



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 03:16 AM EDT

PDB ID : 6SLI  
Title : Structure of the RagAB peptide transporter  
Authors : Madej, M.; Ranson, N.A.; White, J.B.R.  
Deposited on : 2019-08-19  
Resolution : 3.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

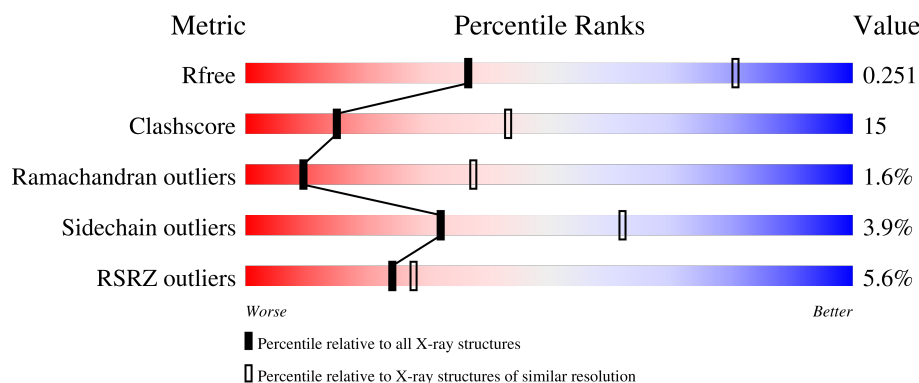
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	488	<div> <div>9%</div> <div>74%</div> <div>24%</div> <div>..</div> </div>
1	C	488	<div> <div>77%</div> <div>21%</div> <div>..</div> </div>
1	F	488	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	I	488	<div> <div>9%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	B	997	<div> <div>2%</div> <div>54%</div> <div>33%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	997	<div><div></div><div>9%</div><div>53%</div><div>34%</div><div>10%</div></div>
2	G	997	<div><div></div><div>9%</div><div>56%</div><div>32%</div><div>10%</div></div>
2	J	997	<div><div></div><div>6%</div><div>56%</div><div>31%</div><div>10%</div></div>
3	H	13	<div><div></div><div>8%</div><div>69%</div><div>23%</div><div>8%</div></div>
3	P	13	<div><div></div><div>8%</div><div>62%</div><div>31%</div><div>8%</div></div>
4	E	13	<div><div></div><div>8%</div><div>38%</div><div>38%</div><div>23%</div></div>
4	K	13	<div><div></div><div>8%</div><div>69%</div><div>23%</div><div>8%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43926 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Lipoprotein RagB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3842	2440	656	737	9			
1	C	482	Total	C	N	O	S	0	0	0
			3842	2440	656	737	9			
1	F	482	Total	C	N	O	S	0	0	0
			3842	2440	656	737	9			
1	I	482	Total	C	N	O	S	0	0	0
			3842	2440	656	737	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	HIS	-	expression tag	UNP F5H948
A	503	HIS	-	expression tag	UNP F5H948
A	504	HIS	-	expression tag	UNP F5H948
A	505	HIS	-	expression tag	UNP F5H948
A	506	HIS	-	expression tag	UNP F5H948
A	507	HIS	-	expression tag	UNP F5H948
C	502	HIS	-	expression tag	UNP F5H948
C	503	HIS	-	expression tag	UNP F5H948
C	504	HIS	-	expression tag	UNP F5H948
C	505	HIS	-	expression tag	UNP F5H948
C	506	HIS	-	expression tag	UNP F5H948
C	507	HIS	-	expression tag	UNP F5H948
F	502	HIS	-	expression tag	UNP F5H948
F	503	HIS	-	expression tag	UNP F5H948
F	504	HIS	-	expression tag	UNP F5H948
F	505	HIS	-	expression tag	UNP F5H948
F	506	HIS	-	expression tag	UNP F5H948
F	507	HIS	-	expression tag	UNP F5H948
I	502	HIS	-	expression tag	UNP F5H948
I	503	HIS	-	expression tag	UNP F5H948
I	504	HIS	-	expression tag	UNP F5H948

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Chain	Residue	Modelled	Actual	Comment	Reference
I	505	HIS	-	expression tag	UNP F5H948
I	506	HIS	-	expression tag	UNP F5H948
I	507	HIS	-	expression tag	UNP F5H948

- Molecule 2 is a protein called RagA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	900	Total	C	N	O	S	0	0	0
			7048	4466	1179	1371	32			
2	D	900	Total	C	N	O	S	0	0	0
			7048	4466	1179	1371	32			
2	G	900	Total	C	N	O	S	0	0	0
			7048	4466	1179	1371	32			
2	J	900	Total	C	N	O	S	0	0	0
			7048	4466	1179	1371	32			

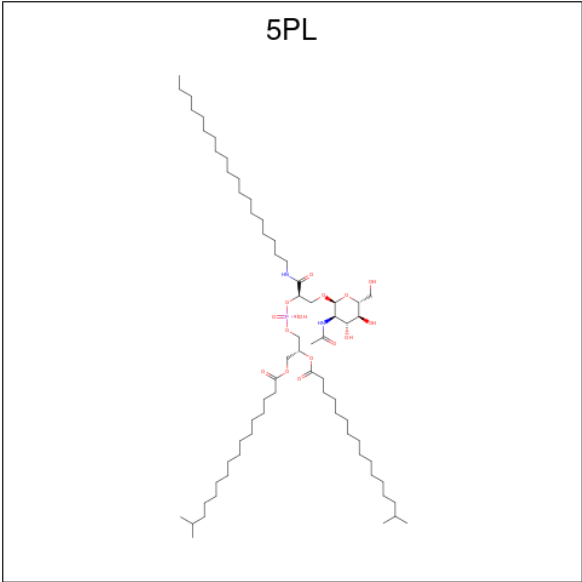
- Molecule 3 is a protein called ALA-SER-THR-THR-GLY-GLY-ASN-SER-GLN-ARG-GLY-SER-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	0	0	0
			81	43	18	20			
3	H	13	Total	C	N	O	0	0	0
			81	43	18	20			

- Molecule 4 is a protein called ASTTGGSQRGGG.

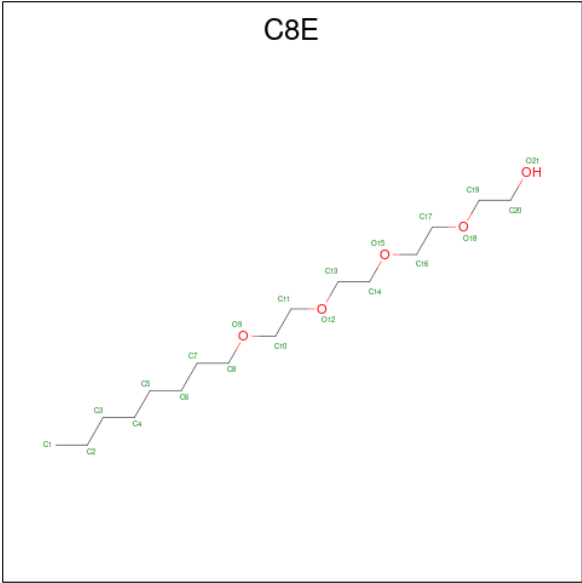
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	13	Total	C	N	O	0	0	0
			79	42	18	19			
4	K	13	Total	C	N	O	0	0	0
			79	42	18	19			

- Molecule 5 is (1R,4S,6R)-6-([2-(ACETYLAMINO)-2-DEOXY-ALPHA-D-GLUCOPYRANOSYL]OXY)METHYL)-4-HYDROXY-1-([(15-METHYLHEXADECANOYL)OXY]METHYL)-4-OXIDO-7-OXO-3,5-DIOXA-8-AZA-4-PHOSPHAHEPTACOS-1-YL 15-METHYLHEXADECANOATE (three-letter code: 5PL) (formula: C<sub>67</sub>H<sub>129</sub>N<sub>2</sub>O<sub>15</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			20	16	4		

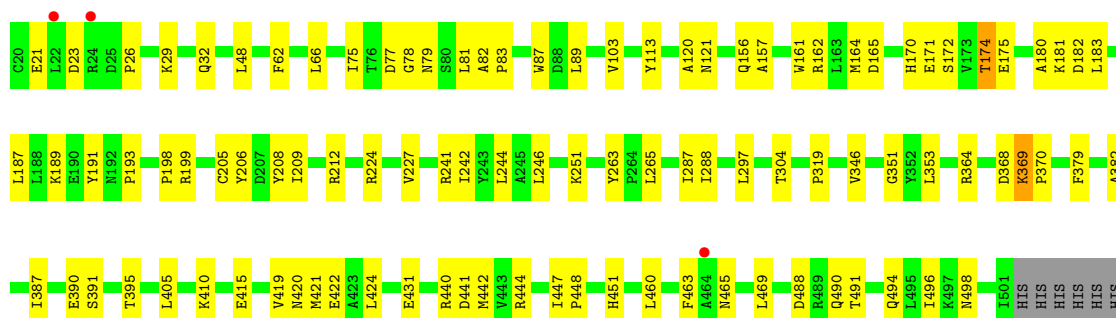
- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



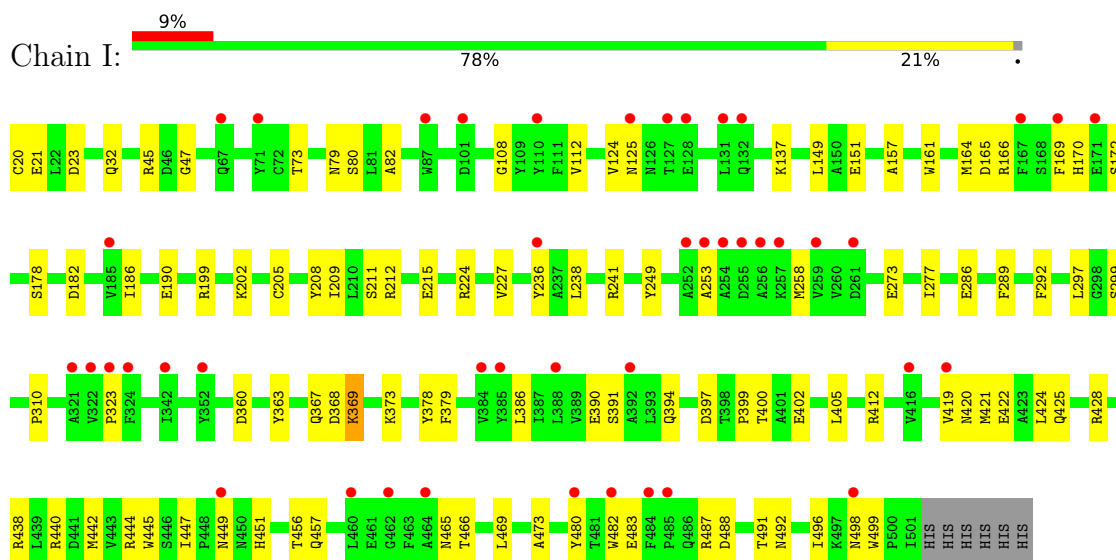
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	11	2		
6	B	1	Total	C	O	0	0
			13	11	2		

- Molecule 1: Lipoprotein RagB

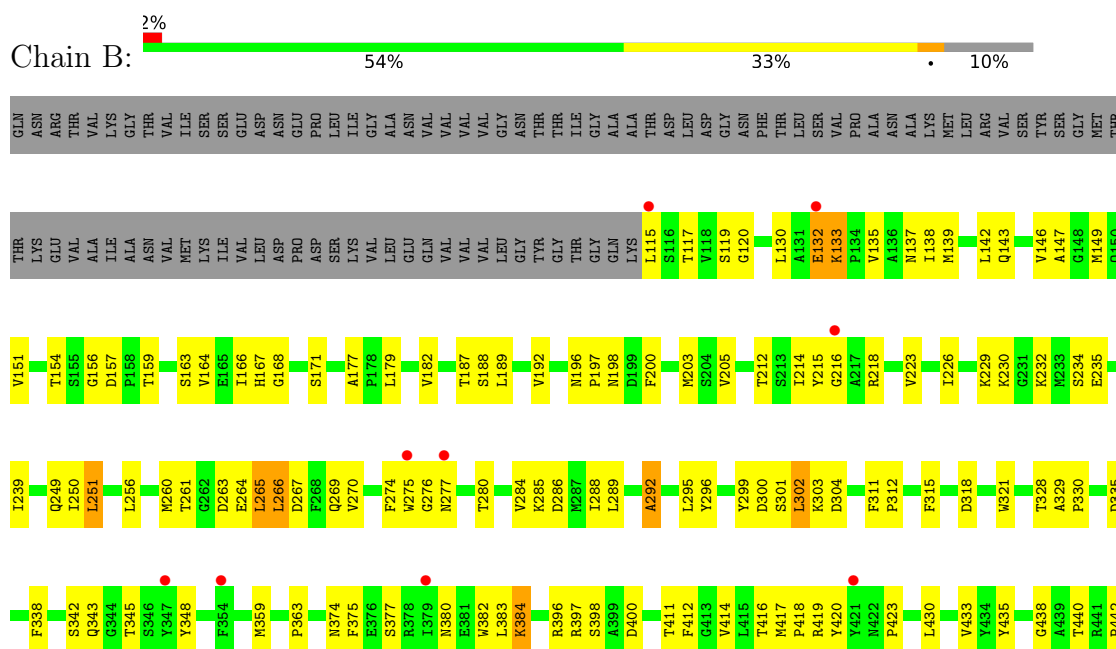




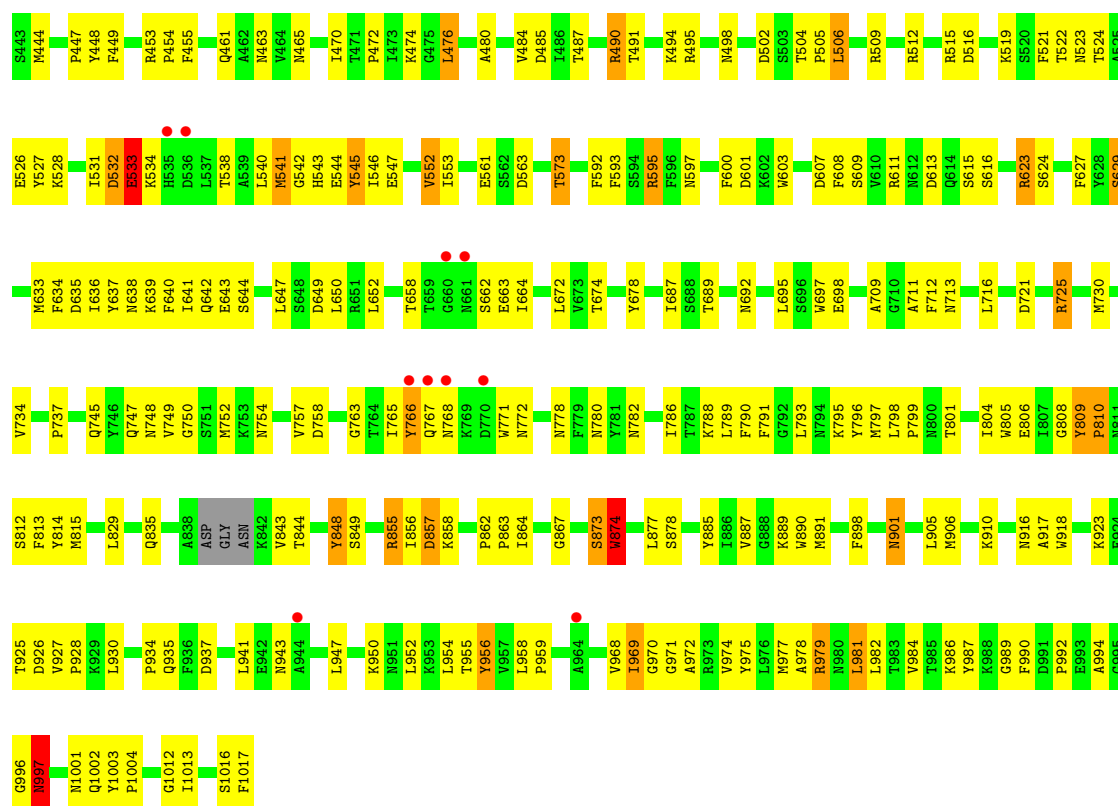
• Molecule 1: Lipoprotein RagB



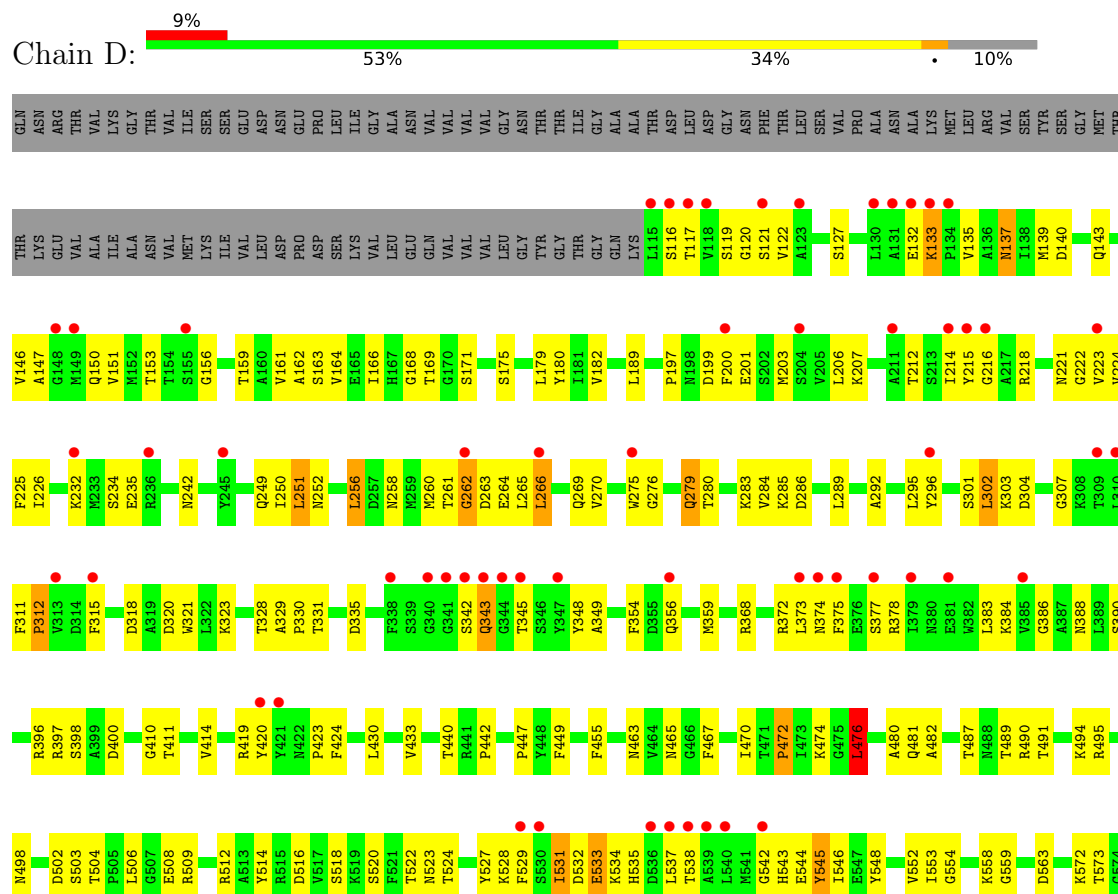
• Molecule 2: RagA protein

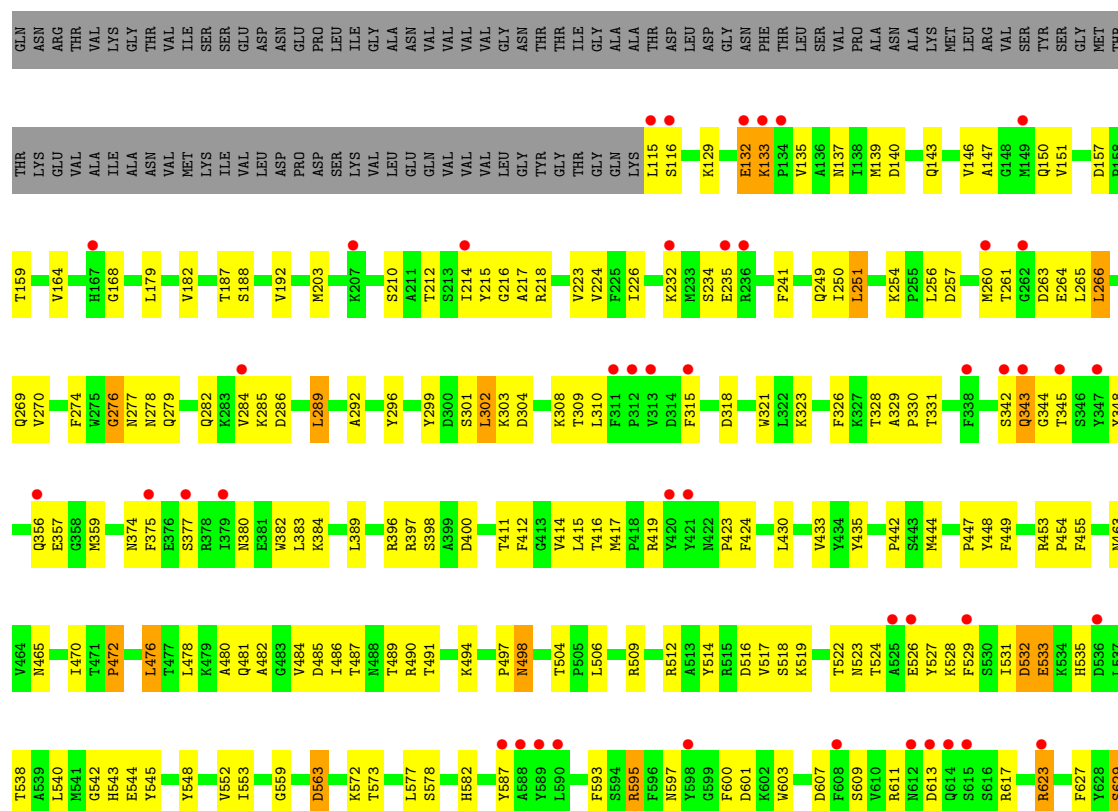




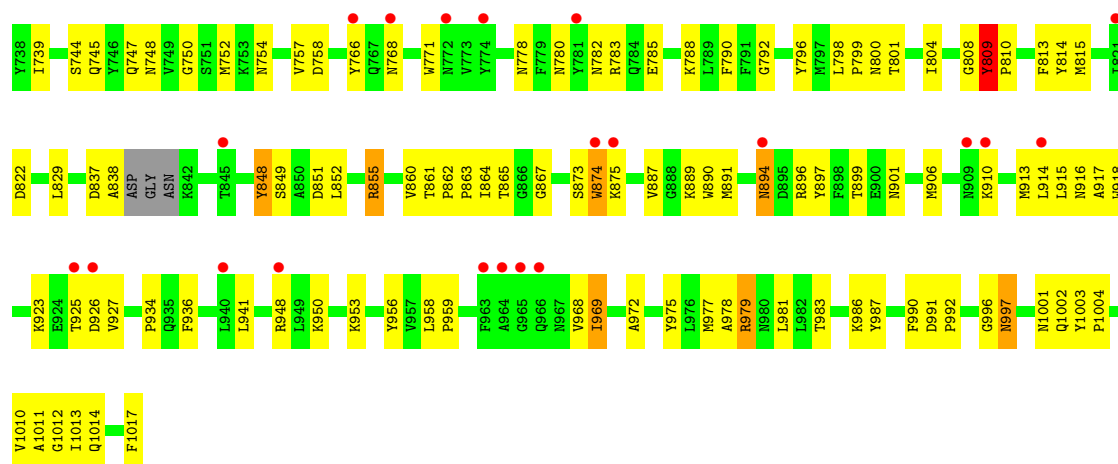


● Molecule 2: RagA protein

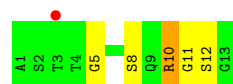








- Molecule 3: ALA-SER-THR-THR-GLY-GLY-ASN-SER-GLN-ARG-GLY-SER-GLY



- Molecule 3: ALA-SER-THR-THR-GLY-GLY-ASN-SER-GLN-ARG-GLY-SER-GLY



- Molecule 4: ASTTGGNSQRGGG



- Molecule 4: ASTTGGNSQRGGG



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.56Å 376.87Å 369.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.92 – 3.38 83.92 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (83.92-3.38) 99.9 (83.92-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.204 , 0.251 0.204 , 0.251	Depositor DCC
$R_{free}$ test set	9223 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.0	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 77.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	43926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5PL, C8E

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	0.64	0/3928	0.84	5/5331 (0.1%)
1	C	0.65	0/3928	0.85	4/5331 (0.1%)
1	F	0.59	0/3928	0.79	3/5331 (0.1%)
1	I	0.47	0/3928	0.66	1/5331 (0.0%)
2	B	0.64	4/7211 (0.1%)	0.88	9/9753 (0.1%)
2	D	0.61	4/7211 (0.1%)	0.84	5/9753 (0.1%)
2	G	0.51	1/7211 (0.0%)	0.76	5/9753 (0.1%)
2	J	0.50	0/7211	0.75	2/9753 (0.0%)
3	H	0.45	0/80	0.74	0/105
3	P	0.53	0/80	0.93	0/105
4	E	0.38	0/78	0.72	0/102
4	K	0.49	0/78	0.70	0/102
All	All	0.58	9/44872 (0.0%)	0.80	34/60750 (0.1%)

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
2	B	0	1
2	D	0	1
2	J	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	498	ASN	C-N	8.83	1.54	1.34
2	B	498	ASN	C-N	6.64	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	498	ASN	C-N	5.95	1.47	1.34
2	B	552	VAL	CB-CG2	-5.62	1.41	1.52
2	D	440	THR	C-N	-5.53	1.21	1.34
2	B	561	GLU	CB-CG	5.52	1.62	1.52
2	D	575	ASN	CA-C	-5.42	1.38	1.52
2	B	561	GLU	CG-CD	5.37	1.60	1.51
2	D	578	SER	C-N	-5.05	1.22	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	498	ASN	C-N-CA	-10.40	95.70	121.70
2	B	498	ASN	C-N-CA	-10.38	95.76	121.70
2	G	498	ASN	C-N-CA	-9.89	96.97	121.70
2	J	498	ASN	C-N-CA	-9.16	98.81	121.70
1	C	188	LEU	CB-CG-CD2	-7.85	97.65	111.00
1	C	241	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	149	LEU	CB-CG-CD2	-6.78	99.47	111.00
2	D	636	ILE	CG1-CB-CG2	-6.78	96.47	111.40
2	G	310	LEU	CA-CB-CG	6.70	130.70	115.30
2	D	256	LEU	CA-CB-CG	6.66	130.63	115.30
1	A	22	LEU	CA-CB-CG	6.48	130.21	115.30
1	F	241	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	279	ARG	NE-CZ-NH2	-5.89	117.35	120.30
2	G	725	ARG	NE-CZ-NH1	-5.80	117.40	120.30
2	B	573	THR	C-N-CA	-5.76	110.20	122.30
1	A	131	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	F	241	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	48	LEU	CA-CB-CG	5.61	128.20	115.30
2	B	440	THR	C-N-CA	5.59	135.68	121.70
2	B	981	LEU	CB-CG-CD2	-5.49	101.67	111.00
2	G	476	LEU	CA-CB-CG	5.49	127.93	115.30
2	B	725	ARG	NE-CZ-NH1	-5.46	117.57	120.30
2	J	440	THR	C-N-CA	5.45	135.34	121.70
1	F	265	LEU	CB-CG-CD2	-5.44	101.76	111.00
2	B	506	LEU	CB-CG-CD2	-5.31	101.98	111.00
2	B	288	ILE	CG1-CB-CG2	-5.29	99.77	111.40
2	D	476	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	428	ARG	NE-CZ-NH1	-5.28	117.66	120.30
2	D	952	LEU	CA-CB-CG	5.23	127.32	115.30
1	I	20	CYS	CA-CB-SG	5.19	123.34	114.00
1	A	183	LEU	CA-CB-CG	5.15	127.14	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	289	LEU	CB-CG-CD2	-5.14	102.26	111.00
2	B	541	MET	CB-CG-SD	-5.12	97.05	112.40
2	B	490	ARG	CG-CD-NE	-5.04	101.22	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ASP	Peptide
2	B	292	ALA	Peptide
2	D	292	ALA	Peptide
2	J	809	TYR	Peptide

## 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	3842	0	3739	76	0
1	C	3842	0	3740	71	0
1	F	3842	0	3740	78	0
1	I	3842	0	3740	71	0
2	B	7048	0	6792	289	1
2	D	7048	0	6791	272	1
2	G	7048	0	6792	243	0
2	J	7048	0	6791	247	0
3	H	81	0	75	5	0
3	P	81	0	75	4	0
4	E	79	0	73	10	0
4	K	79	0	73	3	0
5	B	20	0	21	4	0
6	B	26	0	42	1	0
All	All	43926	0	42484	1303	2

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 (1303) 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)
2:B:142:LEU:HD21	2:B:203:MET:HE3	1.35	1.08
1:I:465:ASN:OD1	2:J:276:GLY:N	1.88	1.05
2:B:142:LEU:CD1	2:B:203:MET:HE1	1.87	1.04
2:B:142:LEU:HD21	2:B:203:MET:CE	1.87	1.04
2:B:754:ASN:HB3	2:B:782:ASN:HD21	1.25	0.98
2:D:261:THR:OG1	2:D:264:GLU:HG3	1.62	0.96
2:B:142:LEU:HD11	2:B:203:MET:CE	1.97	0.94
2:D:279:GLN:HG2	2:D:284:VAL:HG22	1.54	0.89
2:B:380:ASN:HD21	2:B:382:TRP:HE3	1.20	0.89
2:J:470:ILE:HG22	2:J:472:PRO:HD3	1.54	0.88
2:D:808:GLY:O	2:D:855:ARG:NH2	2.07	0.87
2:B:470:ILE:HG22	2:B:472:PRO:HD3	1.56	0.87
2:J:480:ALA:HA	2:J:523:ASN:HB3	1.57	0.87
2:G:265:LEU:O	2:G:269:GLN:HG3	1.74	0.86
1:C:368:ASP:HB3	1:C:369:LYS:HD2	1.56	0.85
2:B:143:GLN:NE2	2:B:151:VAL:O	2.08	0.85
2:B:142:LEU:CD2	2:B:203:MET:CE	2.54	0.84
2:B:977:MET:HG2	2:B:978:ALA:H	1.41	0.84
2:J:637:TYR:HA	2:J:641:ILE:HG22	1.58	0.84
2:G:143:GLN:NE2	2:G:151:VAL:O	2.10	0.84
2:D:917:ALA:HA	2:D:927:VAL:HG13	1.58	0.84
2:G:480:ALA:HA	2:G:523:ASN:HB3	1.61	0.83
2:J:813:PHE:HE2	2:J:890:TRP:HB2	1.44	0.83
1:F:297:LEU:HB2	2:J:573:THR:HG21	1.60	0.82
2:D:637:TYR:HA	2:D:641:ILE:HG22	1.62	0.82
1:C:79:ASN:HB3	4:E:5:GLY:HA2	1.61	0.82
2:D:783:ARG:NH2	2:D:785:GLU:OE1	2.13	0.81
2:D:470:ILE:HG22	2:D:472:PRO:HD3	1.60	0.81
2:G:754:ASN:HB3	2:G:782:ASN:HD21	1.45	0.81
2:B:132:GLU:HG2	2:B:975:TYR:HE2	1.44	0.81
2:G:532:ASP:HB3	2:G:535:HIS:HB2	1.62	0.81
2:B:637:TYR:HA	2:B:641:ILE:HG23	1.62	0.81
1:F:165:ASP:OD2	1:F:440:ARG:NH1	2.14	0.81
1:F:368:ASP:HB3	1:F:369:LYS:HD2	1.62	0.80
2:B:730:MET:HE3	2:B:752:MET:HB2	1.64	0.80
2:B:639:LYS:HD2	2:B:640:PHE:CE1	2.18	0.79
2:B:480:ALA:HA	2:B:523:ASN:HB3	1.62	0.79
2:G:470:ILE:HG22	2:G:472:PRO:HD3	1.65	0.79
1:I:390:GLU:OE1	1:I:444:ARG:NH2	2.15	0.79
2:B:142:LEU:CD2	2:B:203:MET:HE1	2.11	0.79
2:D:265:LEU:O	2:D:269:GLN:HG3	1.83	0.79
2:G:695:LEU:HA	2:G:748:ASN:HD21	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:975:TYR:HB2	2:J:1012:GLY:H	1.47	0.78
2:B:151:VAL:HG12	2:B:164:VAL:HG22	1.66	0.78
2:J:380:ASN:HD21	2:J:382:TRP:HE3	1.28	0.78
2:J:182:VAL:HG22	2:J:226:ILE:HB	1.65	0.78
2:J:754:ASN:HB3	2:J:782:ASN:HD21	1.49	0.78
1:I:23:ASP:HB3	2:J:623:ARG:NH2	1.99	0.77
2:G:140:ASP:OD2	2:G:979:ARG:NH1	2.17	0.77
2:J:948:ARG:NH2	2:J:991:ASP:OD1	2.17	0.76
2:B:856:ILE:HD12	2:B:857:ASP:H	1.49	0.76
2:D:948:ARG:NH2	2:D:991:ASP:OD1	2.17	0.76
1:A:20:CYS:SG	2:B:545:TYR:HE2	2.09	0.75
2:B:142:LEU:HD11	2:B:203:MET:HE1	1.56	0.75
2:B:641:ILE:O	2:B:643:GLU:N	2.20	0.75
2:D:182:VAL:HG22	2:D:226:ILE:HB	1.66	0.75
2:D:143:GLN:NE2	2:D:151:VAL:O	2.20	0.74
2:G:968:VAL:HG13	2:G:969:ILE:HG13	1.69	0.74
2:G:796:TYR:HE1	2:G:798:LEU:HD23	1.53	0.74
2:J:808:GLY:O	2:J:855:ARG:NH2	2.21	0.74
2:G:975:TYR:HB2	2:G:1012:GLY:H	1.52	0.74
1:A:318:ASN:ND2	2:B:438:GLY:O	2.21	0.73
1:C:180:ALA:HA	1:C:183:LEU:HD12	1.69	0.73
1:I:125:ASN:HD21	1:I:190:GLU:HG2	1.54	0.73
1:F:79:ASN:HB3	3:H:5:GLY:HA2	1.70	0.73
2:G:261:THR:OG1	2:G:264:GLU:HG3	1.88	0.73
2:G:808:GLY:O	2:G:855:ARG:NH2	2.21	0.72
2:G:514:TYR:HD2	2:G:552:VAL:HG22	1.52	0.72
2:D:891:MET:SD	2:D:996:GLY:N	2.60	0.72
2:J:695:LEU:HA	2:J:748:ASN:HD21	1.52	0.72
1:F:496:ILE:HD12	1:F:496:ILE:H	1.53	0.72
2:G:301:SER:HB2	2:G:302:LEU:HD23	1.70	0.72
2:B:734:VAL:HG22	2:B:745:GLN:O	1.90	0.71
2:B:119:SER:OG	2:B:607:ASP:OD1	2.09	0.71
2:B:975:TYR:HB2	2:B:1012:GLY:H	1.55	0.71
2:J:433:VAL:HG21	2:J:442:PRO:HB2	1.72	0.71
2:B:265:LEU:O	2:B:269:GLN:HG3	1.90	0.71
2:G:948:ARG:NH2	2:G:991:ASP:OD1	2.20	0.71
2:B:918:TRP:NE1	2:B:923:LYS:HG3	2.06	0.71
2:D:975:TYR:HB2	2:D:1012:GLY:H	1.56	0.71
2:J:267:ASP:O	2:J:271:LYS:HD3	1.91	0.71
2:J:472:PRO:HG2	2:J:476:LEU:HD11	1.73	0.70
2:D:848:TYR:CE2	2:D:935:GLN:HG2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:267:ASP:HB3	2:J:271:LYS:NZ	2.05	0.70
2:B:494:LYS:HG2	2:B:509:ARG:HG3	1.72	0.70
1:C:310:PRO:HG2	2:D:503:SER:HB3	1.73	0.70
2:D:987:TYR:HB2	2:D:992:PRO:HB3	1.72	0.70
1:F:87:TRP:O	1:F:89:LEU:HD13	1.91	0.70
2:G:342:SER:OG	2:J:342:SER:OG	2.03	0.70
2:B:142:LEU:HD13	2:B:203:MET:HE1	1.72	0.69
2:B:143:GLN:OE1	2:B:950:LYS:NZ	2.25	0.69
2:J:901:ASN:HB2	2:J:934:PRO:HD3	1.73	0.69
2:G:641:ILE:O	2:G:643:GLU:N	2.24	0.69
2:J:140:ASP:OD2	2:J:979:ARG:NH1	2.26	0.69
2:B:261:THR:H	2:B:264:GLU:HB2	1.57	0.69
2:B:796:TYR:CE1	2:B:798:LEU:HD23	2.28	0.69
1:A:449:ASN:HB2	1:A:473:ALA:HB3	1.74	0.69
2:B:639:LYS:HD2	2:B:640:PHE:CD1	2.28	0.69
2:J:267:ASP:O	2:J:271:LYS:CD	2.40	0.69
2:B:990:PHE:HB2	2:B:1002:GLN:HE21	1.58	0.69
2:G:348:TYR:HB3	2:G:374:ASN:HB2	1.73	0.69
2:B:504:THR:HB	2:B:506:LEU:HD12	1.74	0.69
2:D:140:ASP:OD2	2:D:979:ARG:NH1	2.26	0.69
1:A:402:GLU:HB3	1:A:419:VAL:HG21	1.75	0.69
2:J:491:THR:HG23	2:J:512:ARG:HB2	1.75	0.69
2:D:132:GLU:HG2	2:D:975:TYR:HE2	1.57	0.68
2:D:151:VAL:HG12	2:D:164:VAL:HG22	1.75	0.68
1:A:79:ASN:HB3	3:P:5:GLY:HA2	1.75	0.68
2:B:615:SER:O	2:B:623:ARG:NH1	2.26	0.68
2:B:796:TYR:HE1	2:B:798:LEU:HD23	1.58	0.68
2:D:901:ASN:O	2:D:910:LYS:HE2	1.94	0.68
2:J:487:THR:CG2	2:J:516:ASP:HB2	2.23	0.68
2:B:650:LEU:HD23	2:B:709:ALA:HB2	1.75	0.67
2:B:848:TYR:HD2	2:B:935:GLN:HG3	1.58	0.67
2:D:758:ASP:HB3	2:D:780:ASN:HD22	1.58	0.67
2:D:487:THR:HG23	2:D:516:ASP:HB2	1.76	0.67
1:F:23:ASP:HB3	2:G:623:ARG:NH2	2.10	0.67
2:G:891:MET:SD	2:G:996:GLY:N	2.64	0.67
2:J:143:GLN:NE2	2:J:151:VAL:O	2.26	0.67
2:G:179:LEU:HB3	2:G:223:VAL:HG12	1.76	0.67
1:I:368:ASP:HB3	1:I:369:LYS:HD2	1.75	0.67
2:B:296:TYR:CG	2:B:302:LEU:HD12	2.30	0.67
2:B:813:PHE:HE2	2:B:890:TRP:HB2	1.59	0.67
2:B:950:LYS:O	2:B:979:ARG:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:522:THR:HB	2:J:544:GLU:HG3	1.76	0.67
2:B:864:ILE:HB	2:B:887:VAL:HG23	1.76	0.67
2:D:251:LEU:HD23	2:D:251:LEU:H	1.59	0.66
2:J:822:ASP:HB2	2:J:829:LEU:HD11	1.77	0.66
2:J:918:TRP:NE1	2:J:923:LYS:HG3	2.09	0.66
2:J:383:LEU:HD12	2:J:384:LYS:H	1.60	0.66
2:D:641:ILE:O	2:D:643:GLU:N	2.27	0.66
2:B:197:PRO:HA	2:B:200:PHE:CD2	2.31	0.66
2:D:261:THR:OG1	2:D:264:GLU:CG	2.42	0.66
2:D:348:TYR:HB3	2:D:374:ASN:HB2	1.77	0.66
1:F:121:ASN:OD1	1:F:156:GLN:NE2	2.28	0.66
2:B:239:ILE:HG23	2:B:338:PHE:CD1	2.30	0.66
2:D:627:PHE:HB3	2:D:658:THR:O	1.96	0.66
2:G:969:ILE:HG23	2:G:1017:PHE:HD2	1.61	0.66
2:D:132:GLU:OE2	2:D:975:TYR:OH	2.09	0.66
2:D:132:GLU:HG2	2:D:975:TYR:CE2	2.30	0.65
2:G:969:ILE:HA	2:G:1017:PHE:HB3	1.78	0.65
2:J:968:VAL:HG13	2:J:969:ILE:HG13	1.78	0.65
2:B:918:TRP:HE1	2:B:923:LYS:HG3	1.61	0.65
2:B:318:ASP:HB2	2:B:419:ARG:HB3	1.79	0.65
2:D:916:ASN:HB3	2:D:925:THR:HG21	1.78	0.65
4:E:10:ARG:H	4:E:10:ARG:HD3	1.62	0.65
2:B:147:ALA:HB1	2:B:758:ASP:HB2	1.78	0.65
2:D:378:ARG:HG2	2:D:384:LYS:HG3	1.79	0.65
2:D:494:LYS:HG2	2:D:509:ARG:HG3	1.77	0.65
2:G:397:ARG:HG3	2:G:455:PHE:HD2	1.60	0.65
2:D:147:ALA:HB1	2:D:758:ASP:HB2	1.79	0.65
1:I:199:ARG:NH1	1:I:498:ASN:OD1	2.29	0.65
2:J:151:VAL:HG12	2:J:164:VAL:HG22	1.79	0.65
2:G:433:VAL:HG21	2:G:442:PRO:HB2	1.77	0.65
2:G:472:PRO:HG2	2:G:476:LEU:HD11	1.78	0.65
2:J:918:TRP:HE1	2:J:923:LYS:HG3	1.61	0.64
2:D:301:SER:HB2	2:D:302:LEU:HD23	1.78	0.64
2:G:480:ALA:HA	2:G:523:ASN:CB	2.27	0.64
2:J:215:TYR:HD2	2:J:223:VAL:HG11	1.62	0.64
2:B:234:SER:OG	2:B:235:GLU:N	2.29	0.64
2:D:783:ARG:HH12	2:D:785:GLU:HB2	1.61	0.64
1:F:23:ASP:HB3	2:G:623:ARG:HH22	1.62	0.64
2:D:296:TYR:CG	2:D:302:LEU:HD12	2.32	0.64
1:F:206:TYR:CE1	1:F:246:LEU:HD11	2.33	0.64
1:F:488:ASP:HA	1:F:491:THR:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:TRP:CZ2	2:D:423:PRO:HG3	2.33	0.64
2:G:916:ASN:HB3	2:G:925:THR:HG21	1.79	0.64
2:J:864:ILE:HB	2:J:887:VAL:HG23	1.80	0.64
2:B:573:THR:HG22	2:B:573:THR:O	1.98	0.64
2:D:275:TRP:CD1	2:D:284:VAL:HG11	2.33	0.64
2:G:796:TYR:CE1	2:G:798:LEU:HD23	2.31	0.64
2:B:182:VAL:HG22	2:B:226:ILE:HB	1.79	0.64
2:B:301:SER:HB2	2:B:302:LEU:HD23	1.79	0.64
2:G:730:MET:HE3	2:G:752:MET:HB2	1.80	0.64
1:A:164:MET:HE2	1:A:205:CYS:HB2	1.80	0.63
2:G:151:VAL:HG12	2:G:164:VAL:HG22	1.79	0.63
2:J:251:LEU:H	2:J:251:LEU:HD23	1.64	0.63
1:C:164:MET:HE2	1:C:205:CYS:HB2	1.78	0.63
1:I:323:PRO:O	1:I:457:GLN:NE2	2.30	0.63
2:B:487:THR:HG23	2:B:516:ASP:HB2	1.79	0.63
2:D:631:GLY:HA3	2:D:655:SER:HB3	1.81	0.63
1:I:402:GLU:HB3	1:I:419:VAL:HG21	1.81	0.63
2:B:383:LEU:HD12	2:B:384:LYS:H	1.64	0.63
2:G:672:LEU:HB2	2:G:689:THR:HG22	1.81	0.63
2:G:494:LYS:HG2	2:G:509:ARG:HG3	1.80	0.63
2:J:274:PHE:CD2	2:J:906:MET:HB2	2.34	0.63
2:D:528:LYS:HB3	2:D:538:THR:HG23	1.80	0.62
2:G:182:VAL:HG22	2:G:226:ILE:HB	1.79	0.62
2:J:132:GLU:HG2	2:J:975:TYR:CE2	2.34	0.62
2:J:978:ALA:HB1	2:J:981:LEU:HD23	1.80	0.62
2:B:809:TYR:HB2	2:B:855:ARG:NH2	2.15	0.62
2:B:848:TYR:CD2	2:B:935:GLN:HG3	2.34	0.62
2:B:968:VAL:HG13	2:B:969:ILE:HG13	1.81	0.62
2:J:143:GLN:OE1	2:J:950:LYS:NZ	2.32	0.62
2:B:975:TYR:CB	2:B:1012:GLY:H	2.13	0.62
2:B:627:PHE:HB3	2:B:658:THR:O	1.99	0.62
2:G:901:ASN:O	2:G:910:LYS:HE2	1.99	0.62
1:A:180:ALA:HA	1:A:183:LEU:HD12	1.82	0.62
2:D:263:ASP:N	2:D:263:ASP:OD1	2.33	0.62
2:G:627:PHE:HB3	2:G:658:THR:O	2.00	0.62
2:B:251:LEU:HD23	2:B:251:LEU:H	1.64	0.62
2:D:997:ASN:OD1	4:E:12:GLY:N	2.32	0.62
2:B:250:ILE:HD12	2:B:359:MET:HE1	1.80	0.61
2:B:809:TYR:HB3	2:B:810:PRO:HD3	1.82	0.61
2:D:159:THR:HG21	2:D:398:SER:HB3	1.82	0.61
2:D:813:PHE:CE2	2:D:941:LEU:HD21	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:ARG:HD3	4:E:10:ARG:N	2.15	0.61
2:J:249:GLN:HG3	2:J:328:THR:HG23	1.82	0.61
2:G:532:ASP:CB	2:G:535:HIS:HB2	2.29	0.61
2:J:641:ILE:O	2:J:643:GLU:N	2.34	0.61
1:C:165:ASP:OD2	1:C:440:ARG:NH1	2.33	0.61
2:G:380:ASN:HD21	2:G:382:TRP:HE3	1.47	0.61
2:J:117:THR:HG23	2:J:120:GLY:H	1.64	0.61
2:J:768:ASN:HB3	2:J:771:TRP:HB3	1.82	0.61
2:D:633:MET:HG3	2:D:634:PHE:N	2.15	0.61
2:D:949:LEU:HD23	2:D:981:LEU:HD11	1.80	0.61
1:F:442:MET:HB2	1:F:447:ILE:HB	1.82	0.61
2:J:215:TYR:CE2	2:J:223:VAL:HG21	2.35	0.61
1:C:451:HIS:HB3	1:C:469:LEU:HD11	1.82	0.61
2:D:234:SER:OG	2:D:235:GLU:N	2.34	0.61
2:J:159:THR:HG21	2:J:398:SER:HB3	1.83	0.60
2:B:521:PHE:HE2	5:B:1101:5PL:HBV2	1.66	0.60
1:C:379:PHE:HE1	1:C:383:GLU:HB3	1.67	0.60
2:D:400:ASP:OD1	2:D:400:ASP:N	2.33	0.60
1:I:299:SER:HB3	1:I:373:LYS:HD3	1.83	0.60
2:J:494:LYS:HG2	2:J:509:ARG:HG3	1.82	0.60
2:J:783:ARG:NH1	2:J:785:GLU:OE1	2.33	0.60
1:C:137:LYS:HA	1:C:137:LYS:HE2	1.83	0.60
2:D:543:HIS:HB2	2:D:592:PHE:HD1	1.66	0.60
2:G:822:ASP:HB2	2:G:829:LEU:HD11	1.83	0.60
1:C:70:MET:HE2	1:C:429:THR:HG23	1.83	0.60
2:G:157:ASP:OD1	2:G:159:THR:HG22	2.01	0.60
2:G:745:GLN:HE21	2:G:746:TYR:H	1.48	0.60
1:C:368:ASP:HB3	1:C:369:LYS:CD	2.27	0.60
2:D:179:LEU:HB3	2:D:223:VAL:HG12	1.84	0.60
1:C:20:CYS:N	2:D:545:TYR:HH	1.99	0.60
2:D:242:ASN:HD22	2:D:335:ASP:HB3	1.66	0.60
2:D:813:PHE:CE1	2:D:860:VAL:HG12	2.37	0.60
2:J:711:ALA:O	2:J:713:ASN:N	2.35	0.60
2:D:166:ILE:HD12	2:D:222:GLY:HA3	1.82	0.60
1:F:390:GLU:OE1	1:F:444:ARG:NH2	2.32	0.60
2:B:292:ALA:HB3	2:B:435:TYR:CE2	2.37	0.59
2:B:296:TYR:CD2	2:B:302:LEU:HD12	2.36	0.59
2:J:862:PRO:HG3	2:J:889:LYS:HB2	1.83	0.59
2:B:958:LEU:HB2	2:B:972:ALA:HB3	1.84	0.59
2:G:251:LEU:HD23	2:G:251:LEU:H	1.66	0.59
2:J:215:TYR:CD2	2:J:223:VAL:HG11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:THR:HG21	2:D:398:SER:CB	2.32	0.59
2:D:809:TYR:HB2	2:D:810:PRO:HD3	1.84	0.59
2:G:329:ALA:HB1	2:G:357:GLU:HG2	1.83	0.59
2:B:768:ASN:HB3	2:B:771:TRP:HB3	1.83	0.59
2:D:754:ASN:HB3	2:D:782:ASN:HD21	1.67	0.59
2:J:574:GLY:O	2:J:577:LEU:HD12	2.02	0.59
2:J:627:PHE:HB3	2:J:658:THR:O	2.01	0.59
2:B:597:ASN:HA	2:B:607:ASP:HB3	1.84	0.59
2:G:805:TRP:CD1	2:G:811:ASN:ND2	2.71	0.59
1:I:23:ASP:HB3	2:J:623:ARG:HH22	1.67	0.59
2:J:265:LEU:O	2:J:269:GLN:HG3	2.02	0.59
2:B:270:VAL:HG22	2:B:284:VAL:HG21	1.85	0.59
2:B:768:ASN:CB	2:B:771:TRP:HB3	2.33	0.59
1:A:496:ILE:HD12	1:A:496:ILE:H	1.68	0.59
2:B:430:LEU:HD23	2:B:447:PRO:HG2	1.84	0.59
2:G:250:ILE:HB	2:G:359:MET:HE3	1.85	0.59
2:B:916:ASN:HB3	2:B:925:THR:HG21	1.83	0.59
1:C:195:TYR:O	2:D:739:ILE:HD11	2.02	0.59
1:I:496:ILE:HD12	1:I:496:ILE:H	1.68	0.59
2:B:249:GLN:HG3	2:B:328:THR:HG23	1.83	0.58
2:B:848:TYR:HD1	2:B:849:SER:N	2.01	0.58
2:D:168:GLY:H	2:D:725:ARG:NH1	2.01	0.58
2:J:997:ASN:OD1	4:K:11:GLY:N	2.28	0.58
4:K:10:ARG:H	4:K:10:ARG:HD2	1.67	0.58
2:B:528:LYS:HB3	2:B:538:THR:HG23	1.84	0.58
1:F:244:LEU:HD22	1:F:387:ILE:HG12	1.85	0.58
2:G:711:ALA:O	2:G:713:ASN:N	2.36	0.58
1:A:206:TYR:CE1	1:A:246:LEU:HD11	2.38	0.58
2:D:783:ARG:NH1	2:D:785:GLU:HB2	2.17	0.58
2:G:758:ASP:HB3	2:G:780:ASN:HD22	1.68	0.58
1:F:263:TYR:CZ	1:F:288:ILE:HG23	2.38	0.58
3:H:9:GLN:HG3	3:H:10:ARG:NH2	2.18	0.58
2:G:282:GLN:HG3	2:G:286:ASP:HB2	1.85	0.58
2:G:487:THR:HG23	2:G:516:ASP:HB2	1.86	0.58
2:G:611:ARG:NH1	2:G:613:ASP:OD1	2.36	0.58
2:G:702:GLN:HG2	2:G:725:ARG:HG3	1.84	0.58
1:I:386:LEU:HD13	1:I:428:ARG:HA	1.85	0.58
2:J:637:TYR:HA	2:J:641:ILE:CG2	2.32	0.58
2:G:277:ASN:O	2:G:278:ASN:ND2	2.36	0.58
1:A:70:MET:HE2	1:A:429:THR:HG23	1.84	0.58
2:D:491:THR:HG23	2:D:512:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:HB3	1:A:373:LYS:HB3	1.86	0.58
2:D:524:THR:HA	2:D:542:GLY:HA3	1.85	0.58
2:D:799:PRO:O	2:D:801:THR:HG23	2.04	0.58
2:G:132:GLU:HG2	2:G:975:TYR:HE2	1.69	0.58
2:G:279:GLN:HG2	2:G:284:VAL:HG22	1.84	0.58
2:G:308:LYS:HG2	2:G:309:THR:HG23	1.86	0.58
2:J:958:LEU:HD22	2:J:959:PRO:HD2	1.85	0.58
2:B:218:ARG:HD3	2:B:663:GLU:HG3	1.85	0.58
1:C:124:VAL:HG21	1:C:156:GLN:OE1	2.04	0.58
1:A:289:PHE:CD2	1:A:378:TYR:HD2	2.22	0.57
2:G:261:THR:H	2:G:264:GLU:HB2	1.68	0.57
2:G:559:GLY:HA3	2:G:572:LYS:HG2	1.85	0.57
1:I:456:THR:HG21	1:I:466:THR:HG22	1.86	0.57
2:J:487:THR:HG22	2:J:516:ASP:HB2	1.86	0.57
1:A:346:VAL:HG22	1:A:353:LEU:HD23	1.84	0.57
2:G:573:THR:HG21	1:I:297:LEU:HB2	1.85	0.57
1:I:186:ILE:HD12	2:J:739:ILE:HG21	1.86	0.57
2:D:232:LYS:H	2:D:232:LYS:HD2	1.68	0.57
2:G:522:THR:HB	2:G:544:GLU:HG3	1.86	0.57
1:I:124:VAL:HG13	1:I:149:LEU:HD11	1.86	0.57
2:J:559:GLY:HA3	2:J:572:LYS:HG2	1.86	0.57
2:B:878:SER:O	2:B:954:LEU:HD12	2.04	0.57
2:G:582:HIS:ND1	2:J:568:LEU:HB2	2.19	0.57
2:B:521:PHE:CE2	5:B:1101:5PL:HBV2	2.40	0.57
2:B:633:MET:HG3	2:B:634:PHE:N	2.20	0.57
2:B:302:LEU:HD23	2:B:302:LEU:H	1.70	0.57
2:B:977:MET:HG2	2:B:978:ALA:N	2.15	0.57
2:G:454:PRO:HD2	2:G:494:LYS:HB2	1.86	0.57
2:G:768:ASN:CB	2:G:771:TRP:HB3	2.34	0.57
2:G:783:ARG:NH1	2:G:785:GLU:OE1	2.25	0.57
2:J:778:ASN:HB3	2:J:867:GLY:H	1.70	0.57
2:B:637:TYR:HA	2:B:641:ILE:CG2	2.33	0.57
2:D:768:ASN:CB	2:D:771:TRP:HB3	2.35	0.57
2:B:196:ASN:ND2	2:B:335:ASP:OD2	2.38	0.57
2:B:250:ILE:HB	2:B:359:MET:CE	2.35	0.57
2:B:275:TRP:CD1	2:B:284:VAL:HG11	2.39	0.57
2:D:720:VAL:HG22	2:D:759:LEU:HB3	1.87	0.57
2:B:132:GLU:HG2	2:B:975:TYR:CE2	2.34	0.57
2:D:383:LEU:HD12	2:D:384:LYS:H	1.70	0.57
1:A:438:ARG:O	1:A:442:MET:HG2	2.05	0.56
2:J:169:THR:O	2:J:752:MET:HE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:916:ASN:HB3	2:J:925:THR:HG21	1.86	0.56
1:C:106:ILE:HG23	1:C:482:TRP:CE3	2.40	0.56
1:C:164:MET:CE	1:C:205:CYS:HB2	2.35	0.56
2:J:284:VAL:HA	2:J:288:ILE:HD12	1.86	0.56
1:C:93:ASN:HD21	2:D:850:ALA:HB2	1.70	0.56
2:D:261:THR:H	2:D:264:GLU:HB2	1.70	0.56
2:D:472:PRO:HG2	2:D:476:LEU:HD11	1.88	0.56
2:D:813:PHE:HE2	2:D:890:TRP:HB2	1.71	0.56
2:G:487:THR:CG2	2:G:516:ASP:HB2	2.35	0.56
2:G:637:TYR:HA	2:G:641:ILE:HG22	1.87	0.56
2:J:633:MET:HG3	2:J:634:PHE:N	2.20	0.56
2:D:953:LYS:HG3	2:D:977:MET:HG2	1.88	0.56
2:J:768:ASN:CB	2:J:771:TRP:HB3	2.35	0.56
2:B:214:ILE:HG22	2:B:593:PHE:CD2	2.41	0.56
2:D:806:GLU:HG2	2:D:808:GLY:H	1.70	0.56
2:B:146:VAL:C	2:B:778:ASN:HD21	2.09	0.56
2:B:524:THR:HA	2:B:542:GLY:HA3	1.87	0.56
2:J:508:GLU:HB3	2:J:558:LYS:HB3	1.88	0.56
2:B:809:TYR:HB2	2:B:855:ARG:HH21	1.71	0.56
2:B:835:GLN:HB3	2:B:843:VAL:CG2	2.36	0.56
2:D:180:TYR:CZ	2:D:189:LEU:HD21	2.41	0.56
2:D:265:LEU:HD13	2:D:909:ASN:HA	1.88	0.56
2:D:491:THR:CG2	2:D:512:ARG:HB2	2.36	0.56
2:D:975:TYR:CB	2:D:1012:GLY:H	2.17	0.56
1:I:390:GLU:HB2	1:I:424:LEU:HD11	1.88	0.56
2:J:296:TYR:CD2	2:J:302:LEU:HD12	2.41	0.56
2:B:795:LYS:HB2	2:B:804:ILE:HD11	1.88	0.56
2:B:997:ASN:OD1	3:P:11:GLY:N	2.30	0.56
2:D:135:VAL:HG12	2:D:137:ASN:N	2.21	0.56
1:F:199:ARG:NH1	1:F:498:ASN:OD1	2.33	0.56
2:G:187:THR:OG1	2:G:188:SER:N	2.37	0.56
2:G:791:PHE:HB2	2:G:793:LEU:HD11	1.88	0.56
1:I:405:LEU:HD23	1:I:419:VAL:HG22	1.87	0.56
2:J:497:PRO:O	2:J:498:ASN:HB2	2.06	0.56
2:B:146:VAL:HG21	2:B:205:VAL:HG21	1.87	0.56
2:B:461:GLN:NE2	2:B:487:THR:HB	2.22	0.56
1:C:496:ILE:HD12	1:C:496:ILE:H	1.70	0.56
2:J:758:ASP:HB3	2:J:780:ASN:HD22	1.70	0.56
1:A:477:PHE:HD1	1:A:479:ALA:H	1.51	0.55
2:G:975:TYR:HB2	2:G:1012:GLY:N	2.21	0.55
2:J:215:TYR:HE2	2:J:223:VAL:HG21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:263:ASP:OD1	2:J:263:ASP:N	2.39	0.55
2:J:430:LEU:HD23	2:J:447:PRO:HG2	1.88	0.55
1:C:192:ASN:OD1	1:C:195:TYR:HB2	2.06	0.55
1:C:368:ASP:CB	1:C:369:LYS:HD2	2.34	0.55
2:D:318:ASP:HB2	2:D:419:ARG:HB3	1.87	0.55
2:B:345:THR:HG22	2:B:377:SER:CB	2.37	0.55
2:B:969:ILE:HA	2:B:1017:PHE:HB3	1.87	0.55
2:B:835:GLN:HB3	2:B:843:VAL:HG21	1.89	0.55
2:B:975:TYR:HB2	2:B:1012:GLY:N	2.20	0.55
1:C:206:TYR:CE1	1:C:246:LEU:HD11	2.41	0.55
2:D:242:ASN:HB2	2:D:335:ASP:HB3	1.87	0.55
1:I:164:MET:CE	1:I:205:CYS:HB2	2.37	0.55
1:C:289:PHE:CD2	1:C:378:TYR:HD2	2.25	0.55
2:D:433:VAL:HG21	2:D:442:PRO:HB2	1.88	0.55
2:D:750:GLY:HA2	2:D:788:LYS:HB3	1.87	0.55
2:G:345:THR:HG22	2:G:377:SER:HB2	1.88	0.55
2:J:216:GLY:HA3	2:J:611:ARG:NH1	2.21	0.55
2:J:975:TYR:HB2	2:J:1012:GLY:N	2.20	0.55
1:F:368:ASP:CB	1:F:369:LYS:HD2	2.36	0.55
2:G:476:LEU:HD13	2:G:478:LEU:HD13	1.88	0.55
2:G:737:PRO:HB2	2:G:739:ILE:HG12	1.89	0.55
2:G:862:PRO:HG3	2:G:889:LYS:HB2	1.87	0.55
2:B:611:ARG:NH1	2:B:613:ASP:OD1	2.40	0.55
2:G:214:ILE:HG22	2:G:593:PHE:CD2	2.42	0.55
2:G:799:PRO:O	2:G:801:THR:HG23	2.07	0.55
1:I:224:ARG:NH1	1:I:227:VAL:HG23	2.22	0.55
2:J:958:LEU:HB2	2:J:972:ALA:HB3	1.89	0.55
2:B:285:LYS:HB2	2:B:315:PHE:CE2	2.41	0.55
2:B:969:ILE:HG22	2:B:970:GLY:H	1.72	0.55
2:D:262:GLY:N	2:D:318:ASP:OD2	2.37	0.55
2:D:864:ILE:HB	2:D:887:VAL:HG23	1.88	0.55
2:D:975:TYR:HB2	2:D:1012:GLY:N	2.22	0.55
2:B:444:MET:HE3	2:B:448:TYR:HE1	1.72	0.55
2:B:532:ASP:O	2:B:533:GLU:HB2	2.05	0.55
2:G:249:GLN:HG3	2:G:328:THR:HG23	1.88	0.55
2:B:652:LEU:HD13	2:D:654:MET:HE1	1.88	0.55
2:B:917:ALA:HB3	2:B:930:LEU:HD22	1.89	0.55
2:J:750:GLY:HA2	2:J:788:LYS:HB3	1.89	0.55
2:B:159:THR:HG21	2:B:398:SER:HB2	1.89	0.54
2:B:730:MET:HE3	2:B:752:MET:CB	2.37	0.54
2:J:261:THR:H	2:J:264:GLU:HB2	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:135:VAL:HG12	2:D:137:ASN:H	1.72	0.54
2:G:282:GLN:CG	2:G:286:ASP:HB2	2.36	0.54
1:I:47:GLY:HA3	2:J:685:LEU:O	2.07	0.54
1:I:73:THR:HG21	1:I:82:ALA:HA	1.88	0.54
2:J:164:VAL:O	2:J:178:PRO:HD3	2.07	0.54
2:D:303:LYS:HG3	2:D:304:ASP:N	2.22	0.54
1:F:488:ASP:OD2	2:G:739:ILE:HG23	2.08	0.54
1:I:449:ASN:HB2	1:I:473:ALA:HB3	1.90	0.54
2:B:711:ALA:O	2:B:713:ASN:N	2.40	0.54
1:C:79:ASN:CB	4:E:5:GLY:HA2	2.35	0.54
2:J:730:MET:HE3	2:J:752:MET:HB2	1.88	0.54
2:D:615:SER:O	2:D:623:ARG:NH1	2.41	0.54
2:B:261:THR:OG1	2:B:264:GLU:HG3	2.08	0.54
2:B:989:GLY:O	2:B:1002:GLN:NE2	2.41	0.54
2:D:891:MET:HE2	2:D:987:TYR:CE1	2.43	0.54
1:F:32:GLN:HG3	2:G:671:ALA:O	2.08	0.54
2:J:476:LEU:HA	2:J:526:GLU:O	2.06	0.54
2:J:901:ASN:O	2:J:910:LYS:HE2	2.08	0.54
2:B:280:THR:O	2:B:284:VAL:HG23	2.07	0.54
2:D:514:TYR:HD2	2:D:552:VAL:HG22	1.72	0.54
2:G:146:VAL:C	2:G:778:ASN:HD21	2.10	0.54
2:G:813:PHE:CD2	2:G:941:LEU:HD11	2.43	0.54
1:C:346:VAL:HG22	1:C:353:LEU:HD23	1.90	0.54
2:B:901:ASN:O	2:B:910:LYS:HE2	2.08	0.54
2:D:119:SER:OG	2:D:607:ASP:OD1	2.20	0.54
2:D:215:TYR:CD2	2:D:223:VAL:HG11	2.43	0.54
2:D:269:GLN:NE2	2:D:906:MET:O	2.41	0.54
2:D:559:GLY:HA3	2:D:572:LYS:HG2	1.90	0.54
2:G:768:ASN:HB2	2:G:771:TRP:HB3	1.90	0.54
1:I:473:ALA:HB1	1:I:480:TYR:CE2	2.43	0.54
2:B:156:GLY:HA3	2:B:1004:PRO:O	2.08	0.54
2:D:116:SER:HB2	2:D:122:VAL:HG21	1.89	0.54
2:D:150:GLN:HA	2:D:865:THR:HG21	1.90	0.54
2:G:639:LYS:HD2	2:G:640:PHE:CE1	2.43	0.54
2:G:674:THR:OG1	2:G:675:VAL:N	2.40	0.54
2:G:977:MET:HB2	2:G:1010:VAL:HB	1.89	0.53
1:I:125:ASN:ND2	1:I:190:GLU:HG2	2.23	0.53
2:J:487:THR:HG23	2:J:516:ASP:HB2	1.89	0.53
1:A:106:ILE:HG23	1:A:482:TRP:CE3	2.43	0.53
2:B:417:MET:HE3	2:B:418:PRO:HD2	1.90	0.53
2:B:721:ASP:O	2:B:757:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:296:TYR:CG	2:G:302:LEU:HD12	2.43	0.53
2:G:587:TYR:HB3	2:G:666:ASN:OD1	2.08	0.53
2:J:179:LEU:HB3	2:J:223:VAL:HG12	1.89	0.53
2:J:463:ASN:ND2	2:J:485:ASP:OD2	2.40	0.53
1:I:236:TYR:CZ	1:I:258:MET:HG2	2.43	0.53
2:J:267:ASP:CB	2:J:271:LYS:NZ	2.71	0.53
2:B:348:TYR:HB3	2:B:374:ASN:HB2	1.90	0.53
2:B:484:VAL:HG22	2:B:519:LYS:HB3	1.88	0.53
1:C:108:GLY:O	1:C:112:VAL:HG22	2.08	0.53
2:D:342:SER:OG	2:D:343:GLN:N	2.41	0.53
2:D:711:ALA:O	2:D:713:ASN:N	2.41	0.53
1:A:488:ASP:HA	1:A:491:THR:HG22	1.91	0.53
1:C:449:ASN:HB2	1:C:473:ALA:HB3	1.91	0.53
2:D:633:MET:C	2:D:634:PHE:HD1	2.12	0.53
2:D:215:TYR:CE2	2:D:223:VAL:HG21	2.44	0.53
2:D:798:LEU:HB2	2:D:801:THR:OG1	2.09	0.53
2:G:958:LEU:HD22	2:G:959:PRO:HD2	1.91	0.53
2:G:813:PHE:HE2	2:G:890:TRP:HB2	1.74	0.53
2:J:187:THR:OG1	2:J:188:SER:N	2.39	0.53
2:J:296:TYR:CG	2:J:302:LEU:HD12	2.43	0.53
2:J:445:THR:HB	2:J:447:PRO:HD2	1.90	0.53
2:B:400:ASP:OD1	2:B:400:ASP:N	2.40	0.53
2:G:745:GLN:HE21	2:G:746:TYR:N	2.07	0.53
2:B:543:HIS:HB2	2:B:592:PHE:HD1	1.74	0.53
2:B:545:TYR:HE1	2:B:547:GLU:HB2	1.73	0.53
2:D:489:THR:HG22	2:D:490:ARG:H	1.74	0.53
2:D:913:MET:C	2:D:915:LEU:H	2.12	0.53
2:J:608:PHE:HB2	2:J:630:VAL:HG22	1.91	0.53
2:B:662:SER:HB2	2:B:697:TRP:CZ3	2.44	0.52
2:D:495:ARG:HH21	2:D:502:ASP:CG	2.12	0.52
2:D:805:TRP:CD1	2:D:811:ASN:ND2	2.76	0.52
2:B:215:TYR:CD2	2:B:223:VAL:HG11	2.44	0.52
2:B:261:THR:N	2:B:264:GLU:HB2	2.23	0.52
1:I:456:THR:CG2	1:I:466:THR:HG22	2.39	0.52
2:J:480:ALA:HA	2:J:523:ASN:CB	2.35	0.52
2:J:790:PHE:O	2:J:792:GLY:N	2.41	0.52
2:B:380:ASN:ND2	2:B:382:TRP:HB3	2.24	0.52
2:D:1014:GLN:O	2:D:1015:LEU:HD12	2.09	0.52
2:J:648:SER:HB2	2:J:710:GLY:O	2.10	0.52
2:B:523:ASN:OD1	5:B:1101:5PL:HBP1	2.09	0.52
2:B:1012:GLY:O	2:B:1013:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:SER:OG	2:D:463:ASN:HB2	2.09	0.52
2:G:400:ASP:OD1	2:G:400:ASP:N	2.41	0.52
2:D:345:THR:HG22	2:D:377:SER:CB	2.40	0.52
1:F:180:ALA:HA	1:F:183:LEU:HD12	1.91	0.52
2:G:218:ARG:HH11	2:G:663:GLU:HG3	1.74	0.52
2:J:157:ASP:OD1	2:J:159:THR:HG22	2.10	0.52
2:J:159:THR:HG21	2:J:398:SER:CB	2.40	0.52
2:J:267:ASP:O	2:J:271:LYS:HD2	2.08	0.52
1:A:161:TRP:HB2	1:A:209:ILE:HD13	1.92	0.52
2:B:142:LEU:CD1	2:B:203:MET:CE	2.60	0.52
2:B:829:LEU:HD23	2:B:844:THR:HB	1.92	0.52
2:D:331:THR:OG1	2:D:356:GLN:HG3	2.10	0.52
2:G:383:LEU:HD12	2:G:384:LYS:H	1.74	0.52
2:J:303:LYS:HG3	2:J:304:ASP:N	2.24	0.52
2:B:159:THR:HG21	2:B:398:SER:CB	2.39	0.52
1:C:66:LEU:HD13	1:C:81:LEU:HD22	1.92	0.52
2:D:156:GLY:HA3	2:D:1004:PRO:O	2.10	0.52
2:D:180:TYR:CE1	2:D:189:LEU:HD21	2.45	0.52
1:F:87:TRP:O	1:F:89:LEU:CD1	2.57	0.52
2:G:750:GLY:HA2	2:G:788:LYS:HB3	1.92	0.52
2:B:433:VAL:HG21	2:B:442:PRO:HB2	1.92	0.52
2:B:641:ILE:HD13	2:D:724:VAL:HG21	1.92	0.52
2:B:901:ASN:HB2	2:B:934:PRO:HD3	1.90	0.52
2:D:397:ARG:HG3	2:D:455:PHE:HD2	1.74	0.52
2:G:318:ASP:HB2	2:G:419:ARG:HB3	1.92	0.52
2:G:430:LEU:HD23	2:G:447:PRO:HG2	1.92	0.52
2:G:597:ASN:HA	2:G:607:ASP:HB3	1.92	0.52
2:J:491:THR:CG2	2:J:512:ARG:HB2	2.39	0.52
2:B:971:GLY:HA3	2:B:1016:SER:HB3	1.90	0.52
2:B:250:ILE:HB	2:B:359:MET:HE1	1.93	0.52
2:G:250:ILE:HB	2:G:359:MET:CE	2.40	0.52
1:A:410:LYS:HB2	1:A:415:GLU:HB2	1.90	0.51
2:B:534:LYS:HB3	2:B:601:ASP:HA	1.92	0.51
2:D:349:ALA:HB2	2:D:373:LEU:HD12	1.90	0.51
2:D:411:THR:O	2:D:414:VAL:HG22	2.10	0.51
2:D:430:LEU:HD23	2:D:447:PRO:HG2	1.92	0.51
1:I:108:GLY:O	1:I:112:VAL:HG22	2.09	0.51
2:J:410:GLY:HA3	2:J:1001:ASN:HD21	1.76	0.51
2:B:285:LYS:HG3	2:B:286:ASP:N	2.25	0.51
2:B:636:ILE:CG2	2:B:650:LEU:HD12	2.41	0.51
2:D:171:SER:HA	2:D:730:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:GLY:HA3	2:D:611:ARG:NH1	2.25	0.51
2:D:878:SER:HB2	2:D:955:THR:OG1	2.10	0.51
2:G:949:LEU:HD23	2:G:981:LEU:HD11	1.92	0.51
2:J:813:PHE:CE2	2:J:890:TRP:HB2	2.34	0.51
1:C:244:LEU:HD23	1:C:387:ILE:HG12	1.92	0.51
2:D:690:ALA:HB3	2:D:745:GLN:OE1	2.10	0.51
2:G:215:TYR:CE2	2:G:223:VAL:HG21	2.46	0.51
2:J:454:PRO:HD2	2:J:494:LYS:HB2	1.92	0.51
2:B:383:LEU:HD12	2:B:384:LYS:N	2.25	0.51
1:C:211:SER:O	1:C:215:GLU:HG3	2.11	0.51
2:D:480:ALA:HA	2:D:523:ASN:HB3	1.91	0.51
2:D:622:ASN:O	2:D:696:SER:OG	2.27	0.51
2:D:672:LEU:HB2	2:D:689:THR:HG22	1.91	0.51
2:D:695:LEU:HA	2:D:748:ASN:HD21	1.76	0.51
2:D:151:VAL:HA	2:D:163:SER:O	2.10	0.51
1:F:465:ASN:HB3	2:G:276:GLY:HA2	1.92	0.51
2:J:183:ASP:OD2	2:J:228:THR:OG1	2.14	0.51
2:J:636:ILE:CG2	2:J:650:LEU:HD12	2.40	0.51
2:D:950:LYS:O	2:D:979:ARG:HA	2.11	0.51
1:F:174:THR:OG1	1:F:175:GLU:N	2.42	0.51
2:J:532:ASP:HB3	2:J:535:HIS:HB2	1.93	0.51
1:A:247:GLY:O	1:A:249:TYR:N	2.38	0.51
2:B:891:MET:HE2	2:B:987:TYR:CE1	2.45	0.51
2:D:349:ALA:HA	2:D:372:ARG:O	2.10	0.51
2:D:374:ASN:ND2	2:D:388:ASN:HD22	2.09	0.51
2:J:987:TYR:HB2	2:J:992:PRO:HB3	1.92	0.51
2:D:218:ARG:HD3	2:D:663:GLU:HG3	1.93	0.51
2:G:987:TYR:HB2	2:G:992:PRO:HB3	1.92	0.51
2:J:397:ARG:HG3	2:J:455:PHE:CD2	2.45	0.51
2:B:412:PHE:CE1	2:B:416:THR:HG21	2.46	0.51
1:F:170:HIS:O	1:F:172:SER:N	2.43	0.51
2:G:734:VAL:HG22	2:G:745:GLN:O	2.11	0.51
3:P:10:ARG:N	3:P:10:ARG:HD3	2.26	0.51
2:G:261:THR:N	2:G:264:GLU:HB2	2.26	0.51
1:C:265:LEU:HD11	1:C:385:TYR:CE2	2.46	0.50
1:C:420:ASN:O	1:C:421:MET:HB3	2.09	0.50
2:G:601:ASP:HB3	2:G:603:TRP:CD1	2.45	0.50
1:I:170:HIS:C	1:I:172:SER:H	2.14	0.50
1:I:491:THR:HG21	2:J:737:PRO:HB3	1.92	0.50
2:B:863:PRO:HD2	2:B:887:VAL:O	2.12	0.50
2:D:672:LEU:H	2:D:689:THR:HG23	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:968:VAL:HG13	2:D:969:ILE:HG13	1.93	0.50
2:J:383:LEU:HD12	2:J:384:LYS:N	2.26	0.50
2:B:171:SER:HB2	2:B:698:GLU:OE2	2.12	0.50
2:B:380:ASN:ND2	2:B:382:TRP:HE3	2.00	0.50
2:D:768:ASN:HB3	2:D:771:TRP:HB3	1.93	0.50
1:F:77:ASP:OD1	1:F:78:GLY:N	2.45	0.50
2:G:1012:GLY:O	2:G:1013:ILE:HG13	2.12	0.50
1:A:491:THR:HG21	2:B:737:PRO:HB3	1.92	0.50
2:B:491:THR:HG23	2:B:512:ARG:HB2	1.93	0.50
2:B:917:ALA:HA	2:B:927:VAL:HG13	1.92	0.50
1:C:161:TRP:CD1	1:C:242:ILE:HG12	2.47	0.50
2:D:121:SER:OG	2:D:207:LYS:NZ	2.42	0.50
2:D:203:MET:HA	2:D:225:PHE:O	2.12	0.50
1:F:319:PRO:HG3	1:F:353:LEU:HD23	1.93	0.50
2:J:234:SER:OG	2:J:235:GLU:N	2.45	0.50
2:J:262:GLY:N	2:J:318:ASP:OD2	2.44	0.50
2:J:708:ALA:HB2	2:J:719:GLU:HG3	1.93	0.50
1:C:421:MET:HA	1:C:424:LEU:HB3	1.92	0.50
2:D:215:TYR:HD2	2:D:223:VAL:HG11	1.76	0.50
2:D:495:ARG:NH2	2:D:502:ASP:OD1	2.45	0.50
2:G:553:ILE:HG13	2:J:490:ARG:NH2	2.26	0.50
2:G:913:MET:C	2:G:915:LEU:H	2.14	0.50
2:J:698:GLU:HB2	2:J:731:LEU:HD13	1.93	0.50
1:A:390:GLU:OE1	1:A:444:ARG:NH2	2.44	0.50
1:C:67:GLN:HA	1:C:84:PHE:O	2.12	0.50
2:G:433:VAL:CG2	2:G:442:PRO:HB2	2.41	0.50
1:I:421:MET:HA	1:I:424:LEU:HB3	1.93	0.50
2:J:250:ILE:HB	2:J:359:MET:HE3	1.93	0.50
2:J:674:THR:HG22	2:J:688:SER:HB2	1.93	0.50
2:B:601:ASP:HB3	2:B:603:TRP:CD1	2.47	0.50
1:I:32:GLN:HG2	2:J:673:VAL:HG23	1.93	0.50
2:J:891:MET:HE2	2:J:987:TYR:CE1	2.47	0.50
2:J:969:ILE:HA	2:J:1017:PHE:HB3	1.94	0.50
2:D:285:LYS:HB2	2:D:315:PHE:CE2	2.47	0.49
2:D:677:ASN:OD1	2:D:683:MET:HA	2.12	0.49
2:G:633:MET:HG3	2:G:634:PHE:N	2.26	0.49
2:G:730:MET:O	2:G:748:ASN:HA	2.12	0.49
1:A:465:ASN:CG	2:B:276:GLY:H	2.12	0.49
2:D:504:THR:HB	2:D:506:LEU:HD12	1.94	0.49
2:D:674:THR:OG1	2:D:675:VAL:N	2.44	0.49
2:D:730:MET:O	2:D:748:ASN:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:GLU:HB2	1:F:424:LEU:HD11	1.94	0.49
1:I:45:ARG:HH21	1:I:151:GLU:CD	2.15	0.49
2:J:281:VAL:O	2:J:285:LYS:HG2	2.12	0.49
2:D:529:PHE:CE2	2:D:537:LEU:HD22	2.46	0.49
4:E:9:GLN:HG3	4:E:10:ARG:NH2	2.26	0.49
2:G:563:ASP:OD1	2:G:563:ASP:N	2.46	0.49
3:H:9:GLN:HG3	3:H:10:ARG:HH21	1.77	0.49
2:J:397:ARG:HG3	2:J:455:PHE:HD2	1.75	0.49
2:G:132:GLU:HG2	2:G:975:TYR:CE2	2.47	0.49
2:D:261:THR:HG1	2:D:264:GLU:HG3	1.73	0.49
2:J:721:ASP:O	2:J:757:VAL:HG23	2.13	0.49
2:B:796:TYR:HE1	2:B:798:LEU:CD2	2.25	0.49
2:D:250:ILE:HD12	2:D:359:MET:HE1	1.95	0.49
2:G:412:PHE:CE1	2:G:416:THR:HG21	2.48	0.49
1:I:249:TYR:CD1	1:I:394:GLN:HG3	2.48	0.49
2:B:130:LEU:HG	2:B:138:ILE:HD11	1.94	0.49
2:B:303:LYS:HG3	2:B:304:ASP:N	2.28	0.49
1:F:368:ASP:HB3	1:F:369:LYS:CD	2.38	0.49
2:G:265:LEU:HD13	2:G:909:ASN:HA	1.95	0.49
2:G:786:ILE:HG21	2:G:789:LEU:HD11	1.92	0.49
2:G:860:VAL:HG23	2:G:861:THR:N	2.28	0.49
1:I:299:SER:CB	1:I:373:LYS:HD3	2.42	0.49
2:J:217:ALA:O	2:J:662:SER:HB3	2.12	0.49
1:A:330:LEU:O	1:A:430:ARG:HD3	2.13	0.49
2:G:972:ALA:O	2:G:973:ARG:HG3	2.12	0.49
2:J:691:GLY:O	2:J:692:ASN:HB2	2.12	0.49
1:A:402:GLU:CB	1:A:419:VAL:HG21	2.43	0.49
1:A:441:ASP:OD1	1:A:444:ARG:NH1	2.45	0.49
1:C:488:ASP:HA	1:C:491:THR:HG22	1.94	0.49
2:G:758:ASP:HB3	2:G:780:ASN:ND2	2.28	0.49
1:A:289:PHE:CD2	1:A:378:TYR:CD2	3.01	0.49
2:B:956:TYR:CD1	2:B:956:TYR:C	2.86	0.49
1:C:441:ASP:OD1	1:C:444:ARG:NH1	2.46	0.49
1:F:346:VAL:HG22	1:F:353:LEU:HD23	1.95	0.49
2:G:577:LEU:HD22	2:J:578:SER:O	2.13	0.49
2:J:733:ASP:OD1	2:J:744:SER:HB3	2.13	0.49
2:B:490:ARG:NH1	2:B:490:ARG:HG3	2.27	0.48
2:B:926:ASP:OD1	2:B:926:ASP:N	2.45	0.48
1:C:66:LEU:CD1	1:C:81:LEU:HD22	2.43	0.48
2:D:175:SER:HB3	2:D:663:GLU:HB2	1.94	0.48
1:F:465:ASN:CG	2:G:276:GLY:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:SER:O	1:I:215:GLU:HG3	2.12	0.48
2:B:639:LYS:C	2:B:639:LYS:HD3	2.33	0.48
2:B:873:SER:OG	2:B:874:TRP:N	2.46	0.48
2:D:603:TRP:CD2	2:D:639:LYS:HE3	2.48	0.48
1:F:66:LEU:CD1	1:F:81:LEU:HD22	2.43	0.48
2:G:514:TYR:CD2	2:G:552:VAL:HG13	2.47	0.48
1:C:356:LYS:NZ	1:C:435:GLU:OE1	2.41	0.48
2:D:266:LEU:O	2:D:270:VAL:HG23	2.13	0.48
2:G:143:GLN:HB3	2:G:950:LYS:HE3	1.95	0.48
2:G:813:PHE:HD2	2:G:941:LEU:HD11	1.79	0.48
2:J:490:ARG:HG3	2:J:490:ARG:NH1	2.29	0.48
2:B:397:ARG:HG3	2:B:455:PHE:CD2	2.48	0.48
2:B:463:ASN:ND2	2:B:485:ASP:OD2	2.47	0.48
2:B:750:GLY:HA2	2:B:788:LYS:HB3	1.95	0.48
2:D:250:ILE:HB	2:D:359:MET:CE	2.43	0.48
2:D:522:THR:HB	2:D:544:GLU:HG3	1.94	0.48
2:G:232:LYS:H	2:G:232:LYS:HD2	1.79	0.48
2:G:975:TYR:CB	2:G:1012:GLY:H	2.22	0.48
2:J:325:LEU:HD12	2:J:414:VAL:HG12	1.94	0.48
1:A:164:MET:CE	1:A:205:CYS:HB2	2.44	0.48
2:B:754:ASN:HB3	2:B:782:ASN:ND2	2.08	0.48
2:D:132:GLU:CG	2:D:975:TYR:HE2	2.27	0.48
2:D:318:ASP:OD1	2:D:318:ASP:N	2.46	0.48
1:A:169:PHE:O	1:A:202:LYS:NZ	2.47	0.48
2:B:363:PRO:HB2	2:B:397:ARG:NH1	2.28	0.48
2:B:791:PHE:HB2	2:B:793:LEU:HD11	1.94	0.48
2:D:215:TYR:HE2	2:D:223:VAL:HG21	1.77	0.48
2:D:261:THR:N	2:D:264:GLU:HB2	2.28	0.48
2:D:758:ASP:HB3	2:D:780:ASN:ND2	2.27	0.48
2:J:216:GLY:HA3	2:J:611:ARG:HH12	1.77	0.48
2:J:913:MET:C	2:J:915:LEU:H	2.15	0.48
1:A:421:MET:HA	1:A:424:LEU:HB3	1.94	0.48
2:G:216:GLY:HA3	2:G:611:ARG:HH12	1.79	0.48
2:G:953:LYS:HG3	2:G:977:MET:HG2	1.96	0.48
1:A:83:PRO:HG3	1:A:91:ILE:HD12	1.96	0.48
2:B:643:GLU:HG2	2:B:644:SER:N	2.29	0.48
1:C:410:LYS:HD3	1:C:415:GLU:OE1	2.14	0.48
2:D:146:VAL:C	2:D:778:ASN:HD21	2.17	0.48
2:G:217:ALA:O	2:G:662:SER:HB3	2.14	0.48
2:G:603:TRP:CG	2:G:639:LYS:HG3	2.48	0.48
1:I:421:MET:O	1:I:425:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:405:TYR:OH	2:J:894:ASN:HB3	2.13	0.48
2:B:295:LEU:CD2	2:B:299:TYR:HE2	2.27	0.48
2:D:602:LYS:O	2:D:602:LYS:HG2	2.13	0.48
1:F:441:ASP:OD1	1:F:444:ARG:NH1	2.47	0.48
1:C:442:MET:HB2	1:C:447:ILE:HB	1.95	0.48
2:D:749:VAL:CG1	2:D:790:PHE:HA	2.44	0.48
2:J:270:VAL:HG21	2:J:281:VAL:HG22	1.95	0.48
1:A:145:ALA:O	1:A:148:PHE:HB2	2.14	0.47
2:D:863:PRO:HD2	2:D:888:GLY:HA3	1.95	0.47
2:D:901:ASN:HB3	2:D:934:PRO:HG3	1.95	0.47
2:G:518:SER:HB3	2:G:548:TYR:HD2	1.79	0.47
2:G:609:SER:OG	2:G:629:SER:HB3	2.14	0.47
2:J:132:GLU:HG2	2:J:975:TYR:HE2	1.79	0.47
2:J:269:GLN:CB	2:J:275:TRP:HE1	2.26	0.47
2:B:947:LEU:HB3	2:B:984:VAL:HG21	1.97	0.47
2:D:531:ILE:HG22	2:D:535:HIS:O	2.14	0.47
1:F:224:ARG:NH1	1:F:227:VAL:HG23	2.29	0.47
2:G:150:GLN:HA	2:G:865:THR:HG21	1.95	0.47
2:G:380:ASN:ND2	2:G:382:TRP:HB3	2.28	0.47
1:A:310:PRO:HD3	1:A:372:LEU:HD11	1.95	0.47
1:A:314:ASP:O	1:A:370:PRO:HG2	2.14	0.47
2:G:528:LYS:HB3	2:G:538:THR:HG23	1.96	0.47
2:J:622:ASN:O	2:J:696:SER:OG	2.27	0.47
2:B:289:LEU:N	2:B:289:LEU:HD23	2.28	0.47
2:B:292:ALA:HB3	2:B:435:TYR:HE2	1.79	0.47
2:D:397:ARG:HG3	2:D:455:PHE:CD2	2.50	0.47
2:D:637:TYR:CD1	2:D:647:LEU:HD23	2.49	0.47
2:D:860:VAL:HG23	2:D:861:THR:N	2.29	0.47
2:D:918:TRP:NE1	2:D:923:LYS:HG3	2.29	0.47
2:D:977:MET:HB2	2:D:1010:VAL:HB	1.95	0.47
3:H:10:ARG:H	3:H:10:ARG:HD3	1.79	0.47
1:I:397:ASP:OD1	1:I:400:THR:OG1	2.31	0.47
2:J:256:LEU:HD23	2:J:256:LEU:H	1.79	0.47
2:B:269:GLN:OE1	2:B:420:TYR:OH	2.23	0.47
2:B:695:LEU:HA	2:B:748:ASN:HD21	1.79	0.47
2:D:280:THR:O	2:D:284:VAL:HG23	2.14	0.47
2:G:423:PRO:HD2	2:G:424:PHE:CD1	2.49	0.47
1:I:172:SER:O	1:I:172:SER:OG	2.32	0.47
1:I:360:ASP:HB3	1:I:363:TYR:HD2	1.78	0.47
2:J:636:ILE:HG21	2:J:650:LEU:HD12	1.95	0.47
2:D:733:ASP:OD1	2:D:744:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:997:ASN:C	2:D:997:ASN:HD22	2.17	0.47
2:G:481:GLN:HG3	2:G:482:ALA:N	2.29	0.47
1:A:23:ASP:HB3	2:B:623:ARG:NH2	2.30	0.47
1:A:124:VAL:HG21	1:A:156:GLN:OE1	2.14	0.47
1:A:289:PHE:CE2	1:A:378:TYR:CD2	3.02	0.47
2:B:117:THR:HG23	2:B:120:GLY:H	1.80	0.47
2:D:127:SER:OG	2:D:201:GLU:O	2.28	0.47
2:D:554:GLY:HA3	2:D:581:GLU:HB2	1.97	0.47
1:F:79:ASN:HB2	2:G:905:LEU:HD11	1.96	0.47
1:F:170:HIS:C	1:F:172:SER:H	2.18	0.47
2:G:345:THR:HG22	2:G:377:SER:CB	2.45	0.47
2:G:982:LEU:HD23	2:G:982:LEU:HA	1.53	0.47
1:I:208:TYR:CZ	1:I:212:ARG:HD2	2.50	0.47
1:I:236:TYR:CE2	1:I:258:MET:HG2	2.50	0.47
1:I:360:ASP:HB3	1:I:363:TYR:CD2	2.49	0.47
1:I:451:HIS:HB3	1:I:469:LEU:HD11	1.96	0.47
2:J:139:MET:HE1	2:J:224:VAL:HG11	1.96	0.47
2:J:139:MET:CE	2:J:224:VAL:HG11	2.45	0.47
2:J:250:ILE:HB	2:J:359:MET:CE	2.45	0.47
2:J:345:THR:HG22	2:J:377:SER:CB	2.44	0.47
2:J:873:SER:O	2:J:874:TRP:HB2	2.14	0.47
2:B:321:TRP:CZ2	2:B:423:PRO:HG3	2.50	0.47
2:B:411:THR:O	2:B:414:VAL:HG22	2.14	0.47
2:B:636:ILE:O	2:B:641:ILE:HG22	2.15	0.47
2:B:809:TYR:CB	2:B:810:PRO:HD3	2.45	0.47
1:F:224:ARG:HD2	1:F:227:VAL:HA	1.96	0.47
1:I:166:ARG:HB3	1:I:482:TRP:CE3	2.50	0.47
1:I:169:PHE:O	1:I:202:LYS:NZ	2.48	0.47
2:J:345:THR:HG22	2:J:377:SER:HB2	1.97	0.47
2:B:958:LEU:HD22	2:B:959:PRO:HD2	1.97	0.47
2:G:303:LYS:HG3	2:G:304:ASP:N	2.28	0.47
2:J:261:THR:OG1	2:J:264:GLU:HG3	2.14	0.47
2:D:117:THR:HG23	2:D:120:GLY:H	1.80	0.47
2:D:809:TYR:CB	2:D:810:PRO:HD3	2.45	0.47
1:I:161:TRP:HB2	1:I:209:ILE:HD13	1.96	0.47
1:I:164:MET:HE2	1:I:205:CYS:HB2	1.97	0.47
2:J:672:LEU:H	2:J:689:THR:CG2	2.27	0.47
2:D:251:LEU:HG	2:D:252:ASN:N	2.30	0.46
2:G:133:LYS:O	2:G:135:VAL:N	2.46	0.46
2:G:484:VAL:HG22	2:G:519:LYS:HB3	1.98	0.46
2:J:476:LEU:HA	2:J:527:TYR:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:849:SER:O	2:J:852:LEU:HB2	2.15	0.46
2:B:216:GLY:HA3	2:B:611:ARG:NH1	2.30	0.46
2:B:232:LYS:H	2:B:232:LYS:HD2	1.80	0.46
2:D:307:GLY:HA2	2:D:311:PHE:CE1	2.50	0.46
2:G:266:LEU:HD23	2:G:266:LEU:HA	1.75	0.46
2:G:677:ASN:OD1	2:G:683:MET:HA	2.15	0.46
2:G:950:LYS:O	2:G:979:ARG:HA	2.16	0.46
2:J:691:GLY:N	2:J:745:GLN:OE1	2.32	0.46
2:D:611:ARG:NH1	2:D:613:ASP:OD1	2.49	0.46
2:D:716:LEU:HD12	2:D:763:GLY:HA2	1.98	0.46
1:I:488:ASP:HA	1:I:491:THR:HG22	1.96	0.46
2:J:813:PHE:CE2	2:J:941:LEU:HD21	2.50	0.46
2:B:321:TRP:CH2	2:B:423:PRO:HG3	2.51	0.46
1:F:157:ALA:HB1	1:F:209:ILE:HG23	1.98	0.46
2:G:270:VAL:HG22	2:G:284:VAL:HG21	1.98	0.46
2:J:950:LYS:O	2:J:979:ARG:HA	2.16	0.46
1:C:390:GLU:HB2	1:C:424:LEU:HD11	1.97	0.46
1:F:410:LYS:HD3	1:F:415:GLU:OE1	2.16	0.46
2:G:147:ALA:HB1	2:G:758:ASP:HB2	1.97	0.46
2:J:267:ASP:CB	2:J:271:LYS:HZ2	2.29	0.46
2:D:862:PRO:HG3	2:D:889:LYS:HB2	1.96	0.46
2:G:212:THR:O	2:G:212:THR:OG1	2.32	0.46
2:G:389:LEU:HD12	2:J:389:LEU:HD12	1.98	0.46
2:G:528:LYS:O	2:G:529:PHE:HB3	2.15	0.46
2:J:266:LEU:O	2:J:270:VAL:HG23	2.15	0.46
1:A:393:LEU:HD13	1:A:421:MET:HB2	1.97	0.46
1:F:164:MET:CE	1:F:205:CYS:HB2	2.46	0.46
1:F:198:PRO:HB3	1:F:494:GLN:HG2	1.97	0.46
2:J:573:THR:HG22	2:J:573:THR:O	2.16	0.46
2:J:626:TRP:CD1	2:J:626:TRP:N	2.83	0.46
2:B:214:ILE:HG22	2:B:593:PHE:CE2	2.50	0.46
2:B:318:ASP:OD1	2:B:318:ASP:N	2.48	0.46
2:J:609:SER:OG	2:J:629:SER:HB3	2.15	0.46
1:A:52:LEU:HD22	1:A:155:LEU:HD21	1.97	0.46
2:B:815:MET:SD	2:B:937:ASP:O	2.73	0.46
2:D:603:TRP:CE3	2:D:639:LYS:HE3	2.50	0.46
2:D:702:GLN:HG2	2:D:725:ARG:HG3	1.97	0.46
2:G:504:THR:HB	2:G:506:LEU:HD12	1.97	0.46
1:A:65:GLU:OE1	1:A:436:GLY:N	2.36	0.46
2:B:453:ARG:N	2:B:454:PRO:HD3	2.30	0.46
2:B:552:VAL:HG12	2:B:553:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:GLY:O	2:B:997:ASN:HB3	2.16	0.46
1:C:164:MET:HE1	1:C:184:GLY:HA3	1.98	0.46
1:F:66:LEU:HD13	1:F:81:LEU:HD22	1.98	0.46
1:F:77:ASP:OD1	1:F:79:ASN:N	2.49	0.46
2:G:129:LYS:HE2	2:G:882:ASP:OD2	2.15	0.46
2:G:415:LEU:HD11	2:G:990:PHE:HE2	1.81	0.46
2:G:656:TYR:CD1	2:G:656:TYR:C	2.89	0.46
2:B:266:LEU:HA	2:B:266:LEU:HD23	1.67	0.45
2:B:302:LEU:HD23	2:B:302:LEU:N	2.30	0.45
2:D:559:GLY:HA3	2:D:572:LYS:CG	2.45	0.45
2:G:234:SER:OG	2:G:235:GLU:N	2.47	0.45
2:G:617:ARG:NH1	2:G:664:ILE:O	2.49	0.45
2:J:860:VAL:HG23	2:J:861:THR:N	2.31	0.45
2:B:154:THR:HA	2:B:994:ALA:HA	1.98	0.45
2:B:635:ASP:OD2	2:B:638:ASN:ND2	2.39	0.45
2:D:266:LEU:HA	2:D:266:LEU:HD23	1.61	0.45
2:D:936:PHE:CZ	4:E:8:SER:HB2	2.51	0.45
2:G:758:ASP:HB3	2:G:780:ASN:HB2	1.98	0.45
2:J:837:ASP:OD1	2:J:838:ALA:N	2.50	0.45
1:C:74:THR:HG22	1:C:464:ALA:HB2	1.98	0.45
2:G:901:ASN:HB2	2:G:934:PRO:HD3	1.98	0.45
2:J:161:VAL:HG11	2:J:189:LEU:HB3	1.99	0.45
2:B:179:LEU:HB3	2:B:223:VAL:HG12	1.98	0.45
2:B:274:PHE:CD2	2:B:906:MET:HB2	2.52	0.45
1:C:93:ASN:ND2	2:D:850:ALA:HB2	2.31	0.45
2:D:199:ASP:OD2	2:D:372:ARG:HD2	2.17	0.45
2:G:139:MET:HE1	2:G:224:VAL:HG11	1.99	0.45
2:G:342:SER:OG	2:G:343:GLN:N	2.50	0.45
1:A:110:TYR:HD1	1:A:167:PHE:CE2	2.34	0.45
1:A:137:LYS:HA	1:A:137:LYS:HE2	1.97	0.45
2:B:480:ALA:HA	2:B:523:ASN:CB	2.38	0.45
2:D:489:THR:HG22	2:D:490:ARG:N	2.31	0.45
2:D:597:ASN:HA	2:D:607:ASP:HB3	1.99	0.45
2:G:491:THR:HG23	2:G:512:ARG:HB2	1.97	0.45
2:G:798:LEU:HD12	2:G:803:THR:OG1	2.17	0.45
2:J:891:MET:SD	2:J:996:GLY:N	2.78	0.45
2:J:917:ALA:HA	2:J:927:VAL:HG13	1.97	0.45
2:B:166:ILE:O	2:B:167:HIS:HB2	2.17	0.45
2:B:765:ILE:O	2:B:765:ILE:HG22	2.16	0.45
1:C:291:GLY:HA2	2:D:678:TYR:OH	2.17	0.45
1:C:146:LYS:O	1:C:149:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:543:HIS:HB2	2:D:592:PHE:CD1	2.49	0.45
2:D:848:TYR:CZ	2:D:935:GLN:HG2	2.51	0.45
1:F:208:TYR:CZ	1:F:212:ARG:HD2	2.50	0.45
1:F:244:LEU:CD2	1:F:387:ILE:HG12	2.46	0.45
2:G:463:ASN:ND2	2:G:485:ASP:OD2	2.49	0.45
2:B:142:LEU:CG	2:B:203:MET:HE1	2.43	0.45
2:D:212:THR:O	2:D:212:THR:OG1	2.28	0.45
2:D:251:LEU:HG	2:D:252:ASN:H	1.82	0.45
2:D:295:LEU:HD21	2:D:442:PRO:HD3	1.98	0.45
1:F:75:ILE:HG22	2:G:274:PHE:CE1	2.51	0.45
1:F:420:ASN:HD21	1:F:422:GLU:HB3	1.82	0.45
2:G:321:TRP:CH2	2:G:423:PRO:HG3	2.52	0.45
2:G:524:THR:HA	2:G:542:GLY:HA3	1.98	0.45
2:G:958:LEU:HD23	2:G:958:LEU:HA	1.71	0.45
1:I:253:ALA:HB2	1:I:391:SER:HB3	1.98	0.45
2:J:461:GLN:NE2	2:J:487:THR:HB	2.32	0.45
2:B:168:GLY:H	2:B:725:ARG:NH1	2.14	0.45
2:B:522:THR:HB	2:B:544:GLU:HG3	1.97	0.45
2:D:520:SER:HB2	2:D:546:ILE:HD12	1.99	0.45
2:D:662:SER:HB2	2:D:697:TRP:CZ3	2.52	0.45
2:D:937:ASP:OD1	2:D:939:HIS:ND1	2.46	0.45
1:F:447:ILE:HG22	1:F:448:PRO:O	2.17	0.45
1:I:292:PHE:CD2	2:J:679:THR:HG22	2.52	0.45
1:I:442:MET:HB2	1:I:447:ILE:HB	1.99	0.45
1:A:391:SER:O	1:A:395:THR:HG23	2.18	0.45
2:B:804:ILE:HG22	2:B:814:TYR:HB2	1.99	0.45
2:B:990:PHE:HB2	2:B:1002:GLN:NE2	2.28	0.45
1:C:77:ASP:OD1	1:C:78:GLY:N	2.50	0.45
2:D:637:TYR:HD1	2:D:647:LEU:HD23	1.82	0.45
2:D:862:PRO:CG	2:D:889:LYS:HB2	2.47	0.45
2:G:260:MET:HG3	2:G:910:LYS:O	2.17	0.45
2:G:724:VAL:HG22	2:G:755:THR:OG1	2.16	0.45
2:J:815:MET:HE1	2:J:941:LEU:HD11	1.97	0.45
2:J:901:ASN:CB	2:J:934:PRO:HD3	2.46	0.45
2:B:813:PHE:CD2	2:B:941:LEU:HD11	2.52	0.44
3:P:10:ARG:HD3	3:P:10:ARG:H	1.81	0.44
2:D:250:ILE:HB	2:D:359:MET:HE3	1.98	0.44
2:G:489:THR:HG22	2:G:490:ARG:H	1.82	0.44
2:G:578:SER:O	2:J:577:LEU:HD22	2.18	0.44
2:J:603:TRP:CD2	2:J:639:LYS:HG3	2.53	0.44
1:A:108:GLY:O	1:A:112:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:856:ILE:CD1	2:B:857:ASP:H	2.25	0.44
2:B:947:LEU:H	2:B:984:VAL:CG2	2.30	0.44
2:D:901:ASN:HB2	2:D:934:PRO:HD3	1.99	0.44
1:F:62:PHE:CD2	1:F:304:THR:HB	2.53	0.44
1:F:451:HIS:CG	1:F:469:LEU:HD11	2.52	0.44
2:G:215:TYR:HE2	2:G:223:VAL:HG21	1.82	0.44
2:G:331:THR:OG1	2:G:356:GLN:HG3	2.18	0.44
2:G:344:GLY:O	2:G:377:SER:HA	2.17	0.44
2:G:813:PHE:CE2	2:G:941:LEU:HD21	2.53	0.44
2:J:261:THR:N	2:J:264:GLU:HB2	2.31	0.44
2:B:212:THR:O	2:B:212:THR:OG1	2.34	0.44
2:D:603:TRP:HB3	2:D:639:LYS:HG3	1.98	0.44
2:D:1002:GLN:O	2:D:1004:PRO:HD3	2.18	0.44
1:F:113:TYR:CE1	1:F:162:ARG:HG3	2.52	0.44
1:F:164:MET:HE2	1:F:205:CYS:HB2	1.98	0.44
1:F:491:THR:HG21	2:G:737:PRO:HB3	1.99	0.44
2:G:486:ILE:HD13	2:G:517:VAL:HG13	1.98	0.44
2:G:790:PHE:HD2	2:G:791:PHE:CD2	2.36	0.44
2:B:812:SER:HB3	2:B:858:LYS:O	2.18	0.44
2:B:856:ILE:HG13	2:B:858:LYS:HD3	1.99	0.44
1:C:486:GLN:HA	1:C:489:ARG:HB2	1.98	0.44
2:D:161:VAL:HG11	2:D:189:LEU:HB3	2.00	0.44
1:F:297:LEU:HB2	2:J:573:THR:CG2	2.39	0.44
2:G:279:GLN:HG2	2:G:284:VAL:CG2	2.48	0.44
1:I:164:MET:HE1	1:I:205:CYS:HB2	1.97	0.44
2:B:917:ALA:HB1	2:B:928:PRO:O	2.17	0.44
1:C:84:PHE:HE1	1:C:106:ILE:HD11	1.83	0.44
2:D:214:ILE:HG22	2:D:593:PHE:CD2	2.53	0.44
2:D:603:TRP:CB	2:D:639:LYS:HG3	2.48	0.44
2:G:143:GLN:OE1	2:G:950:LYS:NZ	2.49	0.44
2:G:986:LYS:HD2	2:G:986:LYS:HA	1.82	0.44
1:I:249:TYR:CE1	1:I:394:GLN:HG3	2.52	0.44
2:B:613:ASP:O	2:B:624:SER:HA	2.17	0.44
2:B:616:SER:HA	2:B:623:ARG:HH12	1.83	0.44
2:B:947:LEU:O	2:B:984:VAL:HG22	2.17	0.44
1:C:27:GLU:OE1	2:D:584:VAL:HG21	2.18	0.44
2:D:168:GLY:H	2:D:725:ARG:HH11	1.65	0.44
2:D:279:GLN:HG2	2:D:284:VAL:CG2	2.35	0.44
2:D:423:PRO:HD2	2:D:424:PHE:CD2	2.53	0.44
2:D:553:ILE:HD13	2:D:553:ILE:HA	1.79	0.44
2:G:941:LEU:HD23	2:G:941:LEU:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238:LEU:HD12	1:I:241:ARG:HD2	1.99	0.44
2:J:146:VAL:C	2:J:778:ASN:HD21	2.21	0.44
2:J:267:ASP:HB3	2:J:271:LYS:HZ2	1.82	0.44
1:A:20:CYS:SG	1:A:20:CYS:O	2.75	0.44
1:A:292:PHE:CD1	1:A:293:ALA:N	2.86	0.44
2:B:495:ARG:NH2	2:B:502:ASP:OD1	2.50	0.44
2:D:260:MET:HG3	2:D:910:LYS:O	2.17	0.44
2:D:573:THR:HG22	2:D:573:THR:O	2.17	0.44
1:F:420:ASN:O	1:F:421:MET:HB3	2.17	0.44
2:G:700:GLN:HG2	2:G:727:THR:HG23	1.99	0.44
2:G:716:LEU:HD12	2:G:763:GLY:HA2	2.00	0.44
1:I:79:ASN:HB3	4:K:5:GLY:HA2	1.99	0.44
2:J:267:ASP:HB3	2:J:271:LYS:HZ1	1.82	0.44
2:J:990:PHE:HB2	2:J:1002:GLN:NE2	2.32	0.44
2:B:484:VAL:HG23	6:B:1102:C8E:H51	1.98	0.44
1:C:189:LYS:HD3	1:C:208:TYR:CE1	2.53	0.44
2:D:703:PHE:O	2:D:723:TYR:HA	2.17	0.44
2:D:813:PHE:HD2	2:D:941:LEU:HD11	1.83	0.44
2:G:836:VAL:HA	2:G:842:LYS:HA	2.00	0.44
2:J:147:ALA:HB1	2:J:758:ASP:HB2	1.99	0.44
2:J:285:LYS:HG3	2:J:286:ASP:N	2.33	0.44
2:J:433:VAL:CG2	2:J:442:PRO:HB2	2.46	0.44
2:J:674:THR:OG1	2:J:675:VAL:N	2.50	0.44
1:C:306:ASN:ND2	1:C:308:ALA:HB2	2.33	0.44
2:D:270:VAL:HG22	2:D:284:VAL:HG21	2.00	0.44
2:J:137:ASN:OD1	2:J:162:ALA:N	2.51	0.44
2:J:953:LYS:HG3	2:J:977:MET:HG2	1.99	0.44
1:A:200:ALA:HB1	1:A:204:GLN:OE1	2.18	0.43
1:A:218:GLU:HB3	1:F:251:LYS:HE2	2.00	0.43
1:A:313:LYS:HA	1:A:370:PRO:HD3	2.00	0.43
2:B:133:LYS:O	2:B:135:VAL:N	2.50	0.43
2:B:878:SER:O	2:B:954:LEU:HA	2.18	0.43
2:D:249:GLN:HG3	2:D:328:THR:HG23	1.99	0.43
2:D:481:GLN:HG3	2:D:482:ALA:N	2.33	0.43
1:F:48:LEU:HD11	1:F:120:ALA:HB2	2.00	0.43
1:F:75:ILE:HG23	1:F:463:PHE:O	2.17	0.43
1:F:161:TRP:HB2	1:F:209:ILE:HD13	2.00	0.43
2:G:540:LEU:HD23	2:G:595:ARG:HD2	2.00	0.43
1:I:310:PRO:HG2	2:J:503:SER:HB3	2.00	0.43
2:J:378:ARG:HG2	2:J:384:LYS:HG3	2.00	0.43
2:J:809:TYR:N	2:J:809:TYR:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:ASN:N	2:B:867:GLY:O	2.51	0.43
2:D:508:GLU:HB3	2:D:558:LYS:HB3	1.99	0.43
1:F:351:GLY:HA3	1:F:460:LEU:HD21	2.00	0.43
2:G:285:LYS:HB2	2:G:315:PHE:CE2	2.53	0.43
2:J:150:GLN:HB2	2:J:865:THR:HG21	2.00	0.43
2:J:381:GLU:CD	2:J:381:GLU:H	2.21	0.43
2:J:891:MET:HE2	2:J:987:TYR:CZ	2.53	0.43
1:A:164:MET:HE1	1:A:184:GLY:HA3	2.01	0.43
1:A:374:VAL:HG23	1:A:375:GLY:N	2.33	0.43
2:B:790:PHE:HB2	2:B:791:PHE:H	1.38	0.43
2:B:795:LYS:HA	2:B:806:GLU:HA	1.99	0.43
2:B:797:MET:O	2:B:799:PRO:HD3	2.18	0.43
1:C:405:LEU:HD12	1:C:405:LEU:HA	1.66	0.43
2:D:139:MET:HE1	2:D:224:VAL:HG11	1.98	0.43
2:D:810:PRO:HB2	2:D:811:ASN:H	1.51	0.43
1:F:405:LEU:HD23	1:F:419:VAL:HG22	1.99	0.43
2:G:417:MET:HB3	2:G:417:MET:HE3	1.73	0.43
2:G:751:SER:OG	2:G:787:THR:HB	2.18	0.43
2:B:146:VAL:HB	2:B:149:MET:HB3	2.00	0.43
2:B:917:ALA:HB3	2:B:930:LEU:CD2	2.48	0.43
1:F:391:SER:O	1:F:395:THR:HG23	2.18	0.43
2:G:159:THR:HG21	2:G:398:SER:CB	2.48	0.43
2:G:188:SER:O	2:G:192:VAL:HG23	2.17	0.43
2:G:603:TRP:CE2	2:G:639:LYS:HE3	2.54	0.43
2:G:864:ILE:HB	2:G:887:VAL:HG23	2.01	0.43
2:G:891:MET:HB3	2:G:891:MET:HE2	1.79	0.43
1:A:198:PRO:HB3	1:A:494:GLN:HG2	2.00	0.43
1:A:227:VAL:HG22	1:A:227:VAL:O	2.19	0.43
2:D:593:PHE:HB3	2:D:611:ARG:HH21	1.83	0.43
2:G:215:TYR:CD2	2:G:223:VAL:HG11	2.54	0.43
1:I:273:GLU:O	1:I:277:ILE:HG13	2.19	0.43
1:A:79:ASN:HB2	2:B:905:LEU:HD11	1.99	0.43
1:A:368:ASP:HB3	1:A:369:LYS:HD2	2.01	0.43
2:B:786:ILE:HG21	2:B:789:LEU:HD11	1.99	0.43
2:B:890:TRP:HB3	2:B:941:LEU:HD22	2.00	0.43
1:C:23:ASP:HB3	2:D:623:ARG:NH2	2.34	0.43
2:D:285:LYS:HG3	2:D:286:ASP:N	2.34	0.43
1:I:289:PHE:CD2	1:I:378:TYR:HD2	2.37	0.43
2:J:597:ASN:HA	2:J:607:ASP:HB3	2.01	0.43
2:J:616:SER:HA	2:J:623:ARG:HH12	1.84	0.43
2:J:641:ILE:HD13	2:J:647:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:SER:OG	2:B:629:SER:HB3	2.18	0.43
2:B:955:THR:HA	2:B:974:VAL:O	2.19	0.43
1:C:195:TYR:CE2	1:C:197:GLY:HA3	2.54	0.43
2:D:156:GLY:N	2:D:1003:TYR:O	2.49	0.43
2:D:987:TYR:CB	2:D:992:PRO:HB3	2.47	0.43
1:F:26:PRO:HB3	2:G:667:TYR:CD2	2.54	0.43
1:F:103:VAL:HG12	1:F:103:VAL:O	2.18	0.43
2:G:115:LEU:HD12	2:G:116:SER:N	2.34	0.43
2:G:906:MET:HA	2:G:910:LYS:HZ1	1.84	0.43
1:I:488:ASP:O	1:I:492:ASN:HB3	2.19	0.43
2:B:151:VAL:HA	2:B:163:SER:O	2.18	0.43
2:B:982:LEU:HD23	2:B:982:LEU:HA	1.83	0.43
1:C:301:THR:HB	1:C:303:THR:HG23	2.01	0.43
1:C:447:ILE:HG22	1:C:448:PRO:O	2.19	0.43
2:D:311:PHE:HA	2:D:312:PRO:HD3	1.78	0.43
2:D:320:ASP:OD1	2:D:323:LYS:HB3	2.18	0.43
2:D:793:LEU:HD12	2:D:793:LEU:H	1.84	0.43
2:D:947:LEU:H	2:D:984:VAL:CG2	2.32	0.43
1:F:161:TRP:NE1	1:F:242:ILE:HG23	2.34	0.43
2:G:329:ALA:HA	2:G:330:PRO:HD3	1.78	0.43
2:G:808:GLY:O	2:G:809:TYR:HB2	2.17	0.43
2:G:978:ALA:HB1	2:G:981:LEU:HD23	2.00	0.43
2:J:672:LEU:H	2:J:689:THR:HG23	1.84	0.43
1:A:310:PRO:HD3	1:A:372:LEU:CD1	2.49	0.43
2:B:187:THR:OG1	2:B:188:SER:N	2.50	0.43
2:B:546:ILE:HG22	2:B:547:GLU:H	1.83	0.43
2:D:133:LYS:O	2:D:135:VAL:N	2.52	0.43
2:D:472:PRO:HG2	2:D:476:LEU:CD1	2.47	0.43
2:D:982:LEU:HD23	2:D:982:LEU:HA	1.63	0.43
1:F:181:LYS:O	1:F:181:LYS:HG2	2.19	0.43
2:G:323:LYS:HE2	2:G:424:PHE:CE2	2.53	0.43
2:G:326:PHE:HD1	2:G:359:MET:HE2	1.84	0.43
2:J:169:THR:OG1	2:J:861:THR:HG21	2.19	0.43
2:J:172:LEU:HG	2:J:730:MET:HE1	2.01	0.43
2:J:292:ALA:HB3	2:J:435:TYR:CE2	2.54	0.43
2:J:785:GLU:HG3	2:J:809:TYR:HA	2.01	0.43
2:J:948:ARG:NH1	2:J:983:THR:OG1	2.52	0.43
1:A:73:THR:HG23	1:A:85:VAL:HG11	2.00	0.43
2:B:289:LEU:HD23	2:B:289:LEU:H	1.84	0.43
2:D:721:ASP:O	2:D:757:VAL:HG23	2.19	0.43
1:F:29:LYS:HD2	2:G:674:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:292:ALA:HB3	2:G:435:TYR:HE2	1.84	0.43
2:B:321:TRP:CZ2	2:B:417:MET:HE2	2.54	0.42
2:B:476:LEU:HA	2:B:526:GLU:O	2.19	0.42
2:B:491:THR:CG2	2:B:512:ARG:HB2	2.48	0.42
2:D:534:LYS:O	2:D:535:HIS:ND1	2.50	0.42
2:D:898:PHE:CD1	2:D:905:LEU:HD22	2.54	0.42
1:F:187:LEU:HD23	1:F:189:LYS:HE2	2.01	0.42
2:G:948:ARG:NH1	2:G:983:THR:OG1	2.51	0.42
2:J:247:ILE:HD13	2:J:328:THR:CG2	2.49	0.42
2:J:953:LYS:HG3	2:J:977:MET:CG	2.49	0.42
1:A:236:TYR:CE2	1:A:258:MET:HG2	2.54	0.42
2:B:215:TYR:CE2	2:B:223:VAL:HG21	2.55	0.42
2:B:997:ASN:C	2:B:997:ASN:HD22	2.22	0.42
1:C:421:MET:O	1:C:425:GLN:HG3	2.19	0.42
2:D:386:GLY:HA3	2:D:467:PHE:CE2	2.55	0.42
2:G:973:ARG:HB2	2:G:1014:GLN:HB3	2.01	0.42
2:J:275:TRP:CG	2:J:284:VAL:HG11	2.54	0.42
1:A:220:LEU:HD12	1:A:232:ARG:HA	2.00	0.42
2:B:766:TYR:HB2	2:B:772:ASN:HA	2.00	0.42
2:G:430:LEU:HD12	2:G:430:LEU:HA	1.80	0.42
1:I:487:ARG:CZ	2:J:735:PRO:HB3	2.50	0.42
2:J:543:HIS:HB2	2:J:592:PHE:HD1	1.83	0.42
2:J:647:LEU:HD21	2:J:650:LEU:HB2	2.01	0.42
2:J:862:PRO:CG	2:J:889:LYS:HB2	2.47	0.42
2:B:541:MET:HE3	2:B:541:MET:HB2	1.72	0.42
2:B:906:MET:HA	2:B:910:LYS:NZ	2.34	0.42
2:B:987:TYR:HB2	2:B:992:PRO:HB3	2.01	0.42
1:C:121:ASN:OD1	1:C:156:GLN:NE2	2.52	0.42
2:D:383:LEU:HD12	2:D:384:LYS:N	2.35	0.42
2:D:827:LYS:HA	2:D:932:GLN:HE22	1.84	0.42
2:G:878:SER:HB2	2:G:955:THR:OG1	2.19	0.42
2:J:380:ASN:ND2	2:J:382:TRP:HB3	2.34	0.42
2:B:239:ILE:HG23	2:B:338:PHE:HD1	1.80	0.42
1:C:465:ASN:OD1	2:D:276:GLY:N	2.50	0.42
2:D:258:ASN:O	2:D:258:ASN:ND2	2.53	0.42
2:D:345:THR:HG22	2:D:377:SER:HB2	2.00	0.42
2:J:153:THR:OG1	2:J:162:ALA:HB2	2.19	0.42
2:J:758:ASP:HB3	2:J:780:ASN:HB2	2.02	0.42
2:J:804:ILE:HB	2:J:814:TYR:HB2	2.01	0.42
1:A:36:THR:HG22	1:A:36:THR:O	2.19	0.42
1:A:263:TYR:HA	1:A:264:PRO:HD2	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:VAL:O	2:B:177:ALA:HA	2.20	0.42
2:B:284:VAL:O	2:B:284:VAL:HG12	2.20	0.42
2:B:798:LEU:HB2	2:B:801:THR:OG1	2.19	0.42
1:C:24:ARG:HA	1:C:24:ARG:HD3	1.82	0.42
1:C:424:LEU:HD13	1:C:424:LEU:C	2.40	0.42
1:I:137:LYS:HE2	1:I:137:LYS:HA	2.00	0.42
1:I:157:ALA:HB1	1:I:209:ILE:HG23	2.01	0.42
2:J:412:PHE:O	2:J:416:THR:OG1	2.29	0.42
2:B:263:ASP:N	2:B:263:ASP:OD1	2.49	0.42
2:D:816:ALA:O	2:D:938:THR:HG23	2.19	0.42
2:D:837:ASP:OD1	2:D:838:ALA:N	2.53	0.42
2:G:559:GLY:HA3	2:G:572:LYS:CG	2.50	0.42
2:G:656:TYR:HA	2:G:702:GLN:O	2.19	0.42
2:G:768:ASN:HB3	2:G:771:TRP:HB3	2.02	0.42
1:I:483:GLU:OE2	1:I:499:TRP:HB2	2.20	0.42
2:J:199:ASP:O	2:J:229:LYS:HG3	2.20	0.42
2:B:260:MET:HG3	2:B:910:LYS:O	2.19	0.42
2:B:311:PHE:HA	2:B:312:PRO:HD3	1.82	0.42
2:D:354:PHE:HB3	2:D:368:ARG:HG2	2.00	0.42
2:D:518:SER:HB3	2:D:548:TYR:HD2	1.84	0.42
2:D:813:PHE:CE2	2:D:890:TRP:HB2	2.51	0.42
2:J:553:ILE:HD13	2:J:553:ILE:HA	1.89	0.42
1:C:259:VAL:HG13	1:C:384:VAL:HG11	2.01	0.42
2:D:790:PHE:HD2	2:D:791:PHE:CD2	2.38	0.42
1:F:89:LEU:CD1	1:F:89:LEU:N	2.83	0.42
1:F:490:GLN:CG	2:G:797:MET:H	2.33	0.42
1:F:496:ILE:HD12	1:F:496:ILE:N	2.29	0.42
2:G:497:PRO:O	2:G:498:ASN:HB2	2.20	0.42
2:J:430:LEU:HA	2:J:430:LEU:HD12	1.57	0.42
1:A:199:ARG:NH1	1:A:498:ASN:OD1	2.49	0.42
2:B:444:MET:HE3	2:B:448:TYR:CE1	2.53	0.42
2:D:159:THR:HG21	2:D:398:SER:HB2	2.02	0.42
2:G:990:PHE:HB2	2:G:1002:GLN:OE1	2.20	0.42
2:J:813:PHE:CE1	2:J:860:VAL:HG12	2.55	0.42
2:J:896:ARG:HA	2:J:899:THR:OG1	2.20	0.42
2:B:188:SER:O	2:B:192:VAL:HG23	2.20	0.41
2:B:198:ASN:O	2:B:229:LYS:NZ	2.47	0.41
2:B:545:TYR:CD1	2:B:545:TYR:C	2.93	0.41
2:B:862:PRO:HG3	2:B:889:LYS:HB2	2.01	0.41
2:B:956:TYR:C	2:B:956:TYR:HD1	2.22	0.41
2:B:969:ILE:HG22	2:B:970:GLY:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:GLN:O	2:B:1004:PRO:HD3	2.20	0.41
2:G:168:GLY:H	2:G:725:ARG:NH1	2.18	0.41
1:I:425:GLN:HG2	1:I:445:TRP:CZ2	2.55	0.41
2:J:543:HIS:HB2	2:J:592:PHE:CD1	2.54	0.41
2:B:269:GLN:NE2	2:B:906:MET:O	2.53	0.41
2:B:730:MET:O	2:B:748:ASN:HA	2.19	0.41
2:B:878:SER:HB2	2:B:955:THR:OG1	2.19	0.41
2:B:885:TYR:HB3	2:B:947:LEU:HD12	2.02	0.41
3:H:2:SER:O	3:H:2:SER:OG	2.31	0.41
2:J:151:VAL:HG12	2:J:164:VAL:HG13	2.02	0.41
2:J:897:TYR:CD2	2:J:936:PHE:CZ	3.08	0.41
1:A:119:GLN:NE2	2:B:687:ILE:HB	2.35	0.41
1:C:173:VAL:HG12	1:C:181:LYS:HE3	2.01	0.41
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.80	0.41
1:C:398:THR:O	1:C:402:GLU:HG2	2.20	0.41
2:D:203:MET:HE2	2:D:203:MET:HB2	1.91	0.41
2:J:734:VAL:HG21	2:J:747:GLN:OE1	2.20	0.41
2:J:874:TRP:HB3	2:J:875:LYS:H	1.56	0.41
2:B:540:LEU:HD23	2:B:595:ARG:HD2	2.02	0.41
2:B:790:PHE:HZ	2:B:805:TRP:CZ3	2.38	0.41
2:D:166:ILE:HB	2:D:221:ASN:O	2.20	0.41
2:G:299:TYR:CE2	2:G:442:PRO:HD3	2.55	0.41
2:G:809:TYR:N	2:G:809:TYR:CD1	2.88	0.41
2:J:180:TYR:CD2	2:J:189:LEU:HD23	2.55	0.41
2:J:320:ASP:OD1	2:J:323:LYS:HB3	2.21	0.41
1:A:49:TYR:HB3	2:B:678:TYR:CE2	2.56	0.41
1:A:385:TYR:HD2	1:A:408:LEU:HB2	1.84	0.41
1:A:421:MET:O	1:A:425:GLN:HG3	2.21	0.41
2:B:329:ALA:HA	2:B:330:PRO:HD3	1.82	0.41
2:B:543:HIS:HB2	2:B:592:PHE:CD1	2.56	0.41
2:B:749:VAL:CG1	2:B:790:PHE:HA	2.50	0.41
2:B:809:TYR:HB3	2:B:810:PRO:CD	2.49	0.41
1:C:208:TYR:CZ	1:C:212:ARG:HD2	2.55	0.41
2:D:296:TYR:CE2	2:D:312:PRO:HG3	2.56	0.41
2:D:1012:GLY:O	2:D:1013:ILE:HG13	2.19	0.41
1:F:156:GLN:NE2	1:F:208:TYR:OH	2.53	0.41
2:G:444:MET:HE3	2:G:448:TYR:CE1	2.56	0.41
1:I:125:ASN:HD21	1:I:190:GLU:CG	2.27	0.41
1:A:45:ARG:CZ	1:A:148:PHE:HE1	2.34	0.41
1:A:62:PHE:CG	1:A:305:LEU:HD11	2.55	0.41
2:B:345:THR:HG22	2:B:377:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ILE:HD13	1:C:266:ILE:HG21	1.85	0.41
2:D:280:THR:HG23	2:D:283:LYS:NZ	2.35	0.41
2:D:329:ALA:HA	2:D:330:PRO:HD3	1.80	0.41
2:D:905:LEU:HD11	4:E:5:GLY:HA3	2.02	0.41
1:F:287:ILE:HD13	1:F:287:ILE:HG21	1.83	0.41
2:G:672:LEU:HD12	2:G:689:THR:HG21	2.03	0.41
2:J:563:ASP:OD1	2:J:563:ASP:N	2.53	0.41
2:J:926:ASP:OD1	2:J:926:ASP:N	2.54	0.41
2:J:986:LYS:HA	2:J:986:LYS:HD2	1.81	0.41
2:B:345:THR:HG22	2:B:377:SER:OG	2.20	0.41
1:C:312:GLY:O	1:C:369:LYS:HG3	2.20	0.41
2:G:254:LYS:HA	2:G:257:ASP:OD2	2.20	0.41
1:I:420:ASN:HD21	1:I:422:GLU:HB3	1.86	0.41
2:J:796:TYR:CE1	2:J:798:LEU:HD23	2.56	0.41
1:A:273:GLU:O	1:A:277:ILE:HG13	2.20	0.41
2:B:218:ARG:HH11	2:B:663:GLU:HG3	1.86	0.41
2:B:758:ASP:HB3	2:B:780:ASN:HD22	1.85	0.41
2:D:918:TRP:HE1	2:D:923:LYS:HG3	1.86	0.41
2:G:831:TYR:HD1	2:G:844:THR:HG22	1.86	0.41
1:I:286:GLU:CD	1:I:412:ARG:HH22	2.23	0.41
2:J:115:LEU:HG	2:J:116:SER:N	2.36	0.41
2:J:194:THR:HA	2:J:368:ARG:HD3	2.02	0.41
2:J:543:HIS:HD2	2:J:544:GLU:O	2.04	0.41
2:J:673:VAL:HG13	2:J:686:SER:O	2.21	0.41
2:J:851:ASP:OD1	2:J:851:ASP:N	2.37	0.41
2:J:1010:VAL:HG12	2:J:1011:ALA:N	2.36	0.41
1:A:20:CYS:SG	2:B:545:TYR:CE2	3.00	0.41
2:B:430:LEU:HD12	2:B:430:LEU:HA	1.70	0.41
2:B:487:THR:CG2	2:B:516:ASP:HB2	2.47	0.41
2:B:716:LEU:HD12	2:B:763:GLY:HA2	2.03	0.41
2:B:734:VAL:HG21	2:B:747:GLN:OE1	2.20	0.41
2:B:943:ASN:O	2:B:986:LYS:HB3	2.21	0.41
2:D:197:PRO:HA	2:D:200:PHE:CD2	2.55	0.41
2:D:410:GLY:HA3	2:D:1001:ASN:HD21	1.86	0.41
2:D:753:LYS:N	2:D:785:GLU:O	2.47	0.41
2:D:863:PRO:HD3	2:D:888:GLY:O	2.21	0.41
2:D:927:VAL:HA	2:D:928:PRO:HD3	1.94	0.41
2:D:1000:LYS:O	2:D:1002:GLN:N	2.54	0.41
4:E:2:SER:O	4:E:2:SER:OG	2.37	0.41
2:G:216:GLY:HA3	2:G:611:ARG:NH1	2.36	0.41
2:G:950:LYS:HB2	2:G:950:LYS:HE2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:ASP:OD2	1:I:440:ARG:NH1	2.53	0.41
2:J:150:GLN:HA	2:J:865:THR:HG21	2.02	0.41
2:J:242:ASN:OD1	2:J:1014:GLN:HG3	2.21	0.41
2:J:292:ALA:HB3	2:J:435:TYR:HE2	1.85	0.41
2:J:293:GLU:HB3	2:J:306:TYR:CZ	2.56	0.41
2:J:468:ALA:O	2:J:479:LYS:HA	2.21	0.41
2:J:862:PRO:HG3	2:J:889:LYS:CB	2.48	0.41
1:A:299:SER:CB	1:A:373:LYS:HD3	2.51	0.41
2:B:249:GLN:HB3	2:B:250:ILE:H	1.74	0.41
2:B:672:LEU:HB2	2:B:689:THR:HG22	2.01	0.41
2:B:952:LEU:HD23	2:B:952:LEU:HA	2.00	0.41
2:D:698:GLU:HB2	2:D:731:LEU:HD13	2.02	0.41
2:D:862:PRO:HG3	2:D:889:LYS:CB	2.51	0.41
1:F:26:PRO:HB3	2:G:667:TYR:CG	2.56	0.41
2:G:476:LEU:HA	2:G:526:GLU:O	2.21	0.41
2:G:862:PRO:HA	2:G:863:PRO:HD3	1.92	0.41
2:G:955:THR:HA	2:G:974:VAL:O	2.20	0.41
2:J:252:ASN:HB3	2:J:990:PHE:HA	2.01	0.41
1:A:397:ASP:OD1	1:A:400:THR:OG1	2.32	0.40
2:B:877:LEU:HD12	2:B:877:LEU:HA	1.82	0.40
2:B:891:MET:SD	2:B:996:GLY:N	2.87	0.40
1:C:465:ASN:CG	2:D:276:GLY:H	2.22	0.40
2:D:169:THR:O	2:D:752:MET:HE1	2.21	0.40
2:D:917:ALA:CA	2:D:927:VAL:HG13	2.42	0.40
2:G:674:THR:HG22	2:G:688:SER:HB2	2.02	0.40
1:I:438:ARG:O	1:I:442:MET:HG2	2.22	0.40
2:J:799:PRO:O	2:J:801:THR:HG23	2.21	0.40
2:J:848:TYR:HD1	2:J:849:SER:N	2.18	0.40
2:J:1012:GLY:O	2:J:1013:ILE:HG13	2.21	0.40
1:A:266:ILE:HG21	1:A:266:ILE:HD13	1.85	0.40
1:A:469:LEU:HD23	1:A:471:ALA:O	2.21	0.40
2:B:139:MET:HG3	2:B:189:LEU:HD11	2.03	0.40
1:C:182:ASP:HA	1:C:202:LYS:HE2	2.04	0.40
2:D:206:LEU:HG	2:D:223:VAL:HG23	2.03	0.40
2:D:648:SER:N	2:D:710:GLY:O	2.55	0.40
2:D:752:MET:SD	2:D:784:GLN:NE2	2.93	0.40
1:F:82:ALA:HB3	1:F:83:PRO:HD3	2.04	0.40
1:F:364:ARG:NE	1:F:370:PRO:HA	2.36	0.40
2:G:277:ASN:OD1	2:G:277:ASN:N	2.52	0.40
2:G:976:LEU:HD22	2:G:976:LEU:HA	1.83	0.40
2:J:417:MET:HE2	2:J:417:MET:HB3	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HD2	2:B:674:THR:HB	2.02	0.40
2:B:285:LYS:O	2:B:286:ASP:C	2.60	0.40
2:B:515:ARG:HE	2:B:515:ARG:HB2	1.73	0.40
2:B:898:PHE:CD1	2:B:905:LEU:HD22	2.56	0.40
2:D:153:THR:OG1	2:D:162:ALA:HB2	2.21	0.40
1:F:191:TYR:CE1	1:F:193:PRO:HG3	2.56	0.40
2:G:411:THR:HB	2:G:990:PHE:CE2	2.56	0.40
2:J:329:ALA:HB1	2:J:357:GLU:HG2	2.03	0.40
2:J:567:LEU:HD12	2:J:567:LEU:HA	1.89	0.40
2:B:157:ASP:CG	2:B:159:THR:HG22	2.42	0.40
2:B:472:PRO:HD2	2:B:476:LEU:HD13	2.03	0.40
2:B:543:HIS:CD2	5:B:1101:5PL:OCO	2.74	0.40
2:D:672:LEU:H	2:D:689:THR:CG2	2.35	0.40
2:G:159:THR:HG21	2:G:398:SER:HB3	2.03	0.40
2:G:241:PHE:HD2	2:G:1015:LEU:HB2	1.85	0.40
2:G:411:THR:O	2:G:414:VAL:HG22	2.22	0.40
2:G:973:ARG:HD3	2:G:1014:GLN:OE1	2.21	0.40
2:G:973:ARG:HH11	2:G:973:ARG:HD2	1.74	0.40
2:J:171:SER:HB2	2:J:698:GLU:OE2	2.22	0.40
2:J:280:THR:O	2:J:284:VAL:HG23	2.21	0.40
2:J:510:ARG:HD3	2:J:512:ARG:CZ	2.51	0.40
1:A:337:ARG:HD3	1:A:412:ARG:HD2	2.04	0.40
4:E:6:GLY:O	4:E:7:ASN:HB3	2.20	0.40
1:F:165:ASP:CG	1:F:440:ARG:NH1	2.75	0.40
1:F:382:ALA:HB1	1:F:431:GLU:HG2	2.03	0.40
2:G:415:LEU:HD11	2:G:990:PHE:CE2	2.56	0.40
2:G:669:HIS:CE1	2:G:670:GLN:HG3	2.57	0.40
2:G:681:ASP:OD2	1:I:367:GLN:HB2	2.22	0.40
2:G:915:LEU:HA	2:G:915:LEU:HD23	1.77	0.40
2:J:156:GLY:HA3	2:J:1004:PRO:O	2.21	0.40
2:J:415:LEU:HD11	2:J:990:PHE:HE2	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:342:SER:OG	2:D:342:SER:OG[3_655]	1.97	0.23
2:B:342:SER:OG	2:B:342:SER:OG[3_755]	2.09	0.11



## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	480/488 (98%)	439 (92%)	38 (8%)	3 (1%)	25	59
1	C	480/488 (98%)	444 (92%)	33 (7%)	3 (1%)	25	59
1	F	480/488 (98%)	444 (92%)	33 (7%)	3 (1%)	25	59
1	I	480/488 (98%)	444 (92%)	33 (7%)	3 (1%)	25	59
2	B	896/997 (90%)	760 (85%)	118 (13%)	18 (2%)	7	33
2	D	896/997 (90%)	760 (85%)	117 (13%)	19 (2%)	7	32
2	G	896/997 (90%)	768 (86%)	111 (12%)	17 (2%)	8	34
2	J	896/997 (90%)	759 (85%)	118 (13%)	19 (2%)	7	32
3	H	11/13 (85%)	7 (64%)	4 (36%)	0	100	100
3	P	11/13 (85%)	7 (64%)	4 (36%)	0	100	100
4	E	11/13 (85%)	7 (64%)	3 (27%)	1 (9%)	1	5
4	K	11/13 (85%)	6 (54%)	4 (36%)	1 (9%)	1	5
All	All	5548/5992 (93%)	4845 (87%)	616 (11%)	87 (2%)	9	37

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	642	GLN
2	B	712	PHE
2	B	809	TYR
2	B	874	TRP
2	D	532	ASP
2	D	533	GLU
2	D	642	GLN
2	D	712	PHE
2	D	809	TYR
2	G	276	GLY
2	G	642	GLN
2	G	712	PHE

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Mol	Chain	Res	Type
2	G	809	TYR
2	G	874	TRP
2	J	533	GLU
2	J	642	GLN
2	J	712	PHE
2	J	809	TYR
2	J	874	TRP
2	B	531	ILE
2	B	532	ASP
2	B	533	GLU
2	B	808	GLY
2	B	810	PRO
2	D	810	PRO
2	D	874	TRP
1	F	21	GLU
2	G	532	ASP
2	G	533	GLU
2	G	800	ASN
2	G	810	PRO
1	I	21	GLU
2	J	532	ASP
2	J	800	ASN
2	J	810	PRO
2	B	997	ASN
1	C	178	SER
2	G	997	ASN
2	J	278	ASN
2	B	474	LYS
2	B	664	ILE
2	D	664	ILE
2	D	800	ASN
2	D	914	LEU
2	D	997	ASN
2	G	664	ILE
2	G	914	LEU
2	G	1001	ASN
2	J	664	ILE
2	J	914	LEU
1	A	399	PRO
1	A	420	ASN
1	A	471	ALA
2	B	873	SER

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Mol	Chain	Res	Type
2	B	1001	ASN
1	C	174	THR
2	D	474	LYS
2	D	969	ILE
2	D	1001	ASN
1	F	171	GLU
1	F	174	THR
2	G	531	ILE
2	J	531	ILE
4	K	2	SER
2	B	969	ILE
2	D	133	LYS
4	E	2	SER
2	G	969	ILE
1	I	178	SER
2	J	133	LYS
2	J	969	ILE
2	J	472	PRO
2	D	262	GLY
2	D	531	ILE
2	G	133	LYS
2	J	216	GLY
2	J	262	GLY
2	J	863	PRO
2	B	133	LYS
2	B	505	PRO
2	D	312	PRO
2	D	472	PRO
1	I	399	PRO
2	J	692	ASN
2	B	692	ASN
1	C	399	PRO
2	G	472	PRO

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	402/408 (98%)	399 (99%)	3 (1%)	84	92
1	C	402/408 (98%)	398 (99%)	4 (1%)	76	87
1	F	402/408 (98%)	399 (99%)	3 (1%)	84	92
1	I	402/408 (98%)	398 (99%)	4 (1%)	76	87
2	B	752/832 (90%)	710 (94%)	42 (6%)	21	52
2	D	752/832 (90%)	715 (95%)	37 (5%)	25	57
2	G	752/832 (90%)	714 (95%)	38 (5%)	24	55
2	J	752/832 (90%)	710 (94%)	42 (6%)	21	52
3	H	8/8 (100%)	7 (88%)	1 (12%)	4	18
3	P	8/8 (100%)	5 (62%)	3 (38%)	0	0
4	E	7/7 (100%)	5 (71%)	2 (29%)	0	1
4	K	7/7 (100%)	6 (86%)	1 (14%)	3	14
All	All	4646/4990 (93%)	4466 (96%)	180 (4%)	32	62

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	MET
1	A	369	LYS
1	A	379	PHE
2	B	115	LEU
2	B	132	GLU
2	B	137	ASN
2	B	230	LYS
2	B	251	LEU
2	B	256	LEU
2	B	265	LEU
2	B	266	LEU
2	B	267	ASP
2	B	277	ASN
2	B	300	ASP
2	B	302	LEU
2	B	343	GLN
2	B	375	PHE
2	B	384	LYS
2	B	396	ARG
2	B	449	PHE
2	B	465	ASN
2	B	476	LEU

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Mol	Chain	Res	Type
2	B	527	TYR
2	B	533	GLU
2	B	545	TYR
2	B	563	ASP
2	B	595	ARG
2	B	600	PHE
2	B	608	PHE
2	B	623	ARG
2	B	629	SER
2	B	647	LEU
2	B	649	ASP
2	B	766	TYR
2	B	767	GLN
2	B	848	TYR
2	B	855	ARG
2	B	857	ASP
2	B	874	TRP
2	B	901	ASN
2	B	956	TYR
2	B	979	ARG
2	B	981	LEU
2	B	997	ASN
2	B	1003	TYR
3	P	8	SER
3	P	10	ARG
3	P	12	SER
1	C	72	CYS
1	C	182	ASP
1	C	369	LYS
1	C	379	PHE
2	D	137	ASN
2	D	251	LEU
2	D	256	LEU
2	D	266	LEU
2	D	279	GLN
2	D	289	LEU
2	D	302	LEU
2	D	343	GLN
2	D	375	PHE
2	D	396	ARG
2	D	420	TYR
2	D	449	PHE

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Mol	Chain	Res	Type
2	D	465	ASN
2	D	476	LEU
2	D	527	TYR
2	D	533	GLU
2	D	545	TYR
2	D	563	ASP
2	D	595	ARG
2	D	600	PHE
2	D	603	TRP
2	D	608	PHE
2	D	616	SER
2	D	647	LEU
2	D	729	ASP
2	D	766	TYR
2	D	835	GLN
2	D	855	ARG
2	D	894	ASN
2	D	905	LEU
2	D	941	LEU
2	D	956	TYR
2	D	979	ARG
2	D	981	LEU
2	D	997	ASN
2	D	1000	LYS
2	D	1003	TYR
4	E	8	SER
4	E	10	ARG
1	F	182	ASP
1	F	369	LYS
1	F	379	PHE
2	G	132	GLU
2	G	137	ASN
2	G	203	MET
2	G	210	SER
2	G	251	LEU
2	G	256	LEU
2	G	263	ASP
2	G	266	LEU
2	G	289	LEU
2	G	302	LEU
2	G	343	GLN
2	G	375	PHE

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Mol	Chain	Res	Type
2	G	396	ARG
2	G	449	PHE
2	G	453	ARG
2	G	465	ASN
2	G	527	TYR
2	G	533	GLU
2	G	543	HIS
2	G	545	TYR
2	G	563	ASP
2	G	595	ARG
2	G	600	PHE
2	G	623	ARG
2	G	629	SER
2	G	647	LEU
2	G	649	ASP
2	G	652	LEU
2	G	767	GLN
2	G	835	GLN
2	G	848	TYR
2	G	855	ARG
2	G	894	ASN
2	G	941	LEU
2	G	956	TYR
2	G	979	ARG
2	G	981	LEU
2	G	1003	TYR
3	H	10	ARG
1	I	80	SER
1	I	182	ASP
1	I	369	LYS
1	I	379	PHE
2	J	115	LEU
2	J	132	GLU
2	J	137	ASN
2	J	210	SER
2	J	232	LYS
2	J	233	MET
2	J	251	LEU
2	J	271	LYS
2	J	289	LEU
2	J	300	ASP
2	J	302	LEU

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Mol	Chain	Res	Type
2	J	343	GLN
2	J	375	PHE
2	J	382	TRP
2	J	384	LYS
2	J	396	ARG
2	J	420	TYR
2	J	444	MET
2	J	449	PHE
2	J	453	ARG
2	J	476	LEU
2	J	493	SER
2	J	527	TYR
2	J	533	GLU
2	J	537	LEU
2	J	545	TYR
2	J	563	ASP
2	J	595	ARG
2	J	600	PHE
2	J	608	PHE
2	J	623	ARG
2	J	629	SER
2	J	647	LEU
2	J	729	ASP
2	J	766	TYR
2	J	848	TYR
2	J	855	ARG
2	J	894	ASN
2	J	956	TYR
2	J	979	ARG
2	J	997	ASN
2	J	1003	TYR
4	K	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	380	ASN
2	B	461	GLN
2	B	754	ASN
2	B	782	ASN
2	B	935	GLN
2	B	939	HIS

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Mol	Chain	Res	Type
2	B	1002	GLN
2	D	242	ASN
2	D	388	ASN
2	D	463	ASN
2	D	748	ASN
2	D	754	ASN
2	D	782	ASN
2	D	932	GLN
2	D	1014	GLN
2	G	380	ASN
2	G	748	ASN
2	G	754	ASN
2	G	782	ASN
1	I	125	ASN
2	J	380	ASN
2	J	543	HIS
2	J	748	ASN
2	J	754	ASN
2	J	782	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

3 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	$\# Z  > 2$
5	5PL	B	1101	1	19,19,85	1.80	5 (26%)	21,21,101	1.81	4 (19%)
6	C8E	B	1102	-	12,12,20	0.43	0	11,11,19	0.56	0
6	C8E	B	1103	-	12,12,20	0.42	0	11,11,19	0.70	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
5	5PL	B	1101	1	-	9/20/20/107	-
6	C8E	B	1102	-	-	5/10/10/18	-
6	C8E	B	1103	-	-	6/10/10/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1101	5PL	OCL-CBL	4.13	1.45	1.33
5	B	1101	5PL	OCK-CBH	-3.41	1.41	1.47
5	B	1101	5PL	OCK-CBU	3.12	1.43	1.34
5	B	1101	5PL	CBM-CBL	2.33	1.57	1.50
5	B	1101	5PL	CBI-CBH	2.25	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	5PL	OCK-CBU-CBV	4.36	120.91	111.50
5	B	1101	5PL	OCL-CBL-CBM	3.59	123.17	111.91
5	B	1101	5PL	CBH-OCK-CBU	-3.12	113.86	117.88
5	B	1101	5PL	OCK-CBH-CBI	2.59	112.13	106.13

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	5PL	CAW-CBH-CBI-OCL
5	B	1101	5PL	OCK-CBH-CBI-OCL

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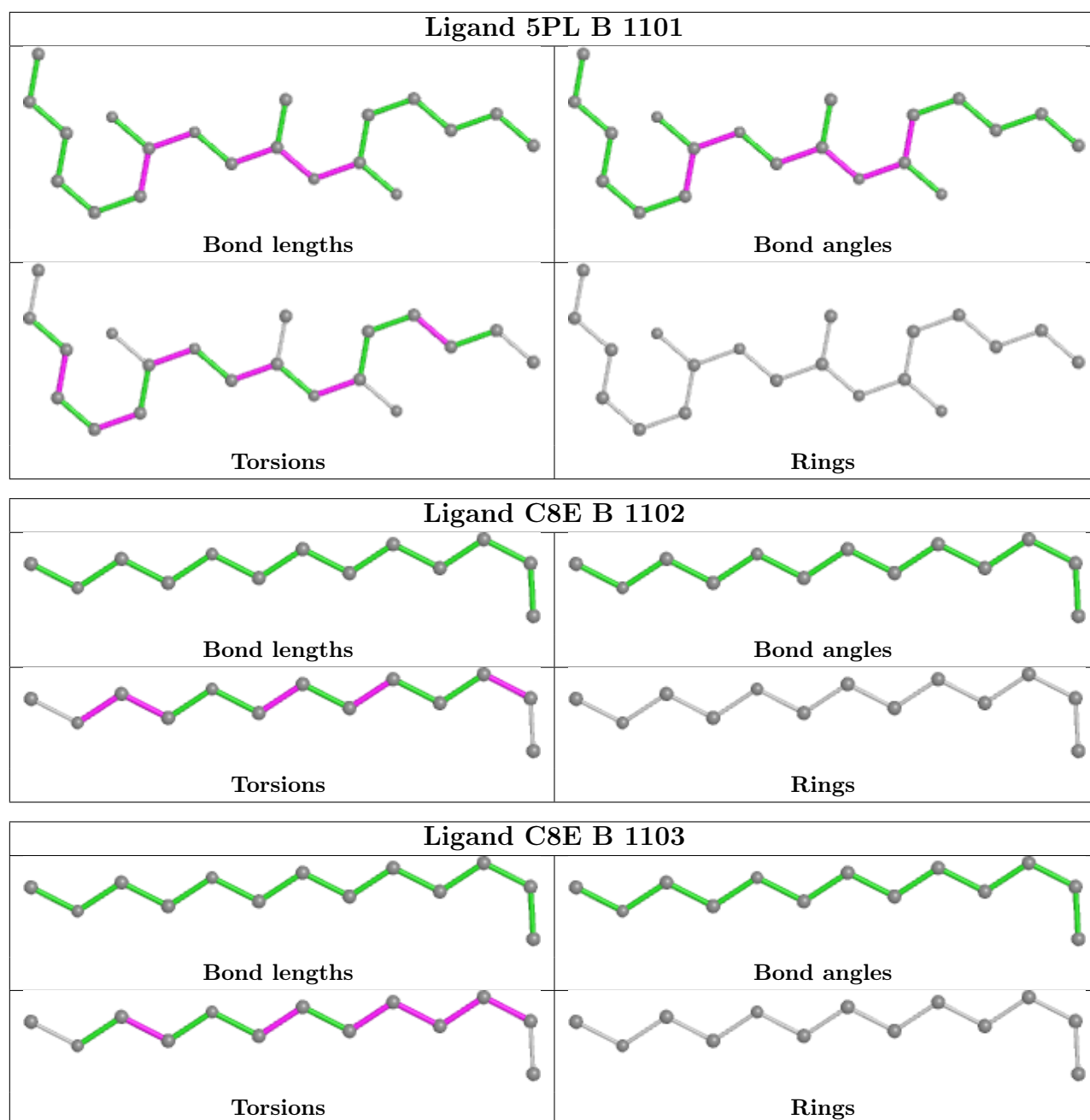
Mol	Chain	Res	Type	Atoms
5	B	1101	5PL	CBV-CBU-OCK-CBH
5	B	1101	5PL	OCN-CBU-OCK-CBH
5	B	1101	5PL	CBM-CBL-OCL-CBI
5	B	1101	5PL	OCO-CBL-OCL-CBI
6	B	1102	C8E	O9-C10-C11-O12
5	B	1101	5PL	CBL-CBM-CBN-CBO
6	B	1103	C8E	C2-C3-C4-C5
6	B	1102	C8E	C4-C5-C6-C7
6	B	1103	C8E	C3-C4-C5-C6
6	B	1103	C8E	C1-C2-C3-C4
6	B	1102	C8E	C10-C11-O12-C13
6	B	1103	C8E	C6-C7-C8-O9
6	B	1102	C8E	C6-C7-C8-O9
6	B	1103	C8E	O9-C10-C11-O12
6	B	1103	C8E	C4-C5-C6-C7
5	B	1101	5PL	CBN-CBO-CBP-CAA
5	B	1101	5PL	CBV-CBW-CBX-CBY
6	B	1102	C8E	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	5PL	4	0
6	B	1102	C8E	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	482/488 (98%)	0.13	4 (0%) 86 89	40, 63, 94, 133	0
1	C	482/488 (98%)	0.00	1 (0%) 95 97	44, 67, 100, 132	0
1	F	482/488 (98%)	0.04	3 (0%) 89 92	48, 76, 105, 146	0
1	I	482/488 (98%)	0.53	44 (9%) 9 12	68, 115, 152, 186	0
2	B	900/997 (90%)	0.26	19 (2%) 63 67	45, 84, 132, 214	0
2	D	900/997 (90%)	0.63	94 (10%) 6 8	56, 115, 180, 265	0
2	G	900/997 (90%)	0.59	87 (9%) 7 10	53, 115, 182, 253	0
2	J	900/997 (90%)	0.47	58 (6%) 19 23	56, 112, 170, 233	0
3	H	13/13 (100%)	0.64	1 (7%) 13 16	94, 107, 140, 141	0
3	P	13/13 (100%)	0.37	1 (7%) 13 16	74, 93, 108, 121	0
4	E	13/13 (100%)	0.44	1 (7%) 13 16	88, 100, 137, 152	0
4	K	13/13 (100%)	0.73	1 (7%) 13 16	102, 120, 133, 153	0
All	All	5580/5992 (93%)	0.38	314 (5%) 24 28	40, 98, 161, 265	0

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	315	PHE	6.2
1	I	236	TYR	6.0
2	D	132	GLU	5.7
2	D	116	SER	5.3
2	D	536	ASP	5.2
2	D	216	GLY	5.0
1	I	324	PHE	5.0
2	G	236	ARG	4.9
2	J	116	SER	4.9
2	D	115	LEU	4.9
2	D	347	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
2	G	821	ILE	4.8
2	G	614	GLN	4.6
2	G	116	SER	4.5
2	D	539	ALA	4.3
2	B	766	TYR	4.3
2	D	344	GLY	4.2
2	J	821	ILE	4.2
2	G	590	LEU	4.2
2	D	530	SER	4.2
2	G	615	SER	4.2
2	B	216	GLY	4.2
2	G	875	LYS	4.2
4	K	13	GLY	4.2
2	G	831	TYR	4.1
2	G	640	PHE	4.1
2	G	823	LYS	4.1
2	J	914	LEU	4.1
2	D	599	GLY	4.0
1	I	167	PHE	4.0
2	D	700	GLN	3.9
2	D	379	ILE	3.9
2	G	872	ALA	3.8
2	J	528	LYS	3.8
2	G	377	SER	3.8
1	I	252	ALA	3.7
2	D	338	PHE	3.7
1	I	321	ALA	3.7
2	D	660	GLY	3.7
2	D	542	GLY	3.7
2	B	767	GLN	3.7
1	I	480	TYR	3.7
2	G	235	GLU	3.6
2	G	115	LEU	3.6
2	G	589	TYR	3.6
2	D	133	LYS	3.5
2	G	700	GLN	3.5
2	G	132	GLU	3.5
2	J	420	TYR	3.5
1	I	185	VAL	3.5
2	J	535	HIS	3.4
2	G	985	THR	3.4
2	J	926	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	345	THR	3.4
1	I	419	VAL	3.4
1	I	388	LEU	3.4
2	D	341	GLY	3.4
2	B	275	TRP	3.4
2	D	215	TYR	3.4
2	D	117	THR	3.3
2	G	774	TYR	3.3
2	J	964	ALA	3.3
2	J	132	GLU	3.3
2	D	375	PHE	3.3
2	J	538	THR	3.3
2	D	865	THR	3.3
2	D	766	TYR	3.3
1	I	460	LEU	3.2
1	I	392	ALA	3.2
2	G	347	TYR	3.2
2	G	313	VAL	3.2
2	G	828	GLN	3.2
2	G	613	ASP	3.1
2	D	661	ASN	3.1
2	B	964	ALA	3.1
2	G	232	LYS	3.1
2	D	640	PHE	3.1
2	J	909	ASN	3.1
2	G	345	THR	3.1
2	G	214	ILE	3.1
2	D	123	ALA	3.1
2	G	723	TYR	3.1
2	G	964	ALA	3.1
2	D	1010	VAL	3.0
2	D	704	ASN	3.0
2	G	338	PHE	3.0
2	G	588	ALA	3.0
2	D	343	GLN	3.0
2	D	385	VAL	3.0
2	J	768	ASN	3.0
2	B	132	GLU	3.0
1	I	342	ILE	3.0
1	I	131	LEU	2.9
2	J	965	GLY	2.9
2	G	312	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	J	115	LEU	2.9
2	G	262	GLY	2.9
2	J	284	VAL	2.9
2	D	342	SER	2.9
2	G	783	ARG	2.9
2	G	167	HIS	2.9
1	I	257	LYS	2.9
1	I	416	VAL	2.9
2	D	377	SER	2.8
2	J	275	TRP	2.8
2	D	591	SER	2.8
2	D	381	GLU	2.8
2	D	130	LEU	2.8
2	G	865	THR	2.8
2	G	813	PHE	2.8
2	D	374	ASN	2.8
1	I	322	VAL	2.8
2	D	926	ASP	2.8
2	G	375	PHE	2.8
1	I	498	ASN	2.8
2	G	784	GLN	2.8
2	G	877	LEU	2.8
2	J	772	ASN	2.8
2	D	638	ASN	2.8
2	G	420	TYR	2.7
2	D	958	LEU	2.7
2	G	873	SER	2.7
1	I	128	GLU	2.7
2	G	659	THR	2.7
2	B	115	LEU	2.7
2	G	790	PHE	2.7
2	D	148	GLY	2.7
1	I	67	GLN	2.7
1	I	171	GLU	2.7
2	J	313	VAL	2.7
2	D	598	TYR	2.7
2	D	985	THR	2.7
1	I	169	PHE	2.7
2	J	356	GLN	2.7
2	D	990	PHE	2.7
2	J	636	ILE	2.7
1	I	110	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	340	GLY	2.6
1	I	352	TYR	2.6
2	D	763	GLY	2.6
2	D	214	ILE	2.6
2	J	940	LEU	2.6
2	J	537	LEU	2.6
2	B	768	ASN	2.6
1	I	482	TRP	2.6
1	I	464	ALA	2.6
2	D	964	ALA	2.6
2	G	207	LYS	2.6
2	D	204	SER	2.6
2	D	783	ARG	2.6
2	D	134	PRO	2.6
2	B	660	GLY	2.5
2	J	216	GLY	2.5
2	D	537	LEU	2.5
2	D	611	ARG	2.5
2	G	782	ASN	2.5
1	I	87	TRP	2.5
2	J	925	THR	2.5
2	G	536	ASP	2.5
2	G	876	GLY	2.5
2	D	309	THR	2.5
1	I	254	ALA	2.5
2	G	608	PHE	2.5
2	J	117	THR	2.5
1	I	259	VAL	2.5
2	J	310	LEU	2.5
2	D	613	ASP	2.5
2	G	914	LEU	2.4
1	I	384	VAL	2.4
2	J	697	TRP	2.4
2	G	842	LYS	2.4
2	J	534	LYS	2.4
2	G	342	SER	2.4
2	G	755	THR	2.4
2	G	134	PRO	2.4
1	I	385	TYR	2.4
2	G	526	GLU	2.4
2	J	311	PHE	2.4
2	B	379	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	121	SER	2.4
2	G	311	PHE	2.4
2	G	754	ASN	2.4
2	G	612	ASN	2.4
2	J	421	TYR	2.3
2	J	595	ARG	2.3
2	G	830	TRP	2.3
2	J	910	LYS	2.3
1	A	480	TYR	2.3
1	I	256	ALA	2.3
2	G	525	ALA	2.3
2	G	833	PRO	2.3
2	J	781	TYR	2.3
2	G	958	LEU	2.3
2	G	638	ASN	2.3
2	D	421	TYR	2.3
2	D	703	PHE	2.3
2	D	275	TRP	2.3
2	B	421	TYR	2.3
2	D	775	ALA	2.3
2	D	821	ILE	2.3
2	B	944	ALA	2.3
2	J	963	PHE	2.3
1	F	464	ALA	2.3
1	I	484	PHE	2.3
2	D	315	PHE	2.3
2	G	260	MET	2.3
2	D	636	ILE	2.3
2	D	529	PHE	2.3
2	B	535	HIS	2.3
2	D	266	LEU	2.3
2	D	1011	ALA	2.3
2	J	134	PRO	2.3
3	H	13	GLY	2.3
2	D	310	LEU	2.3
2	G	959	PRO	2.3
4	E	13	GLY	2.3
1	I	125	ASN	2.3
1	I	127	THR	2.3
2	J	306	TYR	2.3
2	D	373	LEU	2.2
2	D	813	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	379	ILE	2.2
2	J	600	PHE	2.2
2	D	118	VAL	2.2
1	F	24	ARG	2.2
2	G	809	TYR	2.2
2	J	210	SER	2.2
2	D	987	TYR	2.2
2	J	774	TYR	2.2
2	D	223	VAL	2.2
2	D	755	THR	2.2
2	G	343	GLN	2.2
2	G	133	LYS	2.2
2	G	149	MET	2.2
2	J	875	LYS	2.2
2	D	262	GLY	2.2
2	B	354	PHE	2.2
2	D	200	PHE	2.2
2	D	538	THR	2.2
2	D	236	ARG	2.2
2	J	874	TRP	2.2
2	J	347	TYR	2.2
2	G	529	PHE	2.2
1	I	449	ASN	2.2
2	B	277	ASN	2.2
1	I	462	GLY	2.2
2	D	232	LYS	2.2
2	G	765	ILE	2.2
2	J	260	MET	2.2
2	G	816	ALA	2.1
2	J	539	ALA	2.1
2	J	598	TYR	2.1
1	I	323	PRO	2.1
2	J	235	GLU	2.1
2	D	540	LEU	2.1
2	D	155	SER	2.1
2	J	966	GLN	2.1
2	G	962	LEU	2.1
2	B	661	ASN	2.1
2	D	420	TYR	2.1
2	J	766	TYR	2.1
2	B	536	ASP	2.1
2	G	822	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	131	ALA	2.1
2	D	211	ALA	2.1
2	G	598	TYR	2.1
2	G	963	PHE	2.1
2	J	274	PHE	2.1
1	I	261	ASP	2.1
2	D	296	TYR	2.1
2	D	634	PHE	2.1
2	J	529	PHE	2.1
2	G	284	VAL	2.1
2	D	764	THR	2.1
3	P	3	THR	2.1
2	G	722	PHE	2.1
2	G	587	TYR	2.1
2	G	918	TRP	2.1
2	D	828	GLN	2.1
2	J	894	ASN	2.1
1	I	71	TYR	2.1
2	B	347	TYR	2.1
1	C	328	VAL	2.1
1	I	253	ALA	2.1
2	J	948	ARG	2.1
1	A	462	GLY	2.1
1	A	482	TRP	2.1
2	D	356	GLN	2.1
2	G	356	GLN	2.1
2	D	245	TYR	2.1
2	J	588	ALA	2.1
2	J	845	THR	2.1
2	D	833	PRO	2.1
2	D	716	LEU	2.1
1	I	255	ASP	2.1
2	D	946	PHE	2.0
2	G	623	ARG	2.0
1	I	132	GLN	2.0
2	B	770	ASP	2.0
2	G	961	SER	2.0
2	J	613	ASP	2.0
2	G	315	PHE	2.0
2	D	313	VAL	2.0
2	G	421	TYR	2.0
2	G	829	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	272	ALA	2.0
2	G	946	PHE	2.0
1	F	22	LEU	2.0
1	I	101	ASP	2.0
2	J	625	ALA	2.0
1	I	485	PRO	2.0
2	D	149	MET	2.0
1	A	328	VAL	2.0
2	D	979	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

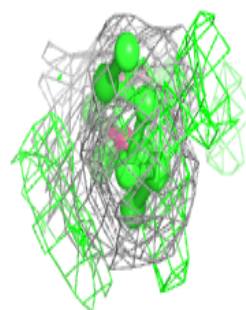
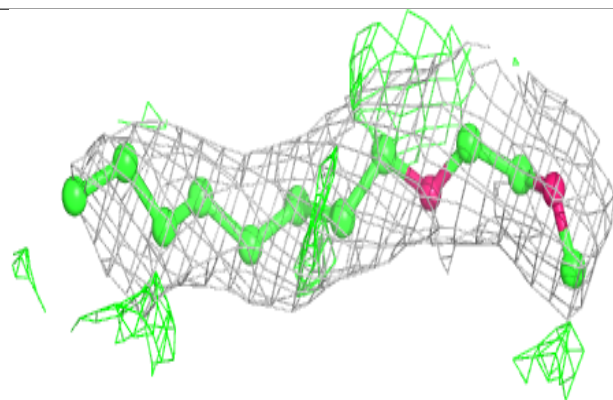
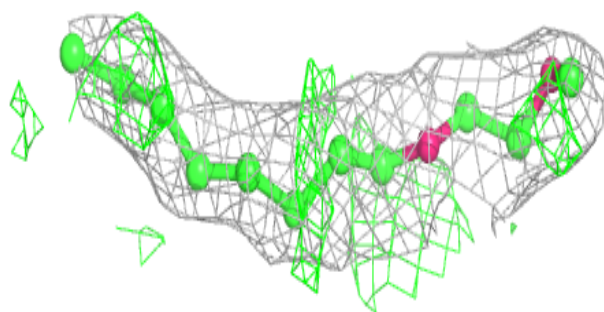
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	C8E	B	1102	13/21	0.84	0.31	66,87,110,110	0
5	5PL	B	1101	20/85	0.87	0.26	87,90,99,100	0
6	C8E	B	1103	13/21	0.93	0.29	36,53,89,92	0

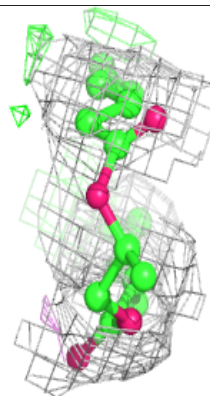
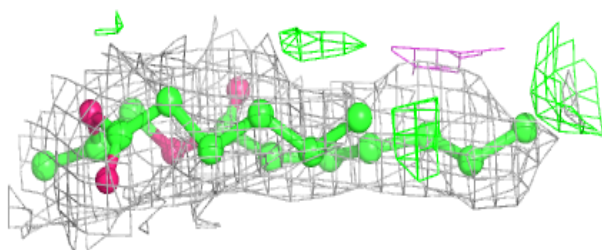
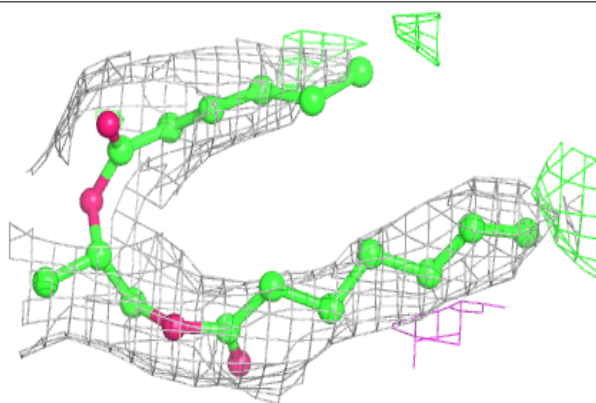
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

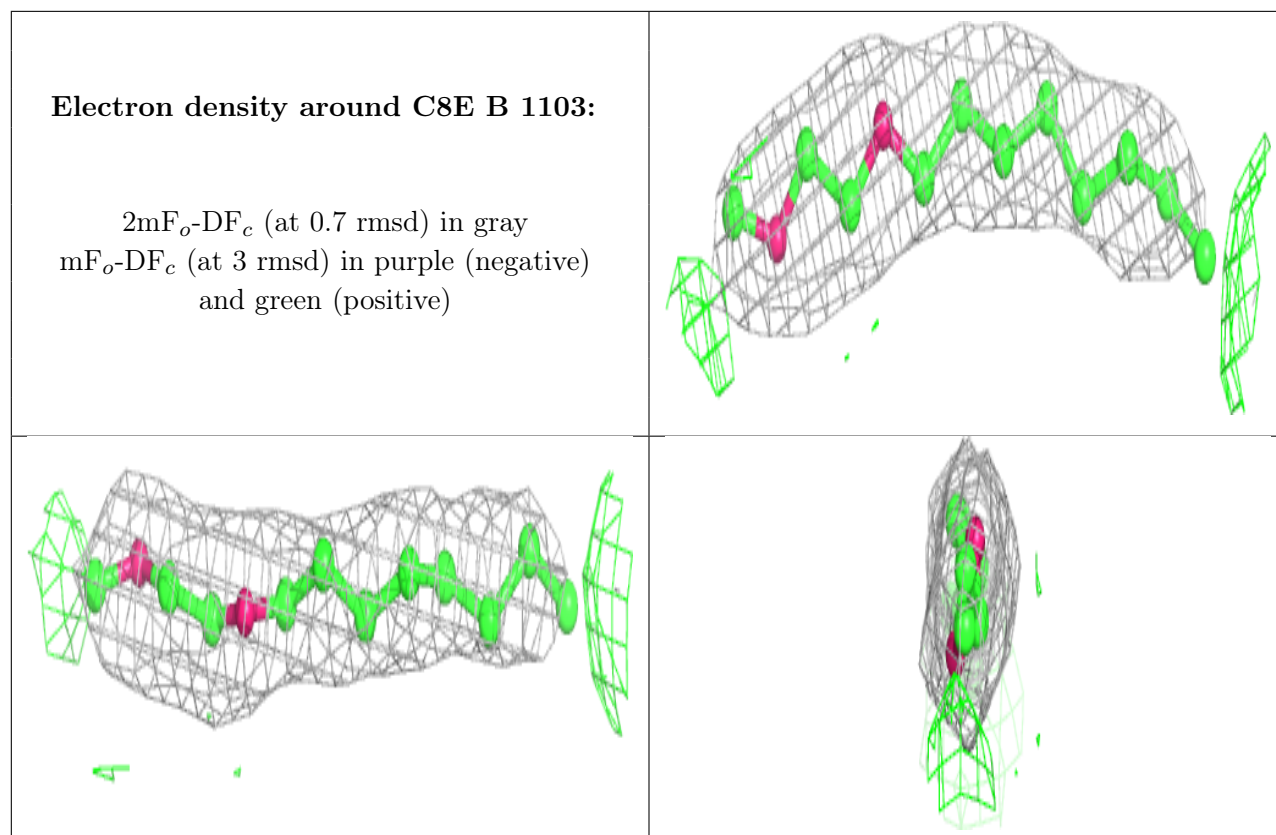
**Electron density around C8E B 1102:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 5PL B 1101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.