
1:A:2568:VAL:HG12	1:A:2575:ILE:HG12	2.00	0.42
1:A:2739:HIS:CD2	1:A:2747:THR:HG21	2.54	0.42
1:A:3453:ASP:OD1	1:A:3454:ILE:N	2.52	0.42
1:A:3622:ASN:ND2	1:A:3625:GLU:HB2	2.35	0.42
1:A:3744:ASP:N	1:A:3750:ASP:OD2	2.52	0.42
1:B:885:TYR:CD2	1:B:896:HIS:HB3	2.54	0.42
1:B:1822:PRO:HG3	1:B:1841:ARG:NH1	2.34	0.42
1:B:2145:ASN:ND2	1:B:2165:PHE:O	2.53	0.42
1:B:3691:ARG:HD3	1:B:3705:CYS:HA	2.00	0.42
1:B:3848:GLU:HA	1:B:3853:VAL:O	2.20	0.42
1:A:964:ASP:HB3	1:A:967:ILE:HG13	2.02	0.42
1:A:3376:ASN:ND2	1:A:3436:TYR:OH	2.53	0.42
1:A:4311:VAL:HG12	1:A:4312:ASN:N	2.33	0.42
1:A:4329:SER:O	1:A:4330:VAL:C	2.63	0.42
1:B:356:GLY:O	1:B:383:GLN:NE2	2.52	0.42
1:B:1362:HIS:CG	1:B:1363:GLU:H	2.38	0.42
1:B:1365:VAL:CG1	1:B:1372:LYS:HD3	2.50	0.42
1:B:2198:ASP:OD2	1:B:2201:ASN:ND2	2.50	0.42
1:B:3517:PHE:HB2	1:B:3528:ILE:HD12	2.02	0.42
1:B:3819:GLY:N	1:B:3829:GLU:OE1	2.51	0.42
1:A:339:ASN:HD22	1:A:344:ARG:HA	1.85	0.42
1:A:441:THR:HG22	1:A:448:VAL:HG22	2.01	0.42
1:A:511:HIS:HB3	1:A:529:TRP:NE1	2.34	0.42
1:A:1205:ASN:HB3	1:A:1212:ASP:CG	2.45	0.42
1:A:1588:MET:SD	1:A:1717:SER:OG	2.77	0.42
1:A:1751:VAL:HG21	1:A:1783:VAL:HB	2.01	0.42
1:A:2469:ASP:N	1:A:2469:ASP:OD1	2.52	0.42
1:A:3135:CYS:SG	1:A:3136:SER:N	2.93	0.42
1:A:3209:LEU:O	1:A:3222:ILE:N	2.52	0.42
1:A:3706:ARG:HD2	1:A:3706:ARG:N	2.35	0.42
1:A:4067:TYR:CE2	1:A:4309:LEU:HD11	2.55	0.42
1:A:4154:ARG:C	1:A:4171:LEU:HD13	2.45	0.42
1:B:570:ARG:NH1	1:B:583:THR:HG22	2.35	0.42
1:B:3577:ASN:HD22	1:B:3583:ASP:CG	2.28	0.42
1:B:3682:THR:O	1:B:3695:LYS:N	2.53	0.42
1:A:698:ASP:OD1	1:A:699:THR:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:TYR:H	1:A:1484:ASP:CG	2.26	0.42
1:A:1784:GLU:OE1	1:A:1785:PHE:N	2.52	0.42
1:A:2644:VAL:HG12	1:A:2646:ASN:O	2.20	0.42
1:A:2758:TYR:HB2	1:A:2766:CYS:HB3	2.02	0.42
1:B:235:ILE:HG23	1:B:239:TRP:HE3	1.83	0.42
1:B:1205:ASN:HB3	1:B:1212:ASP:CG	2.45	0.42
1:B:2099:HIS:CE1	1:B:2194:HIS:HD2	2.38	0.42
1:B:3199:PRO:HG3	1:B:3416:PHE:CE2	2.55	0.42
1:B:3640:PHE:HE2	1:B:3665:ASP:HA	1.84	0.42
1:B:4242:ASP:OD1	1:B:4242:ASP:N	2.52	0.42
1:B:4314:TRP:O	1:B:4316:THR:HG23	2.19	0.42
1:A:507:GLU:HB3	1:A:548:ARG:NH1	2.35	0.42
1:A:558:TRP:CG	1:A:577:ARG:HB2	2.55	0.42
1:A:966:ASN:O	1:A:969:THR:OG1	2.38	0.42
1:A:1576:HIS:CE1	1:B:2213:PRO:HD2	2.55	0.42
1:A:1828:LEU:HD12	1:A:1835:LEU:HD12	2.02	0.42
1:A:4024:THR:HB	1:A:4027:SER:C	2.45	0.42
1:A:4158:TRP:CZ2	1:A:4167:GLU:HB2	2.55	0.42
1:B:441:THR:HB	1:B:469:PRO:HG2	2.01	0.42
1:B:628:ASN:H	1:B:632:GLU:HB2	1.85	0.42
1:B:785:ASN:HD22	1:B:804:HIS:HB2	1.85	0.42
1:B:1352:SER:O	1:B:1356:PHE:N	2.46	0.42
1:B:1514:ILE:HG23	1:B:1523:LEU:HD21	2.02	0.42
1:B:1550:ASN:O	1:B:1589:ARG:NH2	2.52	0.42
1:B:1667:ARG:NH2	1:B:1677:SER:OG	2.53	0.42
1:B:3516:GLN:HA	1:B:3527:PRO:HA	2.02	0.42
1:B:3708:ASN:O	1:B:3712:GLN:HG3	2.20	0.42
1:B:4298:ASN:HB3	1:B:4302:GLN:O	2.20	0.42
1:A:229:CYS:CB	1:A:233:ARG:HG2	2.48	0.41
1:A:490:ARG:HA	1:A:506:THR:HG22	2.01	0.41
1:A:1049:ASP:OD1	1:A:1049:ASP:N	2.50	0.41
1:A:2523:TRP:NE1	1:A:2533:GLU:OE1	2.43	0.41
1:A:3208:TYR:OH	1:A:3760:THR:OG1	2.23	0.41
1:A:3811:VAL:HG21	1:A:3822:ASP:HB3	2.02	0.41
1:A:4098:LEU:HA	1:A:4121:PRO:HA	2.02	0.41
1:A:4183:ASP:HB3	1:A:4220:ARG:HH12	1.85	0.41
1:B:563:THR:HG23	1:B:572:TYR:HB2	2.00	0.41
1:B:597:GLY:HA2	1:B:1158:ASN:OD1	2.20	0.41
1:B:777:ILE:O	1:B:816:LYS:NZ	2.40	0.41
1:B:1112:THR:HA	1:B:1124:LYS:HE3	2.02	0.41
1:B:2115:SER:HB2	1:B:2121:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3255:PHE:CE2	2:K:1:NAG:H5	2.55	0.41
1:B:4102:TYR:OH	1:B:4171:LEU:HG	2.20	0.41
1:A:365:ARG:HB2	1:A:368:ARG:C	2.44	0.41
1:A:1026:CYS:HB3	1:A:1030:SER:HB2	2.02	0.41
1:A:1060:CYS:SG	1:A:1065:ASN:HB3	2.60	0.41
1:A:2212:ARG:HH22	1:B:1597:ILE:H	1.68	0.41
1:A:2213:PRO:HD2	1:B:1576:HIS:CE1	2.55	0.41
1:A:2257:ILE:HG13	1:A:2270:VAL:HG13	2.02	0.41
1:A:3679:ASP:N	1:A:3683:GLU:HB2	2.35	0.41
1:A:3804:GLN:HE21	1:A:3808:GLY:HA2	1.84	0.41
1:A:4008:ILE:H	1:A:4026:GLY:N	2.18	0.41
1:A:4042:ARG:HA	1:A:4045:LYS:HZ1	1.85	0.41
1:B:793:TRP:CE2	1:B:968:GLN:HA	2.55	0.41
1:B:1786:ASP:HB3	1:B:1791:TYR:HB2	2.02	0.41
1:B:2192:PRO:HB3	1:B:2206:TRP:CD1	2.54	0.41
1:B:3192:ARG:HD3	1:B:3192:ARG:HA	1.95	0.41
1:B:4106:ARG:HA	1:B:4144:PRO:HD2	2.02	0.41
1:B:4154:ARG:C	1:B:4171:LEU:HD13	2.45	0.41
1:A:1112:THR:HA	1:A:1124:LYS:HE3	2.01	0.41
1:B:493:MET:HE3	1:B:493:MET:HB3	1.88	0.41
1:B:1216:ASN:O	1:B:1220:ALA:N	2.54	0.41
1:B:1635:VAL:HG12	1:B:1636:ILE:HG13	2.02	0.41
1:B:3082:CYS:N	1:B:3086:ARG:O	2.38	0.41
1:A:462:LEU:HD11	1:A:494:VAL:HG11	2.01	0.41
1:A:873:ASN:ND2	1:A:917:PHE:HD1	2.18	0.41
1:A:1365:VAL:HG21	1:A:1374:LEU:HD12	2.02	0.41
1:A:1446:ILE:HD11	1:A:1482:TRP:CG	2.55	0.41
1:A:2257:ILE:HD11	1:A:2270:VAL:HG22	2.02	0.41
1:A:2729:SER:O	1:A:2735:VAL:HG21	2.21	0.41
1:A:3844:ALA:HB3	1:A:3846:MET:HE3	2.01	0.41
1:A:4199:MET:HE3	1:A:4201:TRP:HZ3	1.85	0.41
1:B:522:GLY:C	1:B:543:MET:HG3	2.45	0.41
1:B:619:TRP:CD1	1:B:644:ARG:HG3	2.56	0.41
1:B:719:ILE:HD11	1:B:743:PHE:HB3	2.01	0.41
1:B:842:PHE:CZ	1:B:852:MET:HB2	2.56	0.41
1:B:1078:GLU:OE1	1:B:1092:CYS:HB2	2.20	0.41
1:B:1853:ASP:OD1	1:B:1853:ASP:N	2.48	0.41
1:B:1864:ASP:HB3	1:B:2083:HIS:CE1	2.55	0.41
1:B:2176:ILE:HB	2:I:1:NAG:H82	2.03	0.41
1:B:2531:LYS:HE2	1:B:2531:LYS:HB2	1.91	0.41
1:B:3093:LEU:HD22	1:B:3130:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3834:THR:HA	1:B:3841:TYR:CZ	2.56	0.41
1:A:2198:ASP:OD2	1:A:2201:ASN:ND2	2.49	0.41
1:A:2475:TRP:O	1:A:2476:ILE:C	2.64	0.41
1:A:2523:TRP:CE2	1:A:2533:GLU:HB2	2.55	0.41
1:A:4067:TYR:CZ	1:A:4072:GLU:HA	2.55	0.41
1:B:470:GLU:OE1	1:B:513:ARG:HD3	2.20	0.41
1:B:868:THR:HG21	1:B:1242:ILE:HG21	2.03	0.41
1:B:1236:GLN:NE2	1:B:3194:ASN:HD22	2.19	0.41
1:B:3502:LEU:HD11	1:B:3507:TYR:HB2	2.01	0.41
1:B:3706:ARG:HD2	1:B:3706:ARG:N	2.35	0.41
1:B:3744:ASP:N	1:B:3750:ASP:OD2	2.52	0.41
1:B:4285:TYR:HD1	1:B:4320:ILE:HD11	1.86	0.41
1:A:248:LYS:C	1:A:250:ASN:N	2.77	0.41
1:A:452:ASP:OD2	1:A:457:ASN:ND2	2.53	0.41
1:A:895:GLU:HG2	1:A:906:ARG:HB2	2.01	0.41
1:A:977:PRO:HB2	1:B:2776:LEU:HB3	2.02	0.41
1:A:1347:LEU:N	1:A:1369:PHE:O	2.53	0.41
1:A:1362:HIS:O	1:A:1363:GLU:C	2.61	0.41
1:A:2099:HIS:ND1	1:A:2194:HIS:HD2	2.19	0.41
1:A:3577:ASN:HD22	1:A:3583:ASP:CG	2.28	0.41
1:B:620:THR:HA	1:B:1132:ASN:HB2	2.01	0.41
1:B:1122:ILE:HD12	1:B:1133:ASP:OD2	2.21	0.41
1:B:1122:ILE:HG13	1:B:1134:CYS:HB3	2.02	0.41
1:B:1794:TRP:HZ3	1:B:1804:VAL:HG12	1.84	0.41
1:B:2096:ASN:O	1:B:2113:ASP:HA	2.20	0.41
1:B:2304:SER:HB3	1:B:2309:ASN:HD22	1.85	0.41
1:B:2513:VAL:HB	1:B:2522:TYR:HB2	2.02	0.41
1:B:2651:CYS:O	1:B:2652:ASN:C	2.61	0.41
1:A:793:TRP:CE2	1:A:968:GLN:HA	2.56	0.41
1:A:1037:ARG:NH1	1:A:1050:ASP:O	2.53	0.41
1:A:1239:GLU:HG3	1:A:1257:LEU:HB3	2.02	0.41
1:A:2707:CYS:CB	1:A:2729:SER:HB3	2.44	0.41
1:A:3640:PHE:N	1:A:3648:ILE:O	2.53	0.41
1:B:1872:PHE:H	1:B:1889:ASP:CG	2.28	0.41
1:B:1961:SER:OG	1:B:1979:GLN:HB2	2.20	0.41
1:B:2093:GLN:HE21	1:B:2093:GLN:HB3	1.65	0.41
1:B:2312:PRO:HA	1:B:2313:PRO:HD3	1.96	0.41
1:B:3243:TRP:HZ2	1:B:3261:LYS:HE3	1.85	0.41
1:B:3268:ARG:HB2	1:B:3304:ARG:HH12	1.86	0.41
1:B:3318:PHE:CZ	1:B:3361:SER:HB2	2.55	0.41
1:B:3614:ASP:OD1	1:B:3614:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3667:PRO:O	1:B:3670:GLU:N	2.54	0.41
1:B:4042:ARG:HA	1:B:4045:LYS:NZ	2.36	0.41
1:B:4246:TRP:CZ2	1:B:4255:GLU:HB2	2.55	0.41
1:A:350:ASP:HB3	1:A:353:GLN:HB2	2.01	0.41
1:A:925:HIS:CG	1:A:938:ARG:HD2	2.56	0.41
1:A:1076:HIS:N	1:A:1094:ASP:OD2	2.30	0.41
1:A:1965:GLY:H	1:A:1976:THR:HG23	1.86	0.41
1:A:4207:GLU:O	1:A:4208:PRO:C	2.62	0.41
1:B:462:LEU:HD11	1:B:494:VAL:HG11	2.03	0.41
1:B:523:TYR:HB3	1:B:525:PHE:CE1	2.56	0.41
1:B:1112:THR:O	1:B:1124:LYS:HG3	2.20	0.41
1:B:1162:ILE:HD12	1:B:1166:PHE:HB2	2.03	0.41
1:B:1373:CYS:SG	1:B:1386:LYS:HG2	2.60	0.41
1:B:3846:MET:CB	1:B:3857:PRO:HD3	2.50	0.41
1:A:535:GLU:HB2	1:A:537:LYS:HE3	2.03	0.41
1:A:556:LEU:HD11	1:A:559:PRO:HB3	2.03	0.41
1:A:681:ASP:OD1	1:A:682:ASN:N	2.53	0.41
1:A:834:HIS:NE2	1:A:836:PHE:HB2	2.36	0.41
1:A:917:PHE:HD2	1:A:958:LEU:HA	1.86	0.41
1:A:1112:THR:O	1:A:1124:LYS:HG3	2.20	0.41
1:A:1390:ASP:HB2	1:A:1408:ARG:NH1	2.35	0.41
1:A:1606:ASP:OD1	1:A:1650:LEU:HD13	2.21	0.41
1:A:1922:GLU:HG3	1:A:1963:PRO:O	2.20	0.41
1:A:2388:ASN:ND2	1:A:2601:TYR:OH	2.53	0.41
1:A:2501:THR:HB	1:A:2665:ILE:HD12	2.03	0.41
1:A:3281:SER:O	1:A:3283:LYS:NZ	2.52	0.41
1:A:3326:LEU:HD12	1:A:3326:LEU:HA	1.87	0.41
1:A:3655:ASP:HB2	1:A:3691:ARG:HH12	1.85	0.41
1:A:4121:PRO:C	1:A:4123:PHE:H	2.29	0.41
1:A:4165:ARG:NH2	1:A:4167:GLU:OE2	2.50	0.41
1:B:612:GLY:HA2	1:B:629:LYS:HE2	2.03	0.41
1:B:768:GLN:HA	1:B:774:GLY:O	2.21	0.41
1:B:1174:CYS:HB2	1:B:1178:SER:H	1.85	0.41
1:B:1352:SER:HB2	1:B:1358:GLY:HA2	2.03	0.41
1:B:1508:ILE:H	1:B:1508:ILE:HG13	1.49	0.41
1:B:1965:GLY:H	1:B:1976:THR:HG23	1.85	0.41
1:B:2438:ASN:O	1:B:2439:LEU:C	2.63	0.41
1:B:2684:TYR:O	1:B:2693:ILE:HG13	2.21	0.41
1:B:2685:LEU:HB3	1:B:2689:ARG:HA	2.03	0.41
1:B:2733:GLU:O	1:B:2737:ALA:N	2.54	0.41
1:B:3458:HIS:HD2	1:B:3460:TYR:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3633:ARG:NH2	1:B:3647:CYS:HB2	2.36	0.41
1:B:4411:GLU:OE1	1:B:4411:GLU:N	2.41	0.41
1:A:747:ASP:OD1	1:A:748:PHE:N	2.50	0.41
1:A:3020:ASP:OD1	1:A:3020:ASP:N	2.54	0.41
1:A:3025:ARG:HD3	1:A:3028:LEU:HD21	2.02	0.41
1:A:3090:MET:HE2	1:B:3091:MET:HG2	2.03	0.41
1:A:3551:ARG:HA	1:A:3559:GLN:NE2	2.36	0.41
1:A:3842:CYS:HB3	1:A:3846:MET:HB2	2.02	0.41
1:A:4170:LYS:HE2	1:A:4174:ARG:HH21	1.86	0.41
1:A:4246:TRP:CZ2	1:A:4255:GLU:HB2	2.56	0.41
1:B:742:PHE:O	1:B:744:VAL:HG23	2.21	0.41
1:B:845:TRP:CD1	1:B:845:TRP:H	2.39	0.41
1:B:1118:ASN:HD21	1:B:1136:ASP:H	1.69	0.41
1:B:1239:GLU:HG3	1:B:1257:LEU:HB3	2.03	0.41
1:B:2502:VAL:HG23	1:B:2679:HIS:CG	2.56	0.41
1:B:3092:LYS:HB3	1:B:3099:ASP:OD2	2.21	0.41
1:B:3312:VAL:HG11	1:B:3337:TRP:CZ2	2.55	0.41
1:B:3834:THR:O	1:B:3835:ARG:C	2.64	0.41
1:B:4257:ILE:HB	1:B:4261:GLY:HA2	2.03	0.41
1:A:1353:CYS:H	1:A:1371:ALA:HB2	1.86	0.40
1:A:1532:THR:HB	1:A:1545:VAL:HG13	2.03	0.40
1:A:1802:HIS:NE2	1:A:1813:VAL:HG22	2.37	0.40
1:A:1831:ILE:HD12	1:A:2018:SER:HA	2.03	0.40
1:A:2550:LEU:HD21	1:A:2553:PRO:HB3	2.03	0.40
1:A:2733:GLU:O	1:A:2734:SER:C	2.64	0.40
1:A:3201:LEU:N	1:A:3212:LEU:O	2.55	0.40
1:A:3391:TYR:CE1	1:A:3400:HIS:HB2	2.57	0.40
1:B:556:LEU:HG	1:B:559:PRO:HD3	2.02	0.40
1:B:1442:SER:OG	1:B:1443:GLN:N	2.54	0.40
1:B:1578:ARG:NE	1:B:1580:GLU:OE2	2.46	0.40
1:B:3110:GLY:C	1:B:3111:ILE:HD12	2.46	0.40
1:B:3200:TYR:CZ	2:J:1:NAG:H3	2.57	0.40
1:B:3858:TYR:O	1:B:3862:ASP:HB2	2.21	0.40
1:B:4203:ASP:C	1:B:4205:GLY:H	2.29	0.40
1:A:347:VAL:HG22	1:A:349:PHE:N	2.35	0.40
1:A:494:VAL:HG12	1:A:501:ARG:HA	2.03	0.40
1:A:932:ARG:HA	1:A:932:ARG:HD3	1.92	0.40
1:A:1163:ASP:HB3	1:A:1166:PHE:CD2	2.56	0.40
1:A:3307:LEU:HD23	1:A:3307:LEU:HA	1.88	0.40
1:A:3789:ASP:OD1	1:A:3789:ASP:N	2.54	0.40
1:A:4009:ASN:O	1:A:4010:GLU:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4092:ASP:OD1	1:A:4092:ASP:N	2.54	0.40
1:B:1060:CYS:SG	1:B:1065:ASN:HB3	2.61	0.40
1:B:2665:ILE:H	1:B:2665:ILE:HG13	1.64	0.40
1:A:423:ARG:NH2	1:A:1087:ASP:OD2	2.47	0.40
1:A:1375:CYS:SG	1:A:1381:LEU:HG	2.62	0.40
1:A:1872:PHE:H	1:A:1889:ASP:CG	2.28	0.40
1:A:3551:ARG:HA	1:A:3559:GLN:HE22	1.86	0.40
1:A:4175:TYR:OH	1:A:4372:GLU:N	2.53	0.40
1:A:4277:LEU:HB3	1:A:4284:LEU:HD21	2.03	0.40
1:B:535:GLU:O	1:B:537:LYS:HG3	2.21	0.40
1:B:746:ILE:CG1	1:B:961:LYS:HB3	2.51	0.40
1:B:1131:ASP:C	1:B:1133:ASP:N	2.77	0.40
1:B:1352:SER:HA	1:B:1355:ASP:CG	2.46	0.40
1:B:3278:ASP:OD2	1:B:3282:ARG:N	2.54	0.40
1:B:3875:LEU:HD22	1:B:3880:ASP:N	2.35	0.40
1:A:356:GLY:HA2	1:A:630:PHE:CG	2.56	0.40
1:A:1122:ILE:HD12	1:A:1133:ASP:OD2	2.21	0.40
1:A:1442:SER:OG	1:A:1443:GLN:N	2.55	0.40
1:A:1743:ASP:OD1	1:A:1744:ASP:N	2.53	0.40
1:A:3278:ASP:OD2	1:A:3282:ARG:N	2.53	0.40
1:A:3450:ARG:HB2	1:A:3452:PHE:CE2	2.56	0.40
1:A:4004:SER:O	1:A:4005:CYS:C	2.64	0.40
1:A:4106:ARG:HA	1:A:4144:PRO:HD2	2.03	0.40
1:A:4236:ILE:HB	1:A:4238:TYR:CZ	2.56	0.40
1:B:1132:ASN:O	1:B:1133:ASP:C	2.64	0.40
1:B:1365:VAL:HB	1:B:1372:LYS:HB3	2.04	0.40
1:B:2126:ARG:NE	1:B:2137:ILE:HD11	2.36	0.40
1:B:3513:SER:HB3	1:B:3593:HIS:ND1	2.36	0.40
1:B:4163:ASN:O	1:B:4165:ARG:HG3	2.22	0.40
1:B:4271:ALA:HB1	1:B:4286:TRP:NE1	2.37	0.40
1:A:603:HIS:CD2	1:A:619:TRP:HB2	2.56	0.40
1:A:632:GLU:HG3	1:A:634:ASN:H	1.85	0.40
1:A:749:ASP:HA	1:A:968:GLN:HE22	1.86	0.40
1:A:1462:VAL:HG13	1:A:1500:ARG:HH21	1.86	0.40
1:A:1508:ILE:H	1:A:1508:ILE:HG13	1.48	0.40
1:A:1975:TYR:OH	1:A:1984:GLU:OE1	2.21	0.40
1:A:3667:PRO:O	1:A:3670:GLU:N	2.54	0.40
1:A:3888:ARG:O	1:A:3889:PHE:C	2.65	0.40
1:A:4098:LEU:HD22	1:A:4380:PRO:HB2	2.04	0.40
1:A:4199:MET:HE3	1:A:4201:TRP:CZ3	2.57	0.40
1:B:379:LEU:HD12	1:B:384:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:TRP:CE3	1:B:968:GLN:HG2	2.56	0.40
1:B:1154:PHE:N	1:B:1162:ILE:O	2.55	0.40
1:B:1390:ASP:HB2	1:B:1408:ARG:NH1	2.35	0.40
1:B:1615:MET:HE3	1:B:1615:MET:HB2	1.90	0.40
1:B:2399:ARG:HG2	1:B:2414:THR:CG2	2.52	0.40
1:B:3331:GLN:O	1:B:3486:GLY:HA3	2.22	0.40
1:B:4314:TRP:O	1:B:4315:LEU:C	2.64	0.40
2:N:1:NAG:H82	2:N:1:NAG:H2	1.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3683/4655 (79%)	3478 (94%)	203 (6%)	2 (0%)	48	76
1	B	3680/4655 (79%)	3478 (94%)	197 (5%)	5 (0%)	48	76
All	All	7363/9310 (79%)	6956 (94%)	400 (5%)	7 (0%)	50	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1160	ARG
1	A	821	VAL
1	A	960	LEU
1	B	821	VAL
1	B	646	TYR
1	B	1135	GLY
1	B	2417	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3150/4105 (77%)	3047 (97%)	103 (3%)	33	60
1	B	3150/4105 (77%)	3038 (96%)	112 (4%)	30	57
All	All	6300/8210 (77%)	6085 (97%)	215 (3%)	34	59

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	GLU
1	A	446	ASN
1	A	453	ILE
1	A	464	VAL
1	A	466	VAL
1	A	488	VAL
1	A	581	ILE
1	A	683	ASP
1	A	746	ILE
1	A	810	VAL
1	A	821	VAL
1	A	887	VAL
1	A	892	ASP
1	A	969	THR
1	A	974	CYS
1	A	1023	THR
1	A	1051	CYS
1	A	1133	ASP
1	A	1184	VAL
1	A	1185	LEU
1	A	1187	CYS
1	A	1198	ASP
1	A	1224	THR
1	A	1238	GLN
1	A	1239	GLU
1	A	1363	GLU
1	A	1403	HIS

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Mol	Chain	Res	Type
1	A	1451	VAL
1	A	1454	GLN
1	A	1508	ILE
1	A	1648	LEU
1	A	1649	THR
1	A	1655	VAL
1	A	1712	LEU
1	A	1755	ILE
1	A	1784	GLU
1	A	1801	ILE
1	A	1820	VAL
1	A	1838	THR
1	A	1976	THR
1	A	2007	LEU
1	A	2036	VAL
1	A	2066	VAL
1	A	2093	GLN
1	A	2327	THR
1	A	2341	VAL
1	A	2421	VAL
1	A	2436	THR
1	A	2491	ASN
1	A	2493	MET
1	A	2501	THR
1	A	2513	VAL
1	A	2543	VAL
1	A	2593	VAL
1	A	2651	CYS
1	A	2705	PHE
1	A	2712	CYS
1	A	2747	THR
1	A	2759	ARG
1	A	2765	ASP
1	A	3035	ASN
1	A	3041	ASN
1	A	3045	ILE
1	A	3056	ASP
1	A	3067	LEU
1	A	3075	CYS
1	A	3078	HIS
1	A	3103	ASN
1	A	3129	THR

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Mol	Chain	Res	Type
1	A	3168	GLU
1	A	3278	ASP
1	A	3298	ASP
1	A	3346	ILE
1	A	3371	THR
1	A	3398	HIS
1	A	3413	ILE
1	A	3415	ILE
1	A	3420	ILE
1	A	3465	VAL
1	A	3552	PHE
1	A	3560	CYS
1	A	3578	CYS
1	A	3590	GLU
1	A	3619	CYS
1	A	3622	ASN
1	A	3629	HIS
1	A	3706	ARG
1	A	3744	ASP
1	A	3784	CYS
1	A	3843	GLN
1	A	3845	THR
1	A	3848	GLU
1	A	3859	TRP
1	A	4045	LYS
1	A	4120	ILE
1	A	4145	ASP
1	A	4156	ILE
1	A	4171	LEU
1	A	4179	LEU
1	A	4190	ILE
1	A	4219	ASP
1	A	4254	ILE
1	A	4273	ASN
1	B	339	ASN
1	B	354	ILE
1	B	452	ASP
1	B	464	VAL
1	B	466	VAL
1	B	479	ASN
1	B	481	ILE
1	B	488	VAL

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Mol	Chain	Res	Type
1	B	579	ASP
1	B	581	ILE
1	B	622	MET
1	B	642	SER
1	B	643	LEU
1	B	644	ARG
1	B	732	VAL
1	B	746	ILE
1	B	821	VAL
1	B	887	VAL
1	B	892	ASP
1	B	969	THR
1	B	974	CYS
1	B	978	THR
1	B	979	HIS
1	B	991	VAL
1	B	1023	THR
1	B	1051	CYS
1	B	1133	ASP
1	B	1184	VAL
1	B	1185	LEU
1	B	1187	CYS
1	B	1198	ASP
1	B	1224	THR
1	B	1262	GLU
1	B	1373	CYS
1	B	1403	HIS
1	B	1451	VAL
1	B	1454	GLN
1	B	1508	ILE
1	B	1612	LEU
1	B	1648	LEU
1	B	1649	THR
1	B	1655	VAL
1	B	1712	LEU
1	B	1755	ILE
1	B	1784	GLU
1	B	1801	ILE
1	B	1820	VAL
1	B	1838	THR
1	B	1976	THR
1	B	2007	LEU

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Mol	Chain	Res	Type
1	B	2036	VAL
1	B	2066	VAL
1	B	2327	THR
1	B	2341	VAL
1	B	2491	ASN
1	B	2493	MET
1	B	2513	VAL
1	B	2543	VAL
1	B	2593	VAL
1	B	2651	CYS
1	B	2705	PHE
1	B	2706	THR
1	B	2712	CYS
1	B	2739	HIS
1	B	2756	TYR
1	B	2776	LEU
1	B	3035	ASN
1	B	3041	ASN
1	B	3045	ILE
1	B	3056	ASP
1	B	3067	LEU
1	B	3075	CYS
1	B	3103	ASN
1	B	3129	THR
1	B	3168	GLU
1	B	3278	ASP
1	B	3298	ASP
1	B	3346	ILE
1	B	3371	THR
1	B	3398	HIS
1	B	3413	ILE
1	B	3415	ILE
1	B	3420	ILE
1	B	3446	ASN
1	B	3552	PHE
1	B	3560	CYS
1	B	3578	CYS
1	B	3590	GLU
1	B	3619	CYS
1	B	3622	ASN
1	B	3629	HIS
1	B	3706	ARG

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Mol	Chain	Res	Type
1	B	3744	ASP
1	B	3780	HIS
1	B	3784	CYS
1	B	3843	GLN
1	B	3858	TYR
1	B	4006	LEU
1	B	4041	ASP
1	B	4045	LYS
1	B	4080	ASP
1	B	4092	ASP
1	B	4120	ILE
1	B	4156	ILE
1	B	4171	LEU
1	B	4179	LEU
1	B	4190	ILE
1	B	4219	ASP
1	B	4254	ILE
1	B	4272	MET
1	B	4298	ASN
1	B	4312	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	369	HIS
1	A	410	HIS
1	A	445	GLN
1	A	489	ASN
1	A	547	ASN
1	A	596	HIS
1	A	661	ASN
1	A	696	GLN
1	A	716	GLN
1	A	768	GLN
1	A	785	ASN
1	A	896	HIS
1	A	976	GLN
1	A	986	HIS
1	A	1009	ASN
1	A	1064	ASN
1	A	1099	HIS

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Mol	Chain	Res	Type
1	A	1144	ASN
1	A	1153	GLN
1	A	1191	GLN
1	A	1231	HIS
1	A	1366	GLN
1	A	1454	GLN
1	A	1495	GLN
1	A	1522	ASN
1	A	1553	ASN
1	A	1575	HIS
1	A	1594	GLN
1	A	1754	HIS
1	A	1931	GLN
1	A	1969	HIS
1	A	2093	GLN
1	A	2194	HIS
1	A	2302	GLN
1	A	2376	GLN
1	A	2402	HIS
1	A	2529	HIS
1	A	2613	GLN
1	A	2636	GLN
1	A	2739	HIS
1	A	3041	ASN
1	A	3055	ASN
1	A	3103	ASN
1	A	3249	GLN
1	A	3303	HIS
1	A	3310	HIS
1	A	3376	ASN
1	A	3400	HIS
1	A	3458	HIS
1	A	3522	ASN
1	A	3600	GLN
1	A	3622	ASN
1	A	3787	ASN
1	A	3809	HIS
1	A	3843	GLN
1	A	3852	HIS
1	A	3998	ASN
1	A	4132	GLN
1	A	4163	ASN

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Mol	Chain	Res	Type
1	A	4240	ASN
1	B	237	GLN
1	B	339	ASN
1	B	353	GLN
1	B	369	HIS
1	B	410	HIS
1	B	445	GLN
1	B	596	HIS
1	B	603	HIS
1	B	661	ASN
1	B	696	GLN
1	B	708	GLN
1	B	729	GLN
1	B	768	GLN
1	B	785	ASN
1	B	834	HIS
1	B	896	HIS
1	B	976	GLN
1	B	1009	ASN
1	B	1099	HIS
1	B	1118	ASN
1	B	1142	ASN
1	B	1153	GLN
1	B	1158	ASN
1	B	1231	HIS
1	B	1236	GLN
1	B	1238	GLN
1	B	1351	ASN
1	B	1366	GLN
1	B	1454	GLN
1	B	1495	GLN
1	B	1522	ASN
1	B	1553	ASN
1	B	1575	HIS
1	B	1594	GLN
1	B	1754	HIS
1	B	1931	GLN
1	B	1969	HIS
1	B	2093	GLN
1	B	2145	ASN
1	B	2194	HIS
1	B	2302	GLN

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Mol	Chain	Res	Type
1	B	2376	GLN
1	B	2396	ASN
1	B	2402	HIS
1	B	2437	GLN
1	B	2529	HIS
1	B	2613	GLN
1	B	2636	GLN
1	B	3041	ASN
1	B	3055	ASN
1	B	3103	ASN
1	B	3115	HIS
1	B	3196	ASN
1	B	3249	GLN
1	B	3300	ASN
1	B	3303	HIS
1	B	3310	HIS
1	B	3376	ASN
1	B	3385	HIS
1	B	3400	HIS
1	B	3458	HIS
1	B	3522	ASN
1	B	3600	GLN
1	B	3622	ASN
1	B	3629	HIS
1	B	3787	ASN
1	B	3804	GLN
1	B	3843	GLN
1	B	4132	GLN
1	B	4163	ASN
1	B	4240	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

33 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.29	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.73	0
2	BMA	C	3	2	11,11,12	0.23	0	15,15,17	0.53	0
2	NAG	D	1	1,2	14,14,15	0.32	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.75	0
2	BMA	D	3	2	11,11,12	0.21	0	15,15,17	0.50	0
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.68	0
2	BMA	E	3	2	11,11,12	0.21	0	15,15,17	0.55	0
2	NAG	F	1	1,2	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.61	0
2	BMA	F	3	2	11,11,12	0.21	0	15,15,17	0.56	0
3	NAG	G	1	3	14,14,15	0.40	0	17,19,21	0.76	0
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	2.00	4 (23%)
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	1.33	2 (11%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	2.00	4 (23%)
2	NAG	I	1	1,2	14,14,15	0.31	0	17,19,21	0.66	0
2	NAG	I	2	2	14,14,15	0.31	0	17,19,21	0.80	0
2	BMA	I	3	2	11,11,12	0.22	0	15,15,17	0.51	0
2	NAG	J	1	1,2	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	J	2	2	14,14,15	0.26	0	17,19,21	0.66	0
2	BMA	J	3	2	11,11,12	0.21	0	15,15,17	0.52	0
2	NAG	K	1	1,2	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
2	NAG	K	2	2	14,14,15	0.25	0	17,19,21	0.68	0
2	BMA	K	3	2	11,11,12	0.22	0	15,15,17	0.56	0
2	NAG	L	1	1,2	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	L	2	2	14,14,15	0.27	0	17,19,21	0.63	0
2	BMA	L	3	2	11,11,12	0.21	0	15,15,17	0.55	0
3	NAG	M	1	1,3	14,14,15	0.42	0	17,19,21	1.05	1 (5%)
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	1.02	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	N	1	1,2	14,14,15	0.39	0	17,19,21	1.21	2 (11%)
2	NAG	N	2	2	14,14,15	0.41	0	17,19,21	1.10	1 (5%)
2	BMA	N	3	2	11,11,12	0.21	0	15,15,17	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	BMA	L	3	2	-	0/2/19/22	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	BMA	N	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	O5-C5-C6	6.53	120.37	107.66
3	G	2	NAG	O5-C5-C6	6.52	120.35	107.66
2	N	2	NAG	O5-C1-C2	3.81	117.18	111.29
3	H	1	NAG	C1-C2-N2	3.69	116.25	110.43
3	H	1	NAG	C2-N2-C7	3.45	127.53	122.90
3	M	1	NAG	C2-N2-C7	3.12	127.08	122.90
3	M	2	NAG	C1-C2-N2	2.89	114.99	110.43
3	G	2	NAG	C4-C3-C2	2.74	115.03	111.02
2	N	1	NAG	C1-C2-N2	2.72	114.71	110.43
3	H	2	NAG	C4-C3-C2	2.71	114.99	111.02
3	M	2	NAG	C2-N2-C7	2.50	126.25	122.90
3	H	2	NAG	O3-C3-C4	2.46	116.18	110.38
3	G	2	NAG	O3-C3-C4	2.45	116.16	110.38
2	N	1	NAG	O5-C1-C2	2.40	115.00	111.29
2	E	1	NAG	C2-N2-C7	-2.17	119.99	122.90
2	K	1	NAG	C2-N2-C7	-2.07	120.12	122.90
3	G	2	NAG	O4-C4-C5	2.04	114.36	109.32
3	H	2	NAG	O4-C4-C5	2.04	114.35	109.32

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C1-C2-N2-C7
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C3-C2-N2-C7
2	K	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C1-C2-N2-C7
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	N	2	NAG	C8-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C1-C2-N2-C7
2	K	2	NAG	C8-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	I	3	BMA	O5-C5-C6-O6
3	M	2	NAG	C3-C2-N2-C7
2	I	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
3	H	1	NAG	C3-C2-N2-C7
2	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	6	0
3	G	1	NAG	7	0
2	E	1	NAG	5	0
2	D	1	NAG	2	0
2	I	1	NAG	2	0
2	J	2	NAG	1	0
2	N	1	NAG	2	0

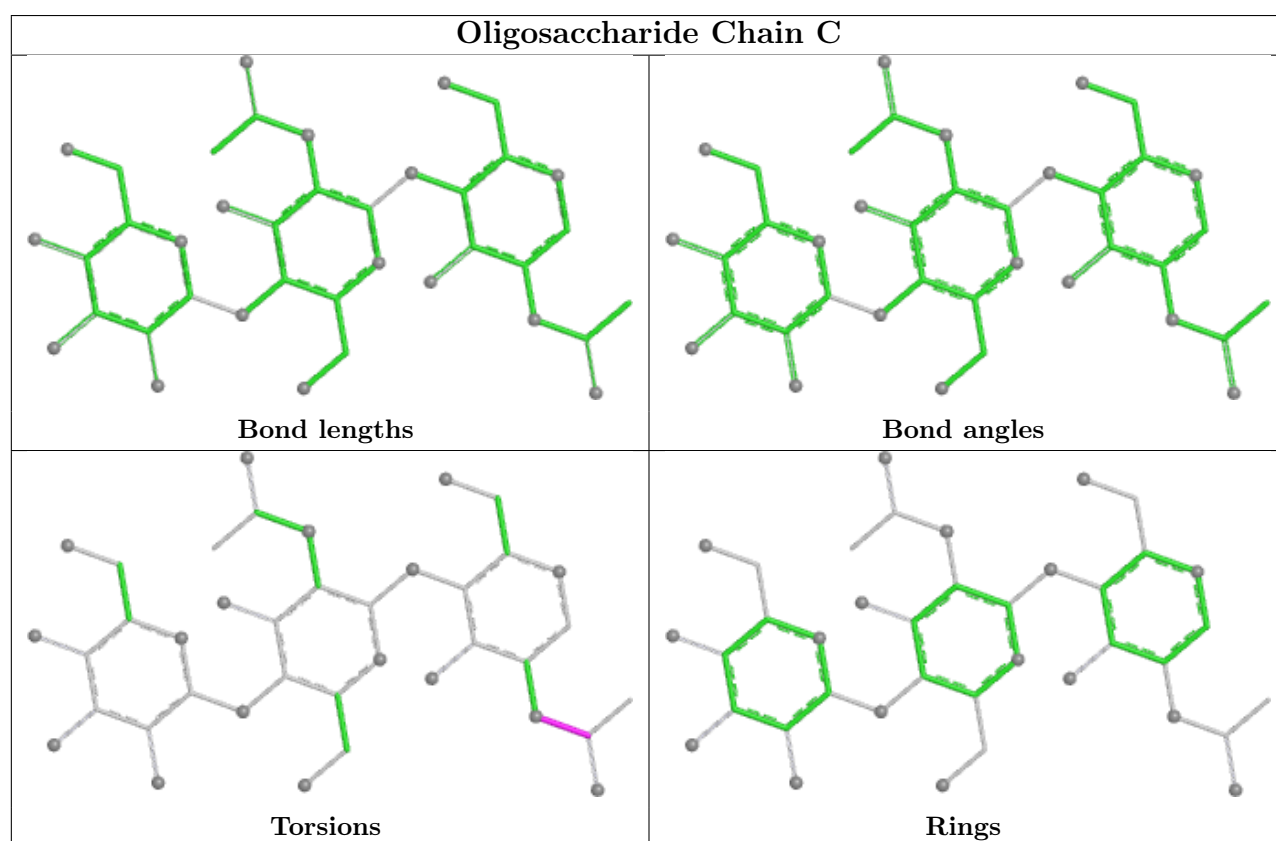
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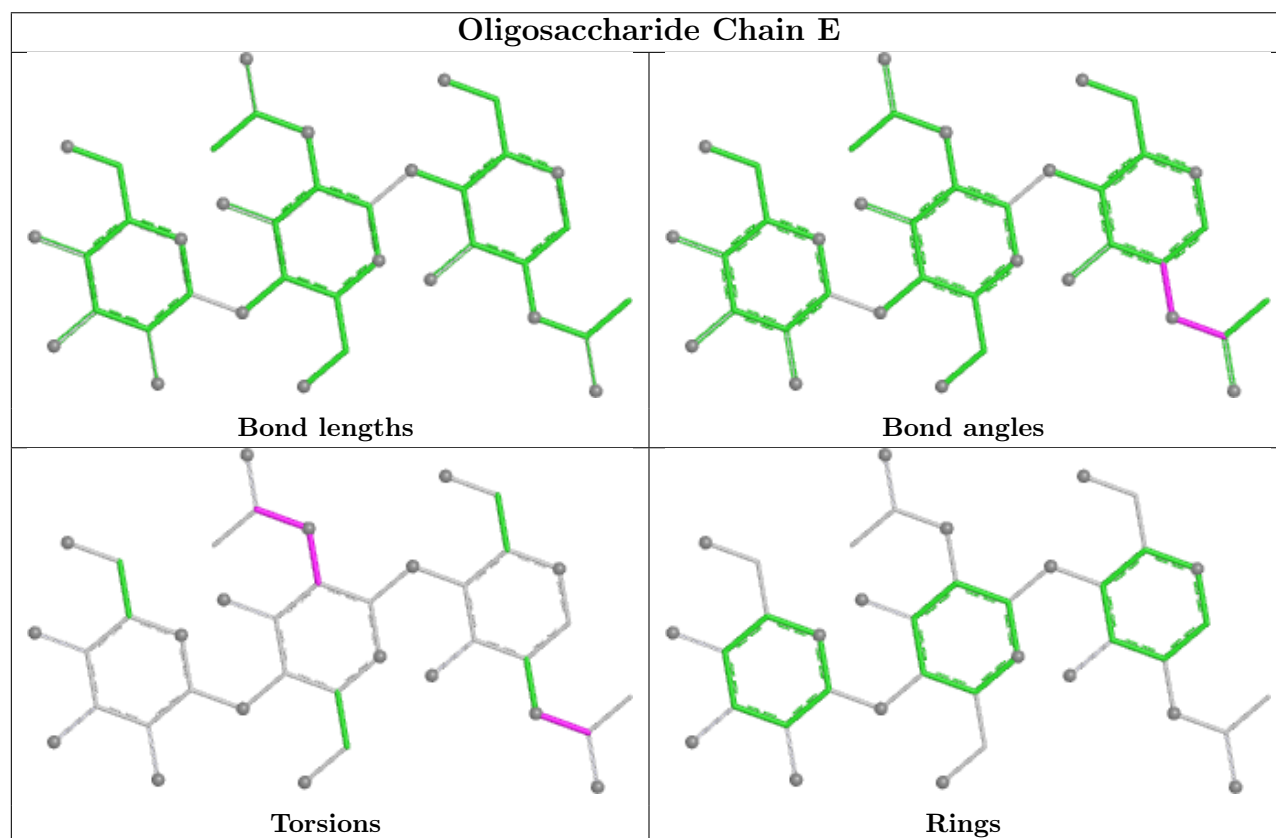
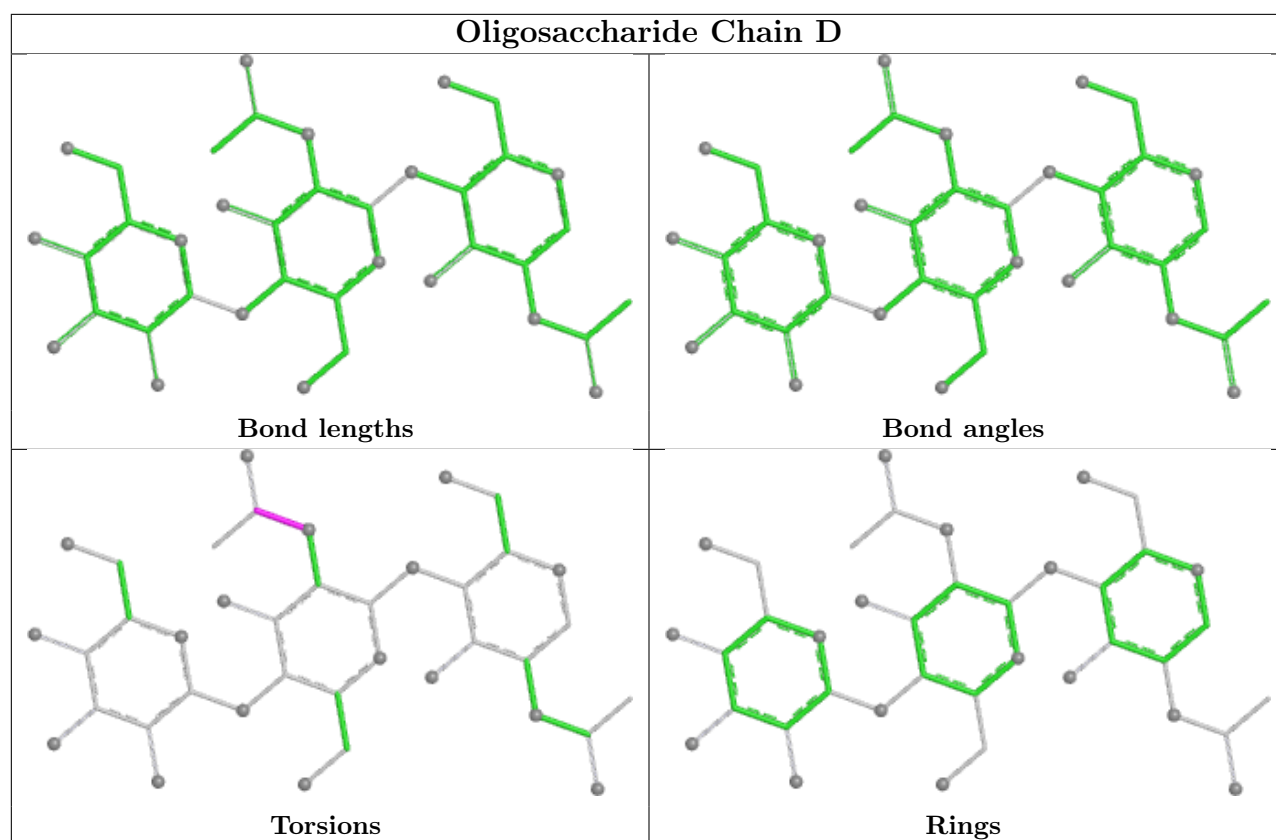


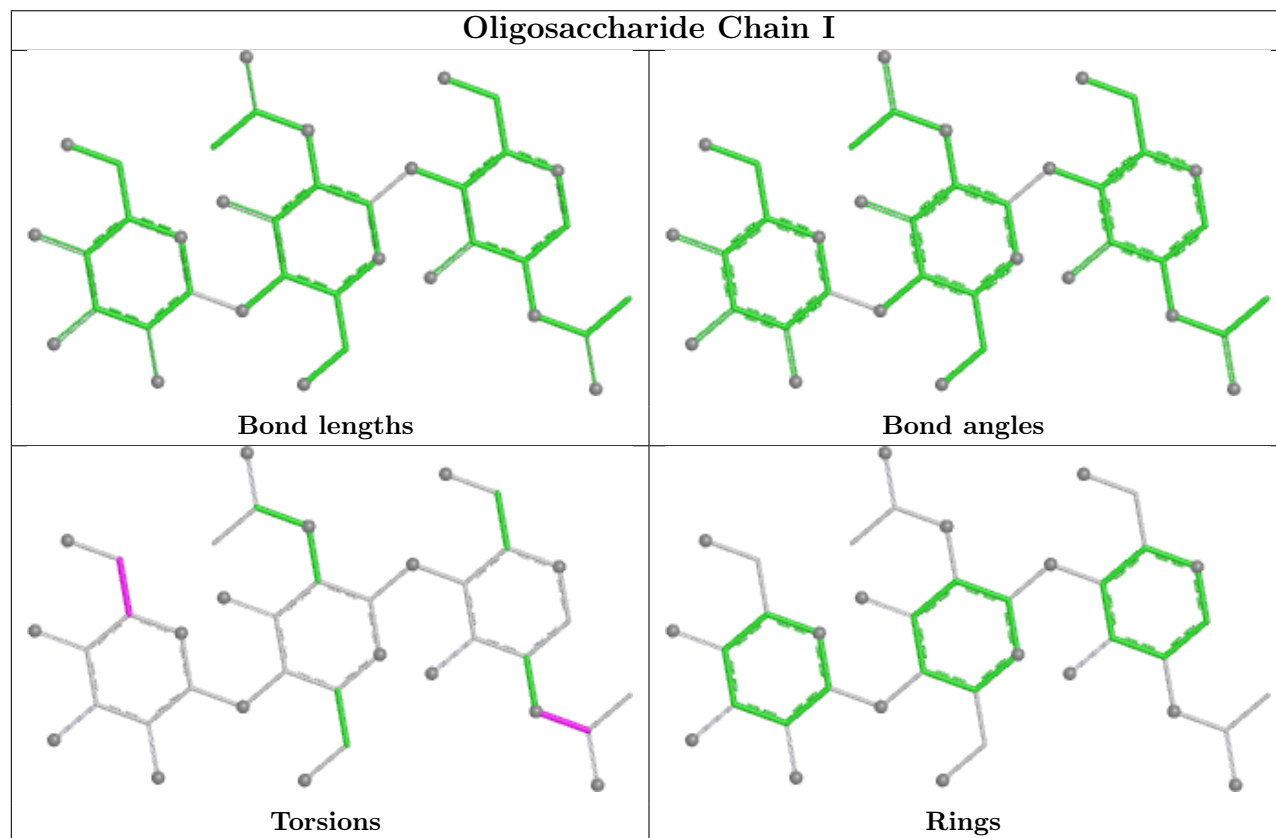
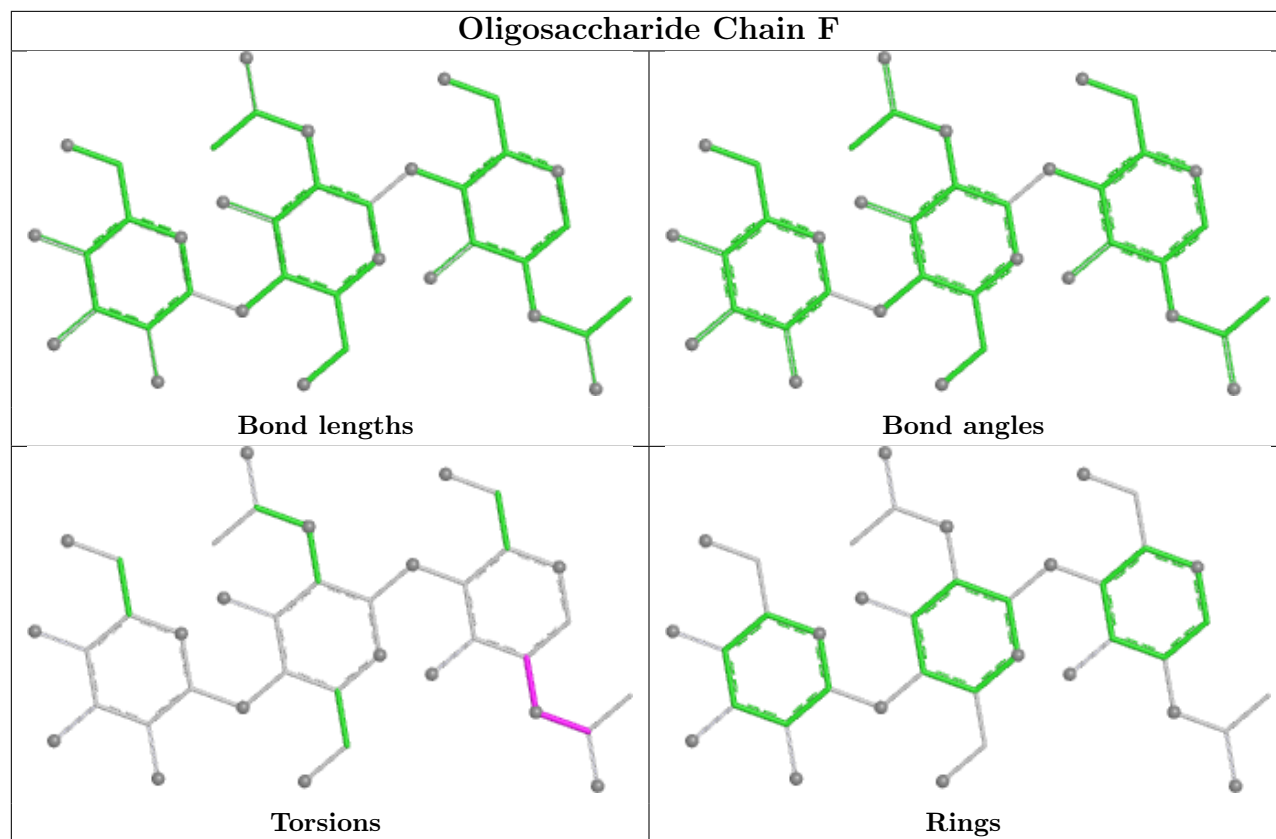
*Continued from previous page...*

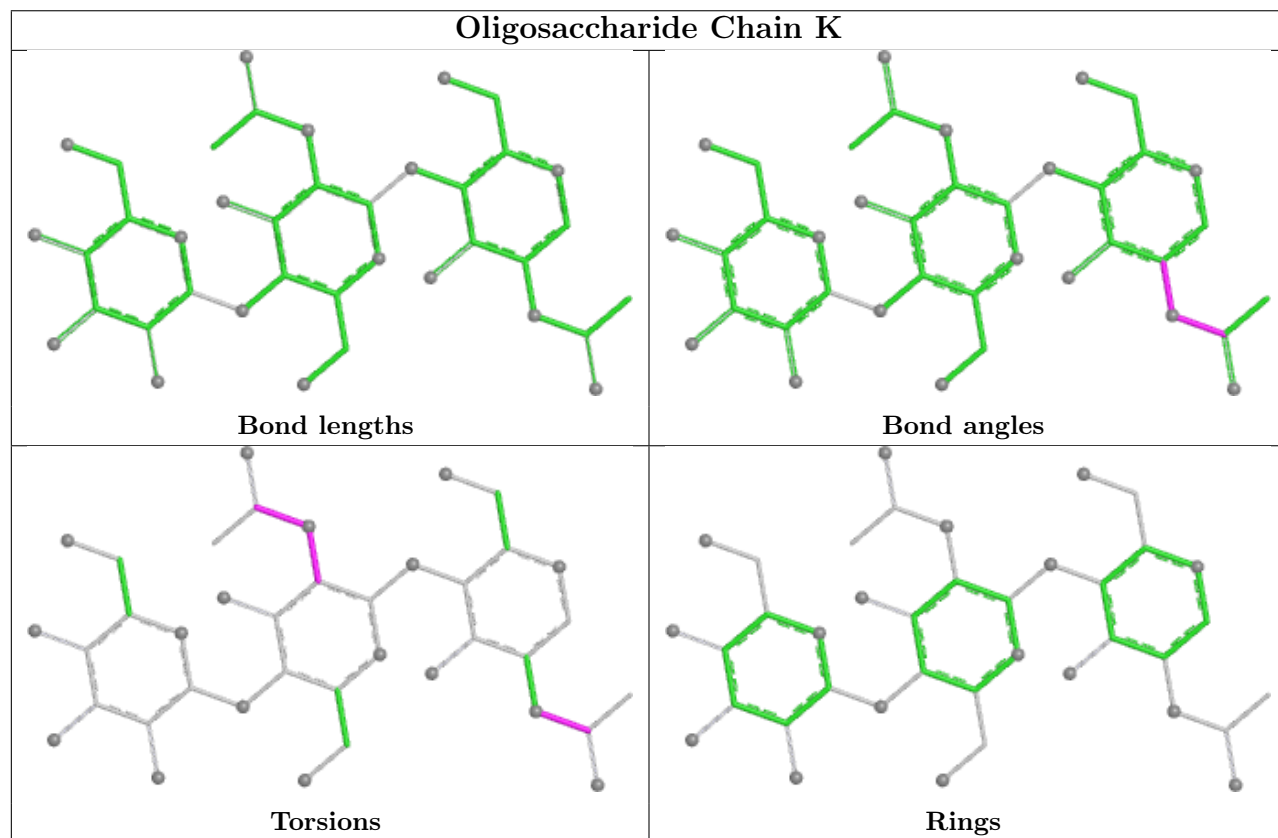
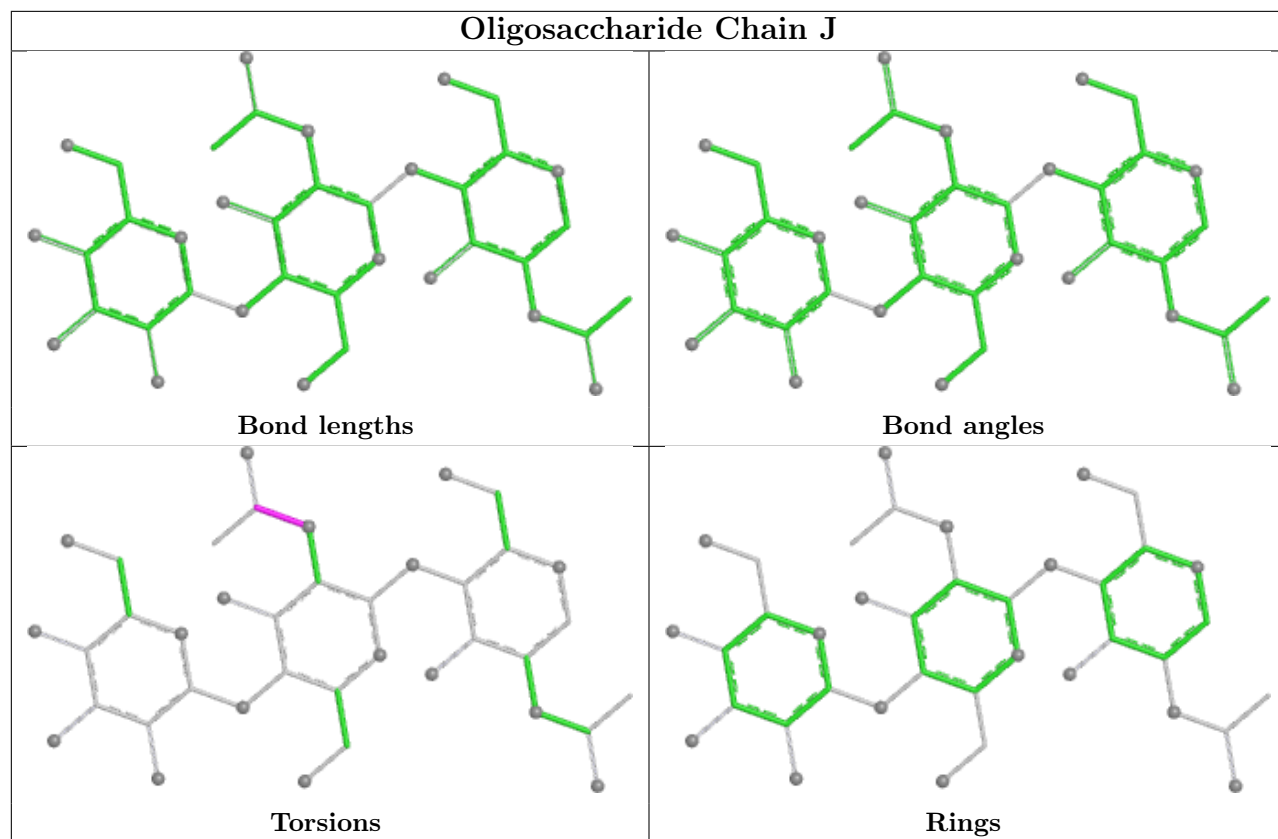
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	2	0
2	C	2	NAG	1	0
3	M	1	NAG	1	0
3	H	1	NAG	1	0
3	G	2	NAG	3	0
2	J	1	NAG	3	0
2	D	2	NAG	1	0
2	C	1	NAG	2	0

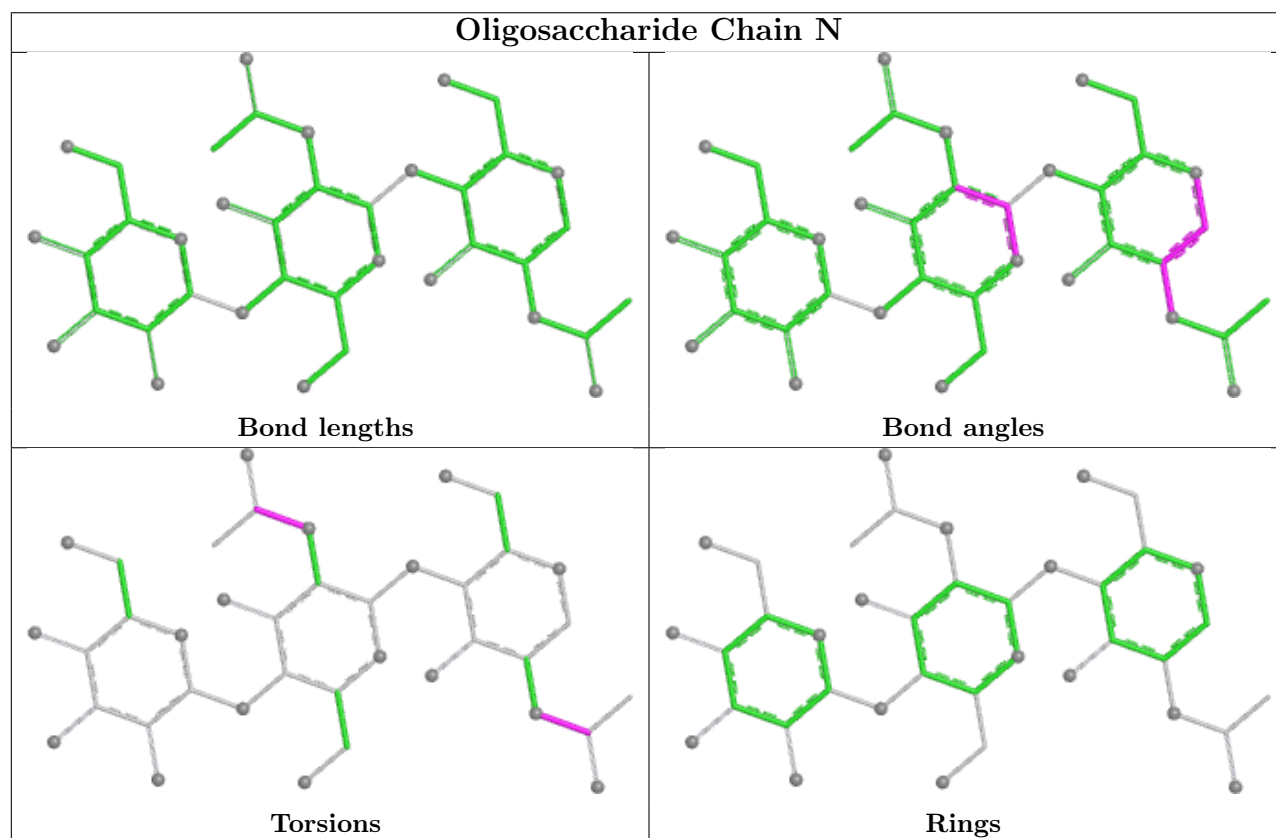
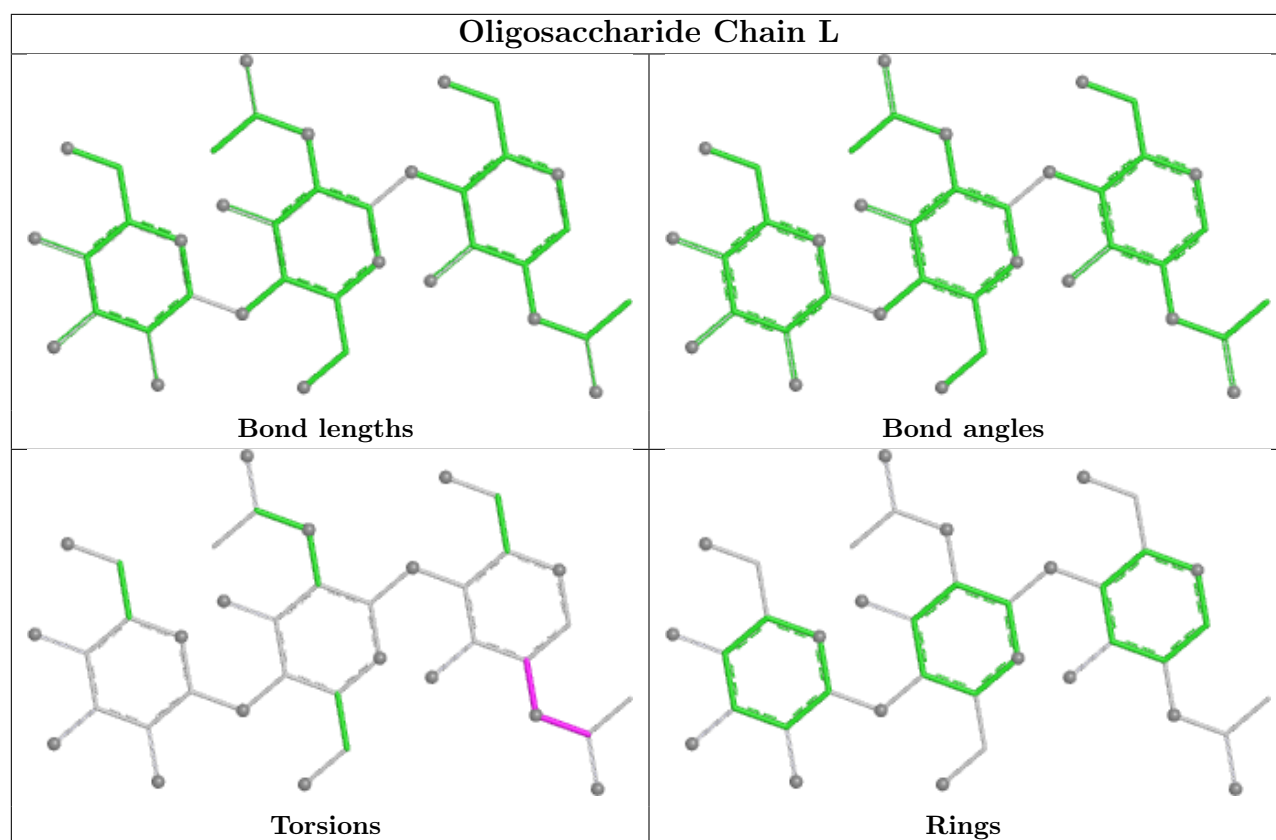
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

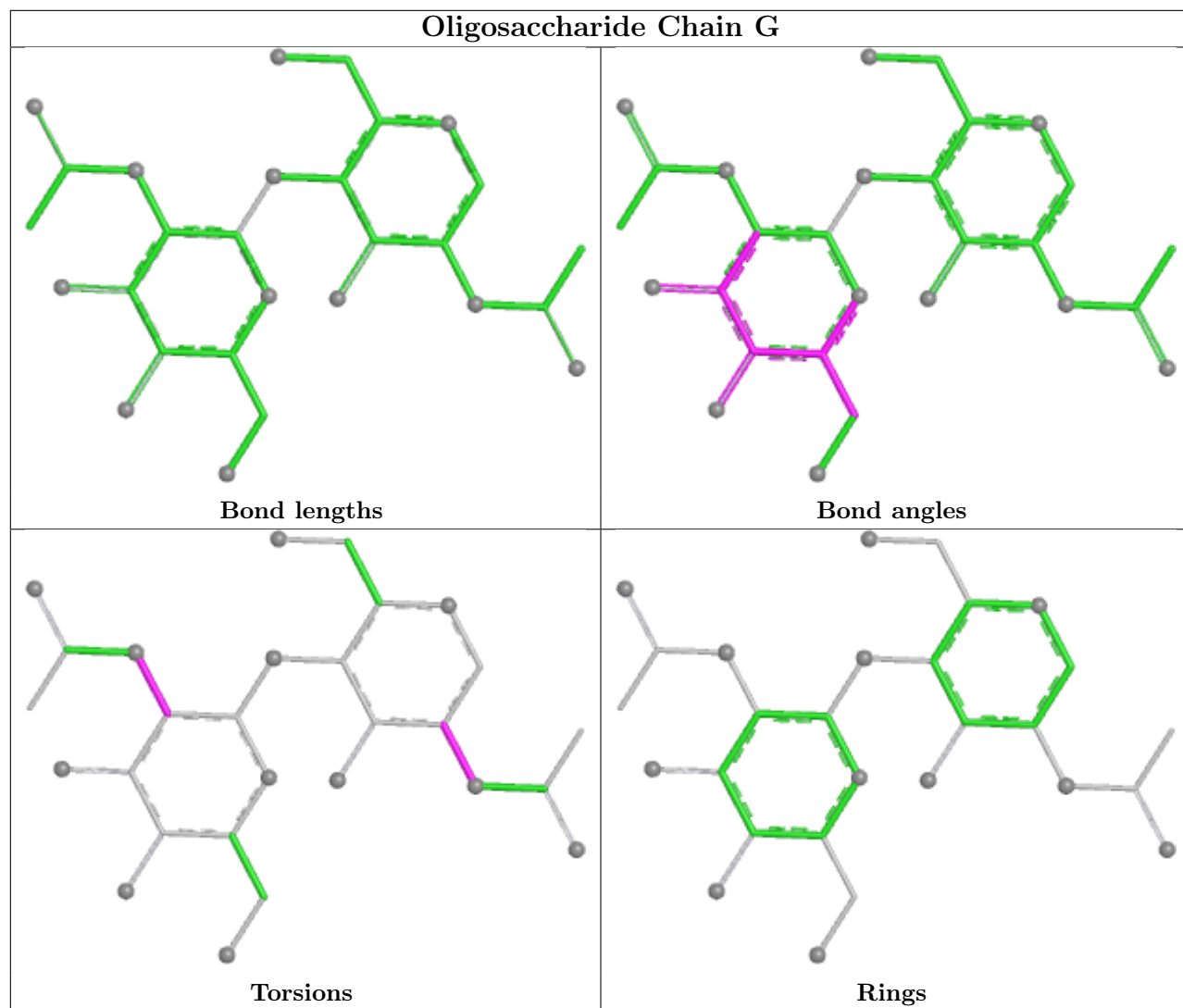


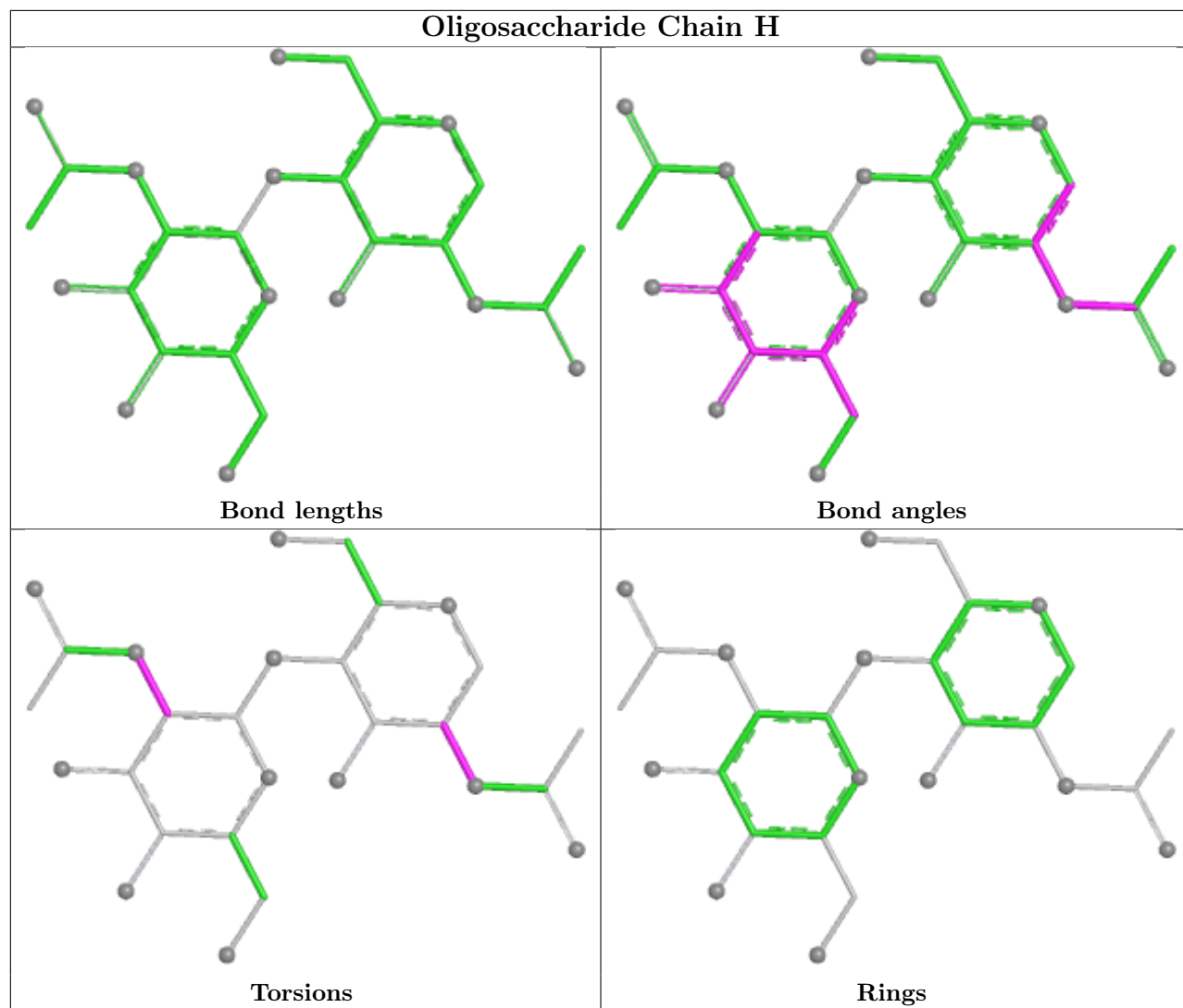


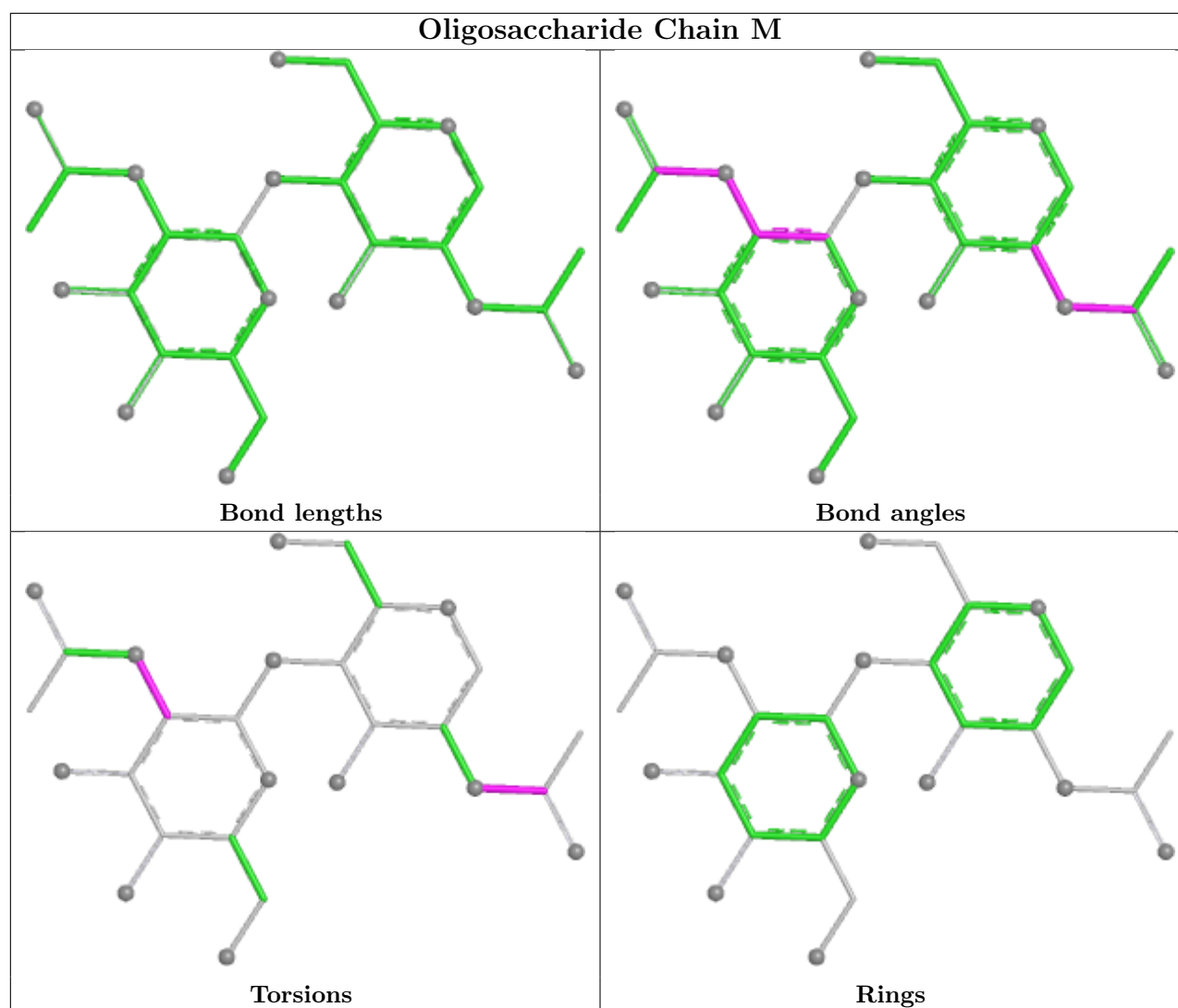












## 5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	4709	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4703	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	B	4705	1	14,14,15	0.28	0	17,19,21	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4708	1	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
4	NAG	A	4706	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4712	1	14,14,15	0.39	0	17,19,21	0.79	1 (5%)
4	NAG	B	4703	1	14,14,15	0.30	0	17,19,21	0.68	0
4	NAG	B	4702	1	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	B	4704	1	14,14,15	0.27	0	17,19,21	0.74	0
4	NAG	A	4701	1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	A	4708	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
4	NAG	B	4710	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	B	4711	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	A	4702	1	14,14,15	0.29	0	17,19,21	0.75	0
4	NAG	A	4709	1	14,14,15	0.27	0	17,19,21	0.69	0
4	NAG	B	4706	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	A	4705	1	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	A	4711	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	A	4710	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	B	4701	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	A	4704	1	14,14,15	0.28	0	17,19,21	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	4709	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4703	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4707	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4708	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4706	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4712	1	-	1/6/23/26	0/1/1/1
4	NAG	B	4703	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4708	1	-	1/6/23/26	0/1/1/1
4	NAG	B	4710	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4702	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4709	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4710	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4707	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4708	NAG	C2-N2-C7	3.44	127.50	122.90
4	A	4712	NAG	C2-N2-C7	2.43	126.15	122.90
4	A	4708	NAG	C2-N2-C7	2.26	125.92	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4707	NAG	C8-C7-N2-C2
4	A	4707	NAG	O7-C7-N2-C2
4	A	4710	NAG	C1-C2-N2-C7
4	A	4710	NAG	C8-C7-N2-C2
4	A	4710	NAG	O7-C7-N2-C2
4	B	4704	NAG	C8-C7-N2-C2
4	B	4704	NAG	O7-C7-N2-C2
4	B	4707	NAG	C3-C2-N2-C7
4	B	4707	NAG	C8-C7-N2-C2
4	B	4707	NAG	O7-C7-N2-C2
4	B	4708	NAG	C3-C2-N2-C7
4	B	4708	NAG	C8-C7-N2-C2
4	B	4708	NAG	O7-C7-N2-C2
4	A	4702	NAG	C8-C7-N2-C2
4	A	4702	NAG	O7-C7-N2-C2
4	B	4702	NAG	C8-C7-N2-C2
4	A	4706	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	4703	NAG	C8-C7-N2-C2
4	A	4703	NAG	C8-C7-N2-C2
4	A	4706	NAG	O7-C7-N2-C2
4	B	4702	NAG	O7-C7-N2-C2
4	B	4703	NAG	O7-C7-N2-C2
4	A	4703	NAG	O7-C7-N2-C2
4	A	4709	NAG	C8-C7-N2-C2
4	A	4707	NAG	C3-C2-N2-C7
4	A	4709	NAG	O7-C7-N2-C2
4	A	4708	NAG	C3-C2-N2-C7
4	A	4712	NAG	C3-C2-N2-C7
4	A	4703	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4703	NAG	1	0
4	A	4702	NAG	1	0
4	B	4701	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

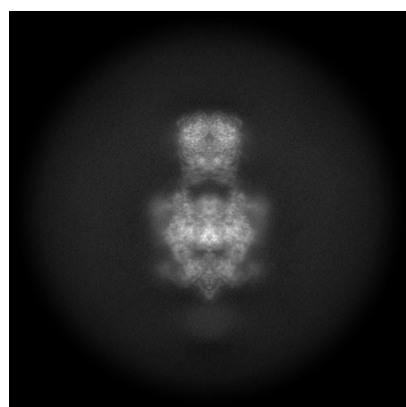
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45967. These allow visual inspection of the internal detail of the map and identification of artifacts.

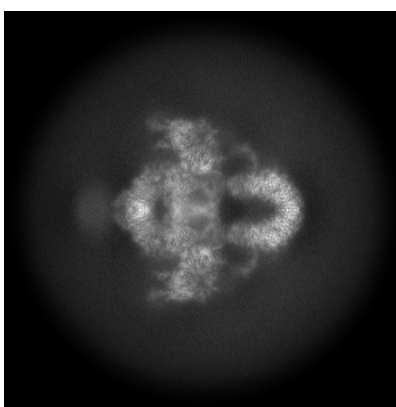
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

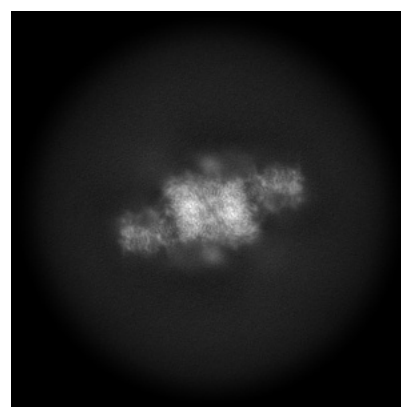
#### 6.1.1 Primary map



X



Y

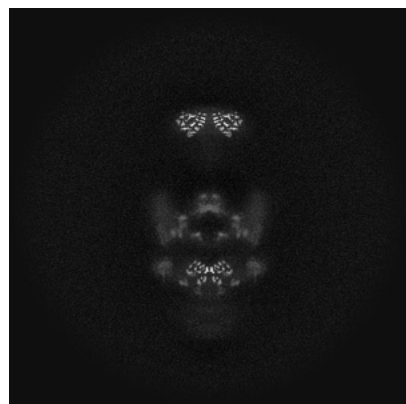


Z

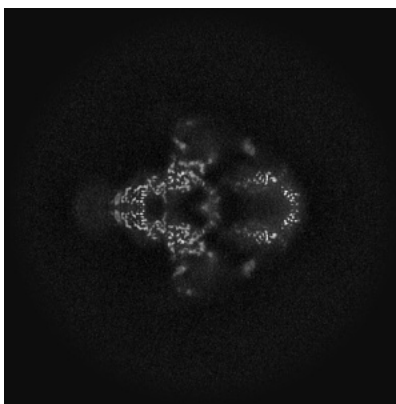
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

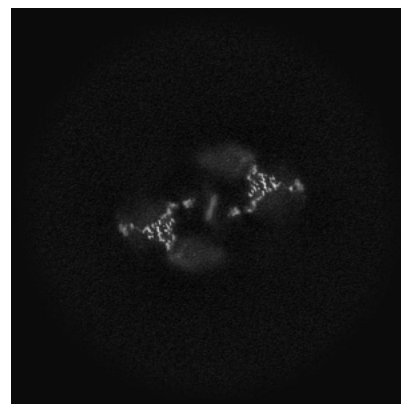
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

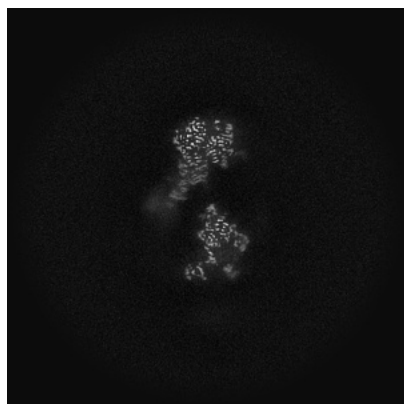


Z Index: 256

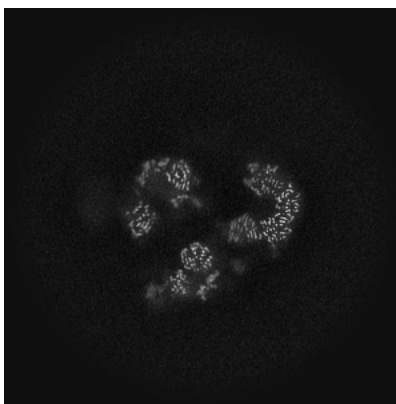
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

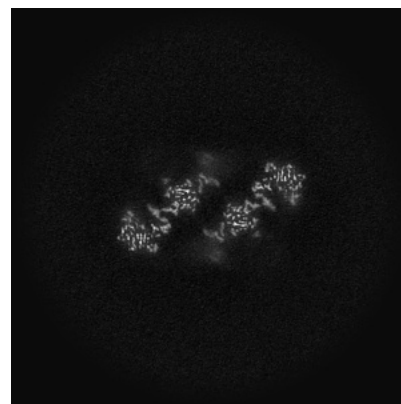
### 6.3.1 Primary map



X Index: 224



Y Index: 233

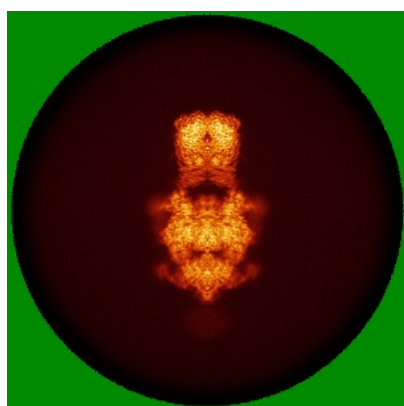


Z Index: 231

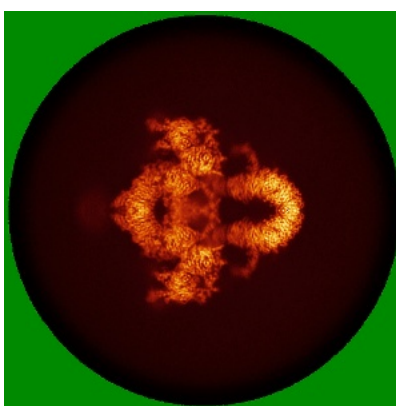
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

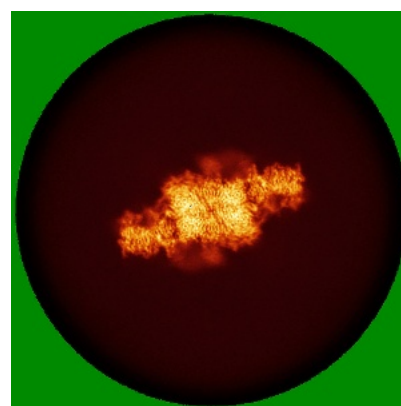
### 6.4.1 Primary map



X



Y

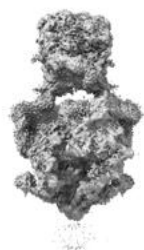


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

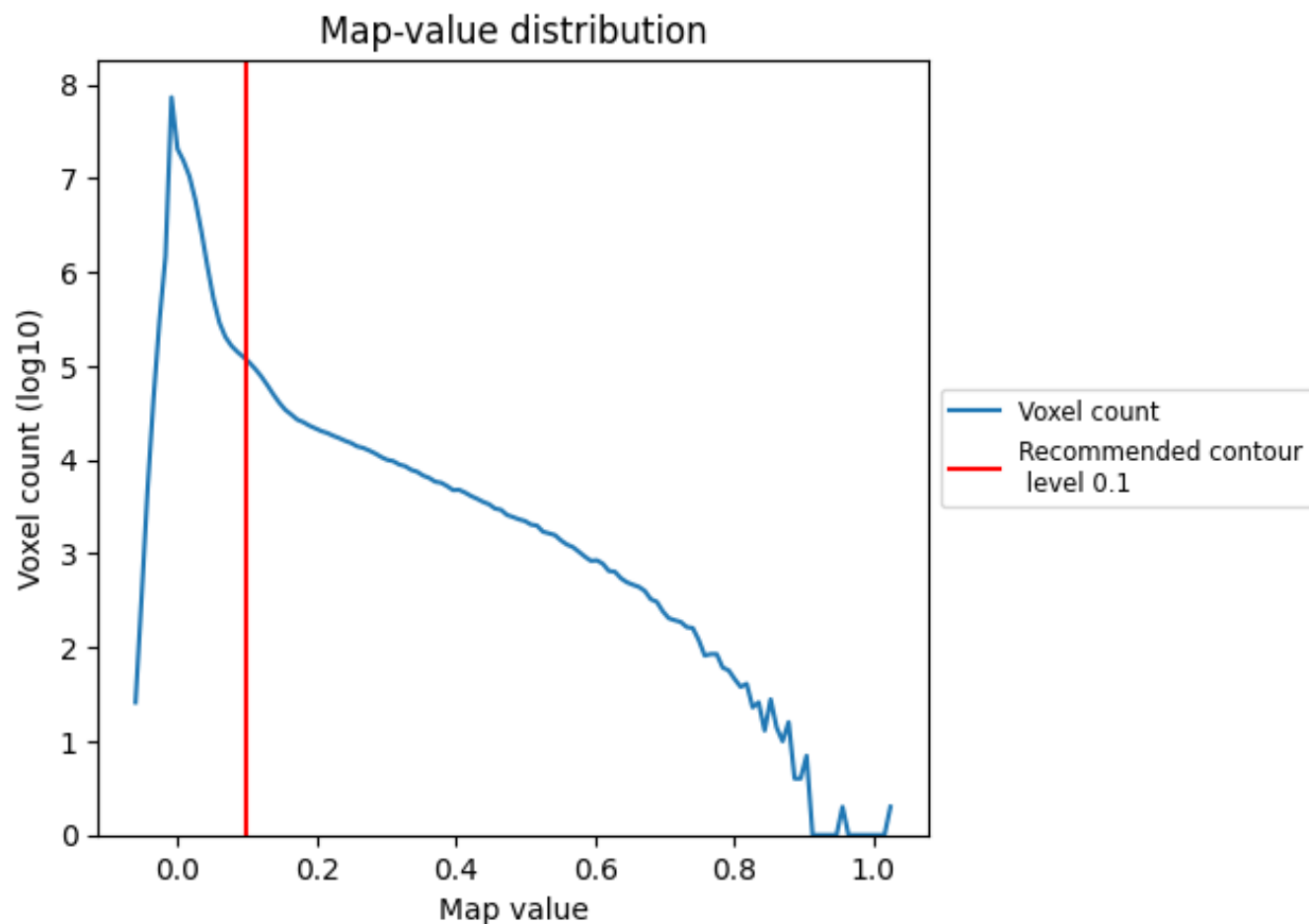
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

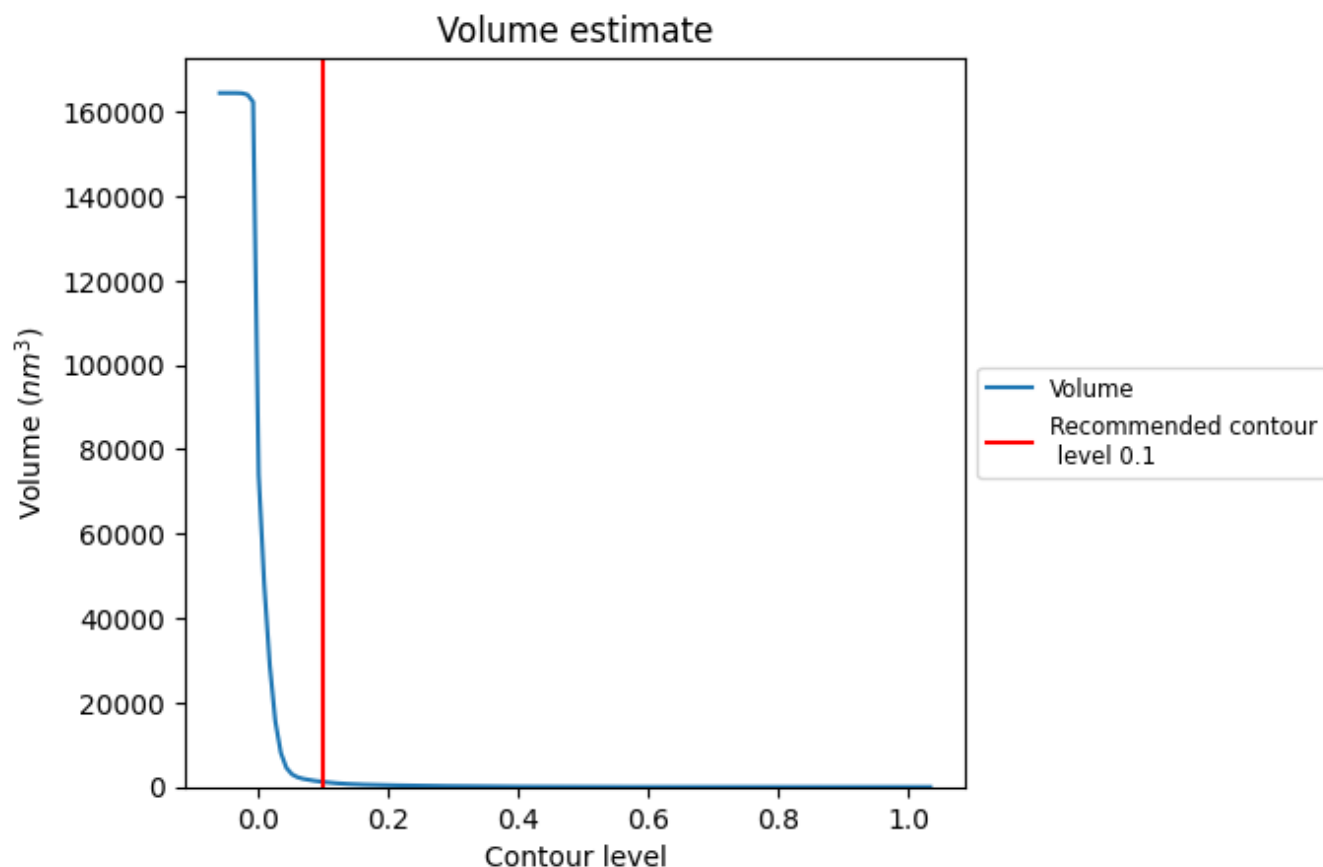
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

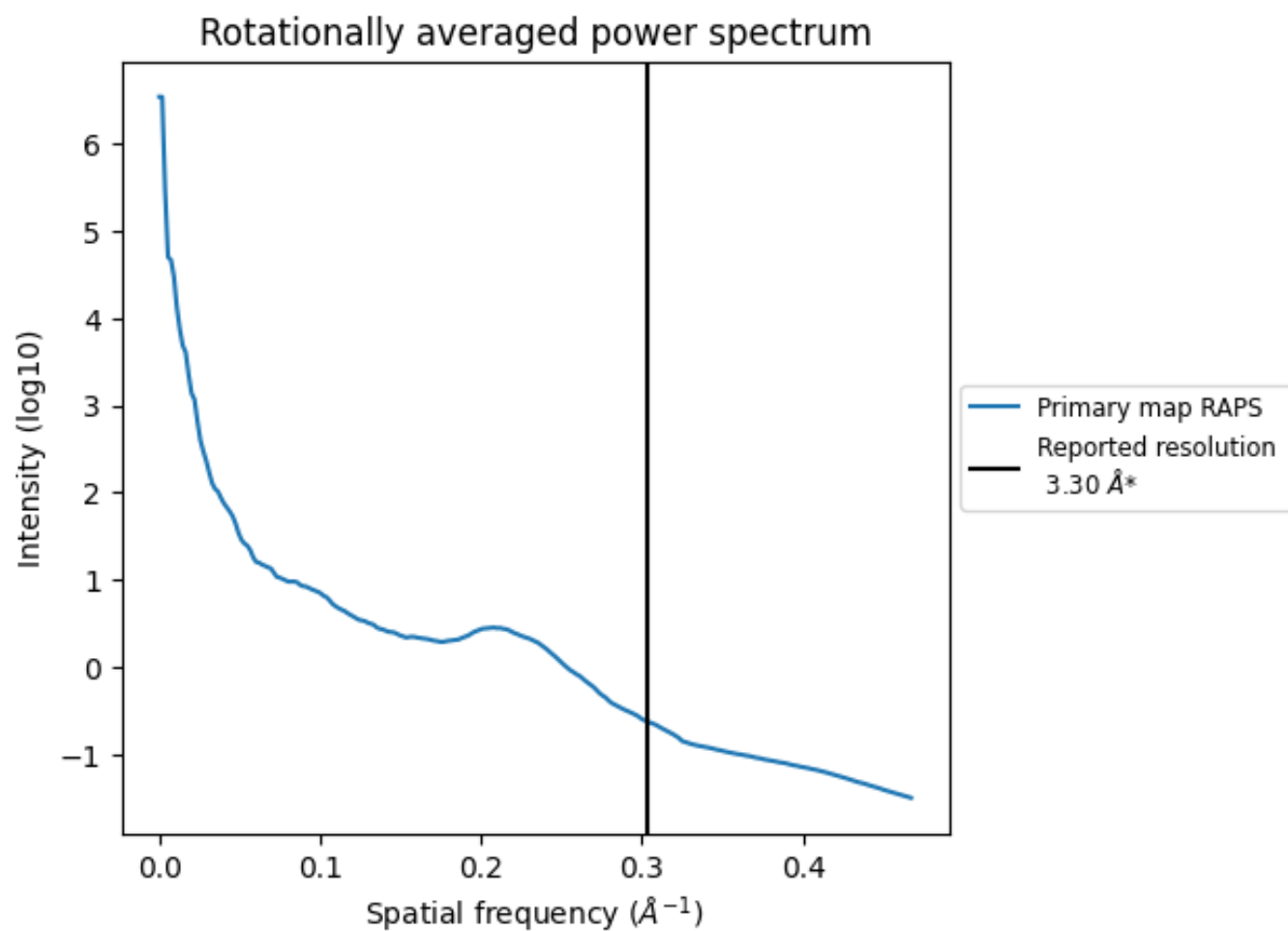


The volume at the recommended contour level is 1187  $\text{nm}^3$ ; this corresponds to an approximate mass of 1072 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$

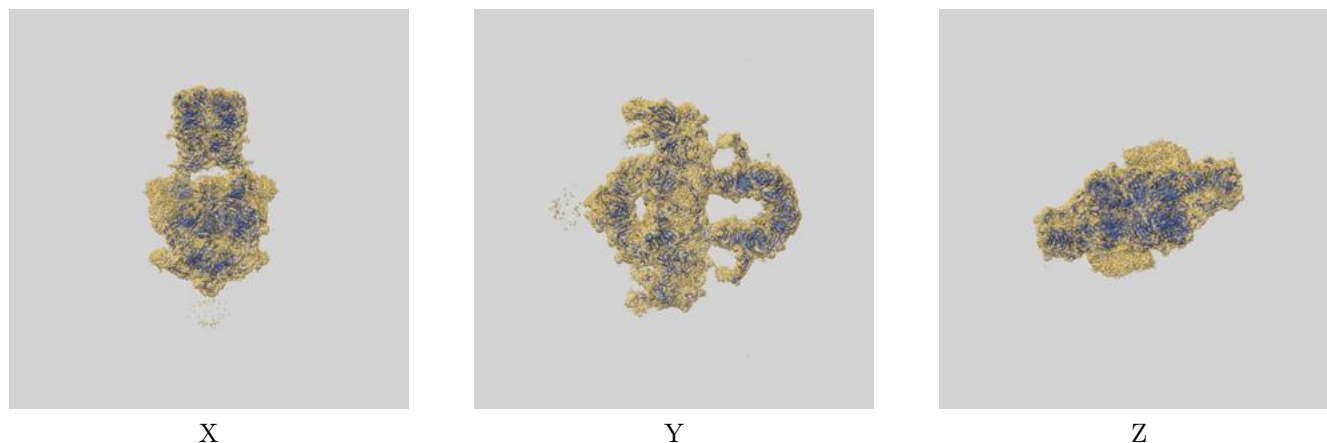
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

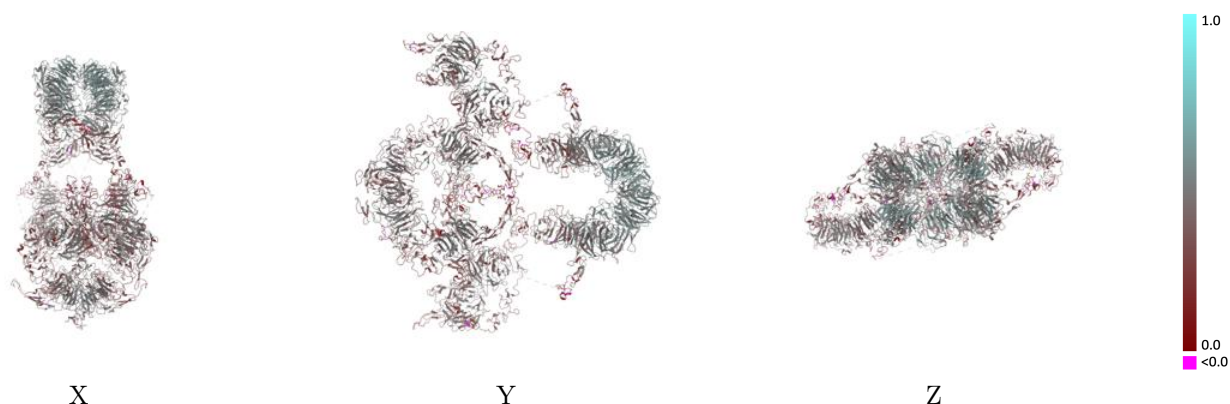
This section contains information regarding the fit between EMDB map EMD-45967 and PDB model 9CWM. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



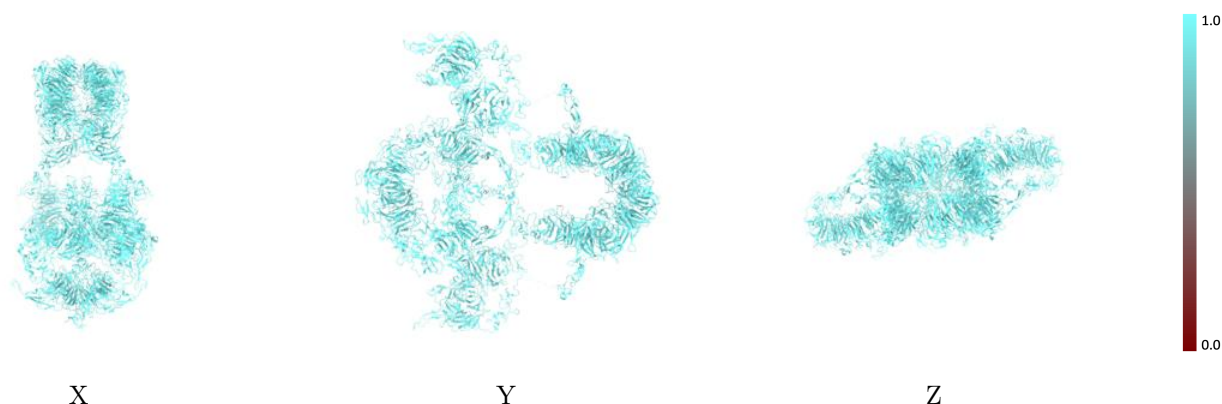
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



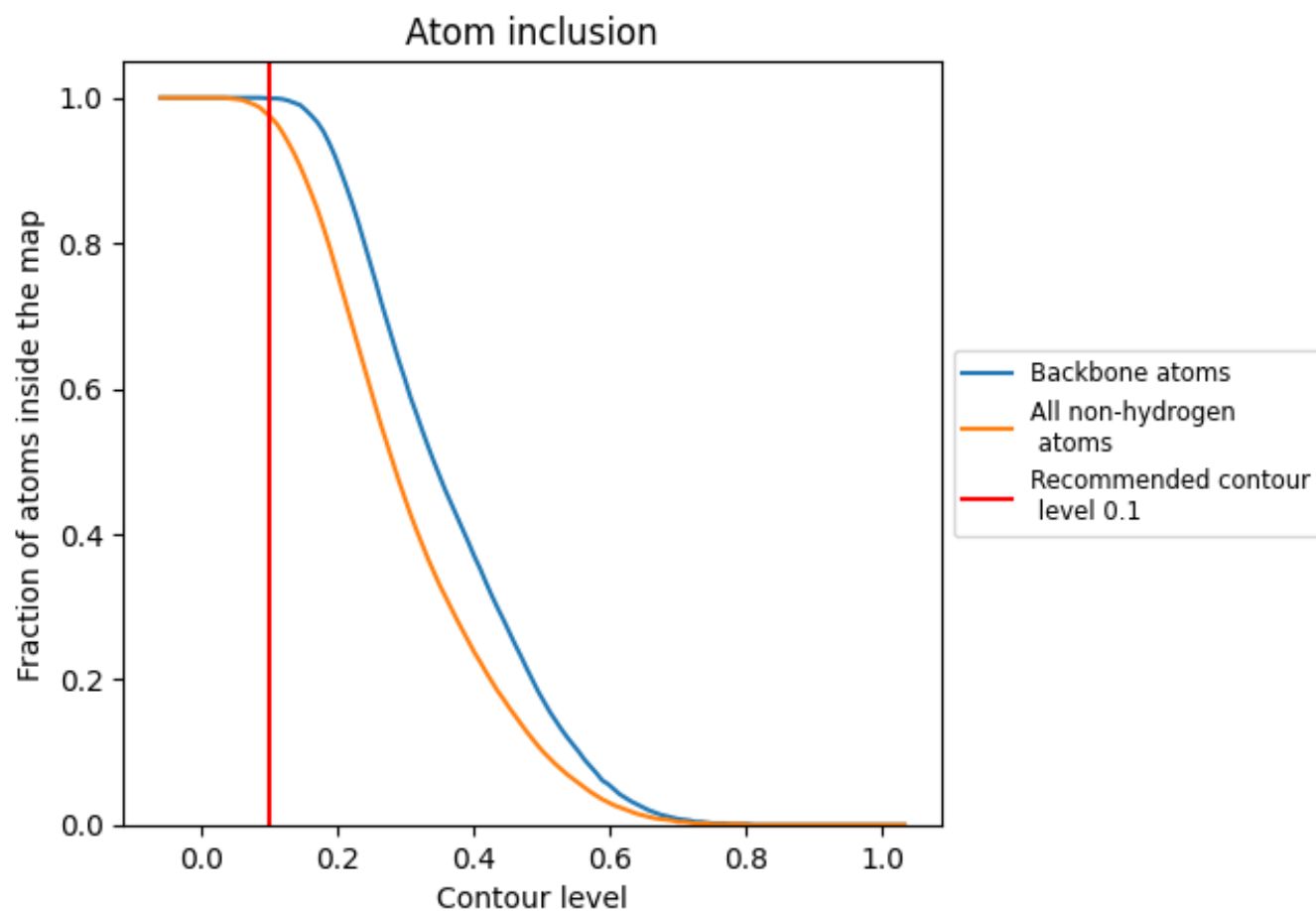
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.4030
A	 0.9760	 0.4050
B	 0.9750	 0.4010
C	 0.9490	 0.4310
D	 0.9490	 0.3520
E	 1.0000	 0.4100
F	 0.8970	 0.1850
G	 0.8930	 0.3650
H	 1.0000	 0.4200
I	 0.9740	 0.4470
J	 0.9490	 0.3580
K	 1.0000	 0.4160
L	 0.8970	 0.2190
M	 0.9640	 0.3420
N	 0.8210	 0.1740

