



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 12:39 PM EDT

PDB ID : 2QO3
Title : Crystal Structure of [KS3][AT3] didomain from module 3 of 6-deoxyerthronolide B synthase
Authors : Khosla, C.; Cane, E.D.; Tang, Y.; Chen, Y.A.; Kim, C.Y.
Deposited on : 2007-07-19
Resolution : 2.59 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

A user guide is available at

<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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

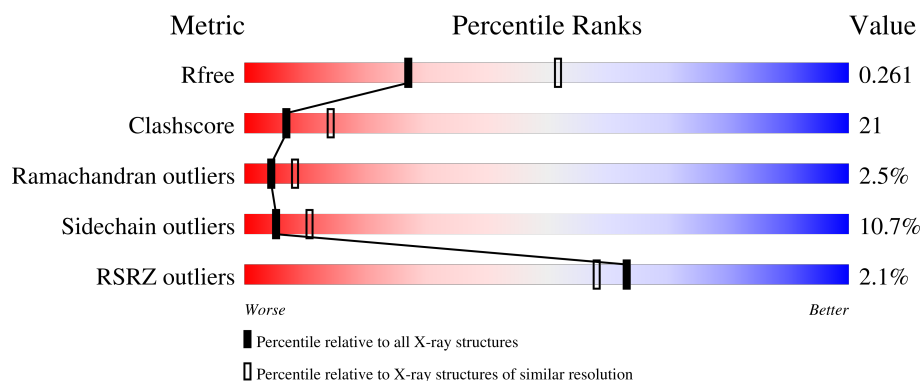
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.59 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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 ≥ 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	915	 2% 60% 30% 5% • 5%
1	B	915	 2% 61% 27% 6% • 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	950	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13148 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 EryAII Erythromycin polyketide synthase modules 3 and 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	0	0	0
			6449	4003	1178	1250	18			
1	B	873	Total	C	N	O	S	0	0	0
			6479	4020	1185	1256	18			

There are 38 discrepancies between the modelled and reference sequences:

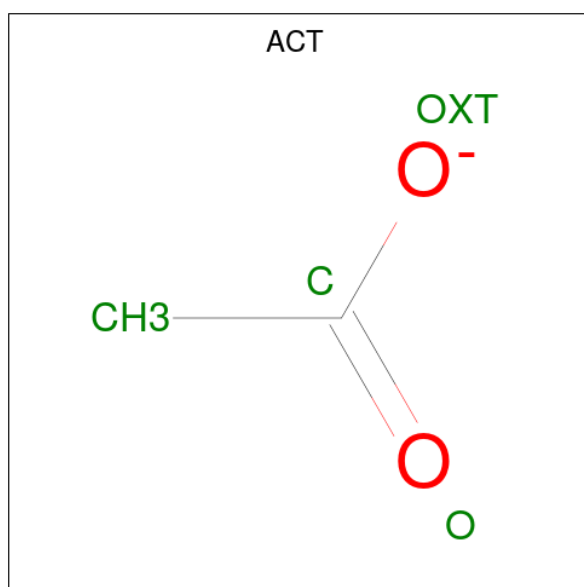
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP A4F7P0
A	923	SER	-	expression tag	UNP A4F7P0
A	924	SER	-	expression tag	UNP A4F7P0
A	925	SER	-	expression tag	UNP A4F7P0
A	926	VAL	-	expression tag	UNP A4F7P0
A	927	ASP	-	expression tag	UNP A4F7P0
A	928	LYS	-	expression tag	UNP A4F7P0
A	929	LEU	-	expression tag	UNP A4F7P0
A	930	ALA	-	expression tag	UNP A4F7P0
A	931	ALA	-	expression tag	UNP A4F7P0
A	932	ALA	-	expression tag	UNP A4F7P0
A	933	LEU	-	expression tag	UNP A4F7P0
A	934	GLU	-	expression tag	UNP A4F7P0
A	935	HIS	-	expression tag	UNP A4F7P0
A	936	HIS	-	expression tag	UNP A4F7P0
A	937	HIS	-	expression tag	UNP A4F7P0
A	938	HIS	-	expression tag	UNP A4F7P0
A	939	HIS	-	expression tag	UNP A4F7P0
A	940	HIS	-	expression tag	UNP A4F7P0
B	26	MET	-	initiating methionine	UNP A4F7P0
B	923	SER	-	expression tag	UNP A4F7P0
B	924	SER	-	expression tag	UNP A4F7P0
B	925	SER	-	expression tag	UNP A4F7P0
B	926	VAL	-	expression tag	UNP A4F7P0
B	927	ASP	-	expression tag	UNP A4F7P0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	928	LYS	-	expression tag	UNP A4F7P0
B	929	LEU	-	expression tag	UNP A4F7P0
B	930	ALA	-	expression tag	UNP A4F7P0
B	931	ALA	-	expression tag	UNP A4F7P0
B	932	ALA	-	expression tag	UNP A4F7P0
B	933	LEU	-	expression tag	UNP A4F7P0
B	934	GLU	-	expression tag	UNP A4F7P0
B	935	HIS	-	expression tag	UNP A4F7P0
B	936	HIS	-	expression tag	UNP A4F7P0
B	937	HIS	-	expression tag	UNP A4F7P0
B	938	HIS	-	expression tag	UNP A4F7P0
B	939	HIS	-	expression tag	UNP A4F7P0
B	940	HIS	-	expression tag	UNP A4F7P0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

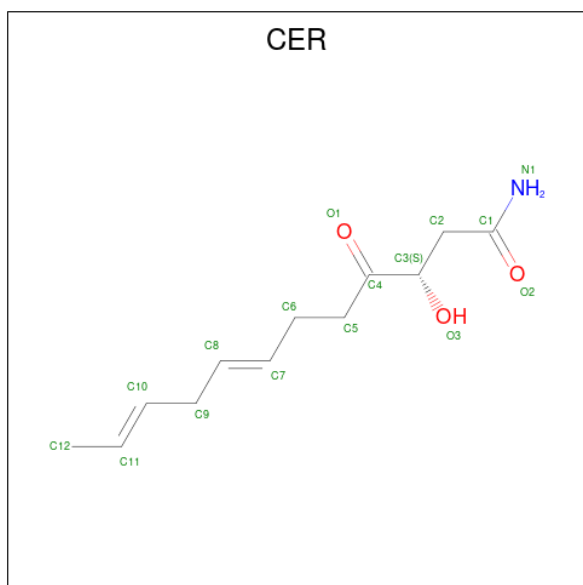


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: C₁₂H₁₉NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	B	1	Total C N O 8 4 1 3	0	0

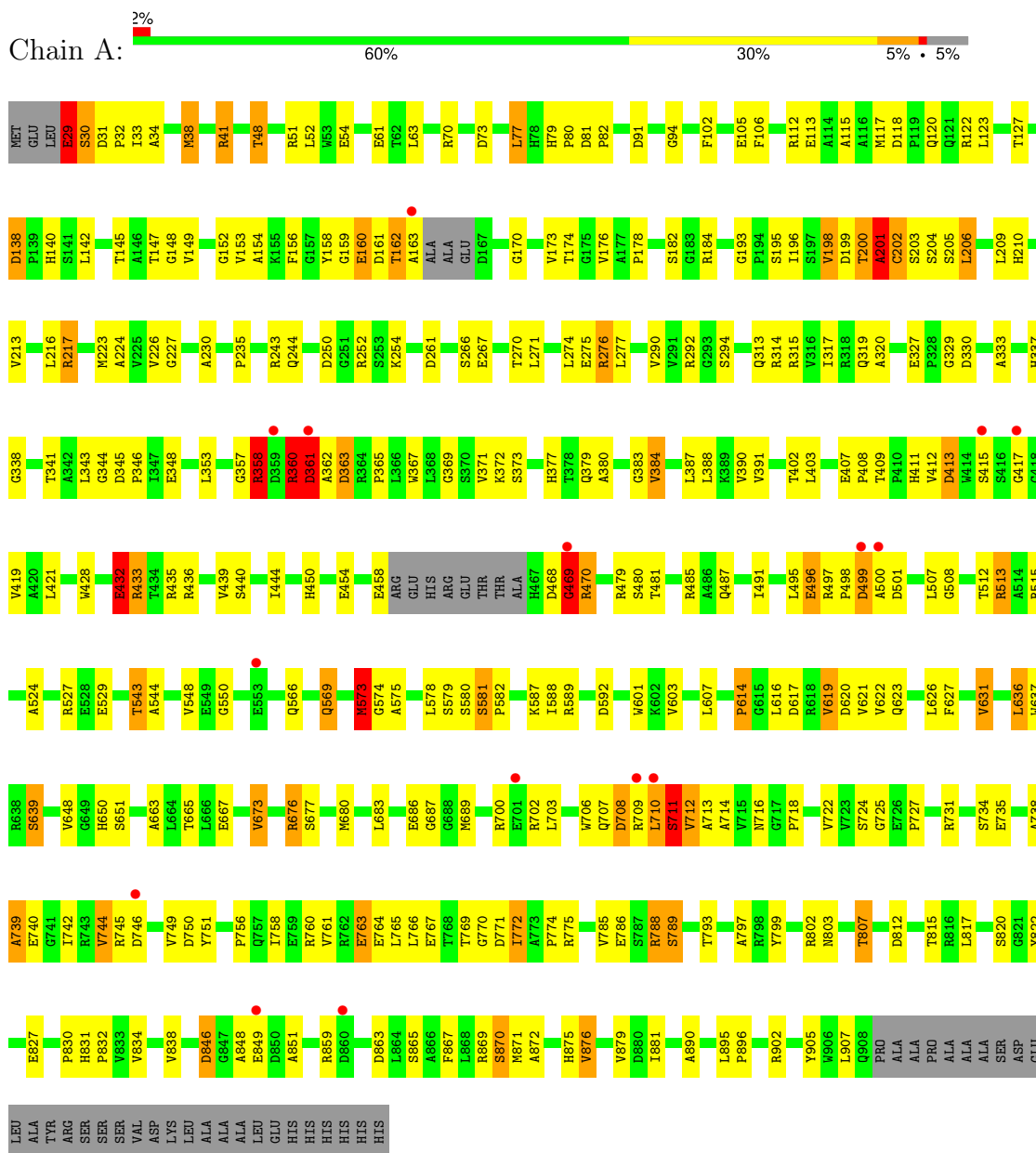
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	95	Total O 95 95	0	0
5	B	99	Total O 99 99	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: EryAII Erythromycin polyketide synthase modules 3 and 4



- Molecule 1: EryAII Erythromycin polyketide synthase modules 3 and 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.20Å 139.00Å 102.34Å 90.00° 106.14° 90.00°	Depositor
Resolution (Å)	41.52 – 2.59 41.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.52-2.59) 99.4 (41.52-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.268 0.210 , 0.261	Depositor DCC
R_{free} test set	3145 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13148	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, ACT, CER

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	0.83	0/6573	0.97	18/8942 (0.2%)
1	B	0.86	1/6603 (0.0%)	0.95	13/8983 (0.1%)
All	All	0.84	1/13176 (0.0%)	0.96	31/17925 (0.2%)

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	11
1	B	0	9
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CG-CD	5.68	1.60	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ALA	O-C-N	-10.90	105.26	122.70
1	A	201	ALA	C-N-CA	10.14	147.05	121.70
1	B	202	CYS	O-C-N	-9.46	107.57	122.70
1	A	360	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	202	CYS	C-N-CA	-7.67	102.53	121.70
1	A	469	GLY	N-CA-C	-7.21	95.07	113.10
1	A	201	ALA	CA-C-N	6.84	132.25	117.20
1	B	299	ASP	CB-CG-OD1	-6.82	112.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	MET	CG-SD-CE	-5.95	90.68	100.20
1	B	63	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	712	VAL	N-CA-C	-5.75	95.47	111.00
1	B	318	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	138	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	184	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	151	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	41	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	151	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	A	276	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	360	ARG	N-CA-C	-5.37	96.49	111.00
1	B	788	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	38	MET	CG-SD-CE	-5.32	91.69	100.20
1	B	422	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	B	700	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	513	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	30	SER	N-CA-C	5.20	125.05	111.00
1	A	217	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	360	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	156	PHE	N-CA-C	-5.11	97.21	111.00
1	B	123	LEU	CA-CB-CG	-5.11	103.55	115.30
1	B	388	LEU	CA-CB-CG	-5.09	103.58	115.30
1	B	314	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLU	Peptide
1	A	201	ALA	Mainchain
1	A	202	CYS	Mainchain
1	A	29	GLU	Peptide
1	A	361	ASP	Peptide
1	A	417	GLY	Peptide
1	A	469	GLY	Peptide
1	A	543	THR	Peptide
1	A	711	SER	Peptide
1	A	822	TYR	Peptide
1	A	849	GLU	Peptide
1	B	159	GLY	Peptide
1	B	29	GLU	Peptide
1	B	30	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	500	ALA	Peptide
1	B	501	ASP	Peptide
1	B	543	THR	Peptide
1	B	711	SER	Peptide
1	B	771	ASP	Peptide
1	B	822	TYR	Peptide

5.2 Too-close contacts [i](#)

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	6449	0	6307	269	0
1	B	6479	0	6340	270	0
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	8	0	5	1	0
4	B	8	0	5	2	0
5	A	95	0	0	22	0
5	B	99	0	0	21	0
All	All	13148	0	12663	532	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (532) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:SER:HB3	1:B:724:SER:N	1.40	1.35
1:B:711:SER:CB	1:B:724:SER:H	1.56	1.19
1:A:711:SER:HB2	1:A:724:SER:H	0.98	1.12
1:A:709:ARG:NH1	1:A:709:ARG:HB2	1.64	1.12
1:B:37:SER:HB2	1:B:135:ALA:HB2	1.34	1.07
1:B:702:ARG:NH2	1:B:737:CYS:SG	2.28	1.06
1:B:444:ILE:HG22	4:B:960:CER:H21	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ARG:HG2	1:A:725:GLY:HA3	1.39	1.02
1:B:711:SER:HB2	1:B:723:VAL:HA	1.40	1.02
1:B:587:LYS:HG3	1:B:635:GLU:HG3	1.38	1.02
1:A:210:HIS:HD2	1:A:294:SER:OG	1.41	1.01
1:A:574:GLY:HA3	1:A:607:LEU:HD13	1.40	0.99
1:A:711:SER:HB2	1:A:724:SER:N	1.77	0.98
1:A:711:SER:CB	1:A:724:SER:H	1.77	0.98
1:B:48:THR:HG22	1:B:51:ARG:H	1.30	0.97
1:B:550:GLY:HA3	1:B:876:VAL:HG13	1.47	0.97
1:B:370:SER:H	1:B:402:THR:CG2	1.77	0.97
1:B:48:THR:HG21	5:B:967:HOH:O	1.67	0.95
1:A:703:LEU:HD22	1:A:709:ARG:HH12	1.30	0.94
1:B:829:SER:HB2	1:B:830:PRO:HD2	1.49	0.93
1:A:812:ASP:HA	1:A:815:THR:HG22	1.50	0.92
1:A:709:ARG:CB	1:A:709:ARG:HH11	1.82	0.91
1:A:48:THR:HG22	1:A:51:ARG:H	1.33	0.91
1:B:711:SER:HB3	1:B:724:SER:H	0.74	0.90
1:B:315:ARG:O	1:B:319:GLN:HG3	1.70	0.90
1:A:875:HIS:HB2	1:A:881:ILE:HD12	1.53	0.89
1:B:359:ASP:O	1:B:360:ARG:HB2	1.73	0.89
1:A:709:ARG:HB2	1:A:709:ARG:HH11	1.30	0.88
1:B:668:ASP:HB3	1:B:772:ILE:HG13	1.56	0.87
1:B:341:THR:HG22	1:B:344:GLY:H	1.38	0.87
1:B:550:GLY:HA3	1:B:876:VAL:CG1	2.03	0.87
1:A:508:GLY:O	1:A:512:THR:HB	1.74	0.87
1:A:209:LEU:CD1	1:A:274:LEU:HD11	2.03	0.86
1:B:683:LEU:HD11	1:B:761:VAL:HG11	1.54	0.86
1:A:170:GLY:O	1:A:174:THR:HG22	1.76	0.84
1:A:636:LEU:O	1:A:639:SER:HB2	1.77	0.84
1:A:763:GLU:CG	1:A:764:GLU:H	1.90	0.84
1:A:210:HIS:CD2	1:A:294:SER:OG	2.28	0.83
1:B:527:ARG:CD	1:B:527:ARG:H	1.91	0.83
1:A:77:LEU:HD11	1:A:235:PRO:HG3	1.60	0.82
1:B:680:MET:HE2	1:B:751:TYR:CD1	2.14	0.82
1:B:573:MET:HE3	1:B:626:LEU:CD1	2.10	0.82
1:A:709:ARG:C	1:A:711:SER:H	1.82	0.82
1:B:515:ARG:CZ	5:B:1049:HOH:O	2.28	0.81
1:B:527:ARG:H	1:B:527:ARG:HD2	1.41	0.81
1:A:709:ARG:NH1	1:A:709:ARG:CB	2.43	0.81
1:B:829:SER:HB2	1:B:830:PRO:CD	2.09	0.81
1:B:711:SER:CB	1:B:723:VAL:HA	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:GLU:OE1	1:B:544:ALA:HB2	1.82	0.80
1:A:120:GLN:HE21	1:A:230:ALA:HA	1.44	0.80
1:B:120:GLN:HE21	1:B:230:ALA:HA	1.46	0.80
1:A:315:ARG:O	1:A:319:GLN:HG3	1.82	0.80
1:B:118:ASP:OD2	1:B:120:GLN:HB2	1.82	0.80
1:B:707:GLN:HA	1:B:707:GLN:NE2	1.97	0.79
1:B:550:GLY:CA	1:B:876:VAL:HG13	2.13	0.79
1:A:292:ARG:HD2	1:A:454:GLU:OE1	1.81	0.79
1:B:496:GLU:OE1	1:B:531:VAL:HG21	1.83	0.79
1:A:198:VAL:HG22	1:B:196:ILE:HD11	1.65	0.78
1:B:336:ALA:HB1	1:B:348:GLU:OE2	1.83	0.78
1:A:38:MET:HE3	1:A:391:VAL:HG11	1.65	0.78
1:B:711:SER:CB	1:B:724:SER:N	2.26	0.78
1:A:33:ILE:HG13	1:A:213:VAL:HG13	1.66	0.78
1:B:711:SER:OG	1:B:723:VAL:HG13	1.84	0.77
1:B:573:MET:CE	1:B:626:LEU:CD1	2.64	0.76
1:A:362:ALA:O	1:A:363:ASP:HB2	1.85	0.76
1:A:763:GLU:HG3	1:A:764:GLU:H	1.51	0.76
1:A:145:THR:HG21	5:A:1035:HOH:O	1.86	0.76
1:B:726:GLU:HG2	1:B:727:PRO:HD2	1.68	0.76
1:B:732:ALA:O	1:B:736:ASP:HB2	1.86	0.75
1:B:737:CYS:HB2	5:B:1059:HOH:O	1.86	0.74
1:A:650:HIS:HE1	1:A:716:ASN:OD1	1.71	0.74
1:B:703:LEU:HD22	1:B:709:ARG:HH21	1.52	0.74
1:A:209:LEU:HD11	1:A:274:LEU:HD11	1.69	0.74
1:B:127:THR:HG22	1:B:271:LEU:HD12	1.67	0.74
1:B:500:ALA:HB3	1:B:893:PHE:CE1	2.22	0.74
1:B:527:ARG:CD	1:B:527:ARG:N	2.50	0.74
1:A:680:MET:HE2	1:A:751:TYR:CD1	2.22	0.73
1:B:760:ARG:HB2	5:B:1044:HOH:O	1.86	0.73
1:A:703:LEU:CD2	1:A:709:ARG:HH12	2.02	0.73
1:B:709:ARG:CZ	1:B:709:ARG:HB3	2.11	0.73
1:A:665:THR:HB	1:A:667:GLU:OE1	1.89	0.73
1:B:765:LEU:O	1:B:769:THR:HG22	1.88	0.73
1:B:174:THR:HG22	5:B:997:HOH:O	1.88	0.72
1:B:444:ILE:CG2	4:B:960:CER:H21	2.17	0.72
1:A:786:GLU:OE1	1:A:802:ARG:NH1	2.22	0.72
1:A:740:GLU:OE1	1:A:742:ILE:HD11	1.90	0.72
1:B:299:ASP:HB3	1:B:312:ALA:CB	2.19	0.72
1:B:808:VAL:HG12	5:B:963:HOH:O	1.88	0.72
1:B:692:VAL:HG22	1:B:744:VAL:HG12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HG21	5:A:963:HOH:O	1.89	0.71
1:B:698:ALA:O	1:B:702:ARG:HG3	1.91	0.71
1:A:763:GLU:CG	1:A:764:GLU:N	2.53	0.71
1:B:731:ARG:O	1:B:735:GLU:HG2	1.91	0.71
1:B:370:SER:N	1:B:402:THR:CG2	2.53	0.70
1:B:508:GLY:O	1:B:512:THR:HB	1.90	0.70
1:A:313:GLN:OE1	1:A:348:GLU:HA	1.91	0.70
1:B:334:VAL:HG23	1:B:366:LEU:HD11	1.73	0.70
1:B:636:LEU:O	1:B:639:SER:HB2	1.92	0.70
1:B:526:THR:HG22	1:B:529:GLU:HB2	1.74	0.69
1:A:763:GLU:HG3	1:A:764:GLU:N	2.07	0.69
1:A:765:LEU:O	1:A:769:THR:HG22	1.93	0.69
1:B:680:MET:HE1	1:B:758:ILE:HD11	1.73	0.69
1:A:651:SER:OG	2:A:950:ACT:O	2.07	0.69
1:B:652:GLN:HG3	5:B:1032:HOH:O	1.93	0.69
1:B:107:PHE:O	1:B:109:VAL:HG23	1.93	0.69
1:A:193:GLY:O	1:B:298:GLN:HB2	1.93	0.68
1:A:337:HIS:O	1:A:372:LYS:HE3	1.93	0.68
1:B:469:GLY:O	1:B:470:ARG:HB2	1.93	0.68
1:B:78:HIS:HB3	5:B:974:HOH:O	1.93	0.68
1:B:707:GLN:HA	1:B:707:GLN:HE21	1.59	0.68
1:A:498:PRO:O	1:A:499:ASP:CB	2.41	0.68
1:B:359:ASP:HB3	5:B:1051:HOH:O	1.93	0.67
1:B:664:LEU:HD22	1:B:772:ILE:HD11	1.76	0.67
1:B:308:PRO:HG2	1:B:347:ILE:HD12	1.77	0.67
1:A:315:ARG:NH1	5:A:989:HOH:O	2.20	0.67
1:A:205:SER:HB3	1:A:384:VAL:HG22	1.77	0.67
1:A:227:GLY:HA3	1:A:270:THR:O	1.94	0.67
1:A:500:ALA:CB	1:A:527:ARG:HD2	2.24	0.67
1:B:366:LEU:HD23	1:B:419:VAL:HG22	1.77	0.67
1:B:152:GLY:O	1:B:153:VAL:HG23	1.95	0.66
1:A:314:ARG:NH1	3:A:2:CL:CL	2.65	0.66
1:B:707:GLN:C	1:B:709:ARG:H	1.99	0.66
1:A:485:ARG:HD2	5:A:1037:HOH:O	1.95	0.66
1:A:587:LYS:HE2	1:A:631:VAL:HG13	1.78	0.66
1:B:38:MET:HE1	1:B:391:VAL:HB	1.77	0.66
1:A:250:ASP:OD1	1:A:252:ARG:HB2	1.95	0.65
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.62	0.65
1:A:812:ASP:HA	1:A:815:THR:CG2	2.24	0.65
1:B:200:THR:HG22	1:B:200:THR:O	1.94	0.65
1:A:709:ARG:C	1:A:711:SER:N	2.49	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:MET:CE	1:A:626:LEU:HD23	2.26	0.65
1:A:620:ASP:HA	1:A:677:SER:HB3	1.77	0.65
1:A:123:LEU:O	1:A:127:THR:HG23	1.96	0.65
1:B:702:ARG:CZ	1:B:737:CYS:SG	2.84	0.65
1:B:683:LEU:HD11	1:B:761:VAL:CG1	2.26	0.65
1:B:680:MET:CE	1:B:751:TYR:CD1	2.80	0.64
1:B:286:GLU:OE1	1:B:395:ARG:NH2	2.30	0.64
2:A:950:ACT:H2	5:A:975:HOH:O	1.97	0.64
1:B:120:GLN:NE2	1:B:230:ALA:HA	2.12	0.64
1:A:498:PRO:O	1:A:499:ASP:HB2	1.98	0.64
1:B:687:GLY:HA2	1:B:727:PRO:HD3	1.80	0.64
1:B:299:ASP:HB2	1:B:309:SER:HB3	1.80	0.63
1:A:145:THR:CG2	5:A:1035:HOH:O	2.44	0.63
1:B:37:SER:CB	1:B:135:ALA:HB2	2.22	0.63
1:A:444:ILE:HA	5:A:1043:HOH:O	1.99	0.63
1:A:680:MET:CE	1:A:751:TYR:CD1	2.82	0.63
1:B:140:HIS:O	1:B:143:ARG:HG3	1.98	0.63
1:B:527:ARG:N	1:B:527:ARG:HD3	2.12	0.63
1:B:650:HIS:HE1	1:B:716:ASN:OD1	1.80	0.63
1:A:200:THR:O	1:A:200:THR:CG2	2.46	0.62
1:B:359:ASP:O	1:B:360:ARG:CB	2.46	0.62
1:A:573:MET:HE3	1:A:626:LEU:HD23	1.81	0.62
1:A:216:LEU:HD22	1:A:275:GLU:HA	1.81	0.62
1:A:458:GLU:HA	1:A:458:GLU:OE2	1.99	0.62
1:A:569:GLN:HG2	1:A:622:VAL:HG13	1.81	0.62
1:A:702:ARG:HG3	5:A:1031:HOH:O	1.98	0.62
1:B:469:GLY:O	1:B:470:ARG:CB	2.48	0.61
1:B:849:GLU:O	1:B:849:GLU:HG3	2.00	0.61
1:A:38:MET:HE1	1:A:391:VAL:HB	1.82	0.61
1:A:159:GLY:HA3	5:A:1039:HOH:O	2.01	0.61
1:A:205:SER:CB	1:A:384:VAL:HG22	2.31	0.60
1:A:369:GLY:HA3	1:A:402:THR:OG1	2.01	0.60
1:A:895:LEU:HB3	1:A:896:PRO:HD2	1.83	0.60
1:B:200:THR:O	1:B:200:THR:CG2	2.50	0.60
1:B:223:MET:CE	5:B:999:HOH:O	2.49	0.60
1:B:276:ARG:HG2	5:B:975:HOH:O	2.02	0.60
1:A:544:ALA:HB2	5:A:996:HOH:O	2.00	0.60
1:B:494:LEU:HD12	1:B:896:PRO:HD3	1.83	0.60
1:B:573:MET:CE	1:B:626:LEU:HD12	2.32	0.59
1:A:709:ARG:HB2	1:A:709:ARG:CZ	2.32	0.59
1:A:362:ALA:O	1:A:363:ASP:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ASN:ND2	5:B:972:HOH:O	2.34	0.59
1:A:687:GLY:HA2	1:A:727:PRO:HD3	1.85	0.59
1:B:802:ARG:NH2	5:B:1015:HOH:O	2.33	0.59
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.66	0.59
1:A:105:GLU:HB2	5:A:1018:HOH:O	2.01	0.59
1:A:573:MET:HE3	1:A:626:LEU:CD2	2.33	0.59
1:A:428:TRP:NE1	1:A:435:ARG:HG2	2.18	0.59
1:B:683:LEU:HD23	1:B:686:GLU:OE1	2.03	0.59
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.68	0.59
1:B:48:THR:CG2	1:B:51:ARG:H	2.11	0.58
1:B:299:ASP:CB	1:B:312:ALA:CB	2.81	0.58
1:A:153:VAL:HG12	1:A:154:ALA:N	2.18	0.58
1:A:200:THR:CG2	1:A:203:SER:OG	2.51	0.58
1:A:200:THR:O	1:A:201:ALA:HB3	2.02	0.58
1:A:198:VAL:HG22	1:B:196:ILE:CD1	2.31	0.58
1:A:227:GLY:HA3	1:A:271:LEU:HD23	1.86	0.58
1:A:496:GLU:O	1:A:497:ARG:C	2.40	0.58
1:A:848:ALA:HB1	1:A:851:ALA:H	1.66	0.58
1:B:152:GLY:O	1:B:153:VAL:CG2	2.51	0.58
1:B:734:SER:HB2	1:B:744:VAL:HG21	1.84	0.58
1:B:293:GLY:HA2	5:B:1017:HOH:O	2.04	0.57
1:B:495:LEU:CD1	1:B:505:VAL:HG21	2.34	0.57
1:A:61:GLU:OE1	1:A:252:ARG:NH1	2.37	0.57
1:A:149:VAL:HB	1:A:195:SER:HB2	1.85	0.57
1:A:515:ARG:HG3	5:A:1028:HOH:O	2.05	0.57
1:B:200:THR:HG22	1:B:203:SER:OG	2.03	0.57
1:B:370:SER:H	1:B:402:THR:HG22	1.68	0.57
1:A:667:GLU:CD	1:A:667:GLU:H	2.07	0.57
1:B:494:LEU:HD21	1:B:893:PHE:HE2	1.68	0.57
1:B:532:ARG:O	1:B:536:GLU:HG3	2.04	0.57
1:A:875:HIS:HA	1:A:879:VAL:O	2.04	0.57
1:A:550:GLY:HA3	1:A:876:VAL:HG13	1.86	0.57
1:B:251:GLY:HA2	5:B:969:HOH:O	2.04	0.56
1:B:370:SER:N	1:B:402:THR:HG21	2.21	0.56
1:B:711:SER:CB	1:B:723:VAL:CA	2.83	0.56
1:A:252:ARG:HH11	1:A:252:ARG:CG	2.18	0.56
1:A:469:GLY:H	1:A:470:ARG:HG3	1.70	0.56
1:A:711:SER:OG	1:A:712:VAL:N	2.32	0.56
1:A:875:HIS:HB2	1:A:881:ILE:CD1	2.32	0.56
1:B:573:MET:HE2	1:B:830:PRO:HG3	1.87	0.56
1:B:475:VAL:HG13	1:B:515:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:LEU:O	1:A:686:GLU:HB2	2.04	0.56
1:B:232:MET:SD	1:B:237:VAL:HG21	2.46	0.56
1:B:713:ALA:O	1:B:807:THR:HA	2.06	0.56
1:B:48:THR:HG22	1:B:51:ARG:N	2.12	0.55
1:B:243:ARG:HA	1:B:243:ARG:NE	2.21	0.55
1:B:279:GLU:OE2	1:B:282:ARG:NH2	2.37	0.55
1:A:831:HIS:HD2	1:A:859:ARG:H	1.53	0.55
1:A:627:PHE:HB2	1:A:673:VAL:HG21	1.87	0.55
1:A:176:VAL:O	1:A:178:PRO:HD3	2.07	0.55
1:B:711:SER:HG	1:B:723:VAL:HG13	1.71	0.55
1:A:444:ILE:HG23	4:A:960:CER:H21	1.88	0.55
1:B:120:GLN:HE21	1:B:231:VAL:H	1.53	0.55
1:A:713:ALA:HB3	1:A:722:VAL:HG12	1.89	0.55
1:B:526:THR:HG22	1:B:529:GLU:H	1.70	0.55
1:B:739:ALA:O	1:B:740:GLU:HB2	2.05	0.55
1:B:842:VAL:HG13	1:B:843:GLU:N	2.21	0.55
1:B:341:THR:HG22	1:B:344:GLY:N	2.17	0.55
1:A:769:THR:HG23	1:A:797:ALA:HB1	1.88	0.54
1:A:412:VAL:HG12	1:A:413:ASP:N	2.23	0.54
1:A:619:VAL:HG12	1:A:623:GLN:HG3	1.89	0.54
1:A:38:MET:CE	1:A:391:VAL:HG11	2.35	0.54
1:A:227:GLY:HA2	1:A:384:VAL:HG21	1.89	0.54
1:B:125:LEU:HD22	1:B:188:THR:HG21	1.90	0.54
1:A:834:VAL:O	1:A:838:VAL:HG23	2.07	0.54
1:A:709:ARG:HB3	1:A:711:SER:HB3	1.90	0.54
1:A:680:MET:HE2	1:A:751:TYR:CG	2.43	0.53
1:A:706:TRP:O	1:A:708:ASP:N	2.42	0.53
1:B:796:ASP:HB3	1:B:798:ARG:H	1.73	0.53
1:B:138:ASP:OD1	1:B:514:ALA:HA	2.09	0.53
1:B:223:MET:HE1	5:B:999:HOH:O	2.07	0.53
1:A:345:ASP:N	1:A:346:PRO:HD2	2.23	0.53
1:A:357:GLY:O	1:A:358:ARG:HB2	2.08	0.53
1:A:206:LEU:HD13	1:A:383:GLY:HA3	1.91	0.52
1:A:361:ASP:OD1	1:A:361:ASP:N	2.41	0.52
1:A:592:ASP:OD1	1:A:603:VAL:HB	2.09	0.52
1:A:120:GLN:NE2	1:A:230:ALA:HA	2.18	0.52
1:B:361:ASP:C	1:B:363:ASP:H	2.11	0.52
1:B:369:GLY:HA2	1:B:402:THR:HG21	1.91	0.52
1:B:563:PHE:N	1:B:563:PHE:CD1	2.78	0.52
1:A:38:MET:HG3	1:A:388:LEU:HD22	1.91	0.52
1:A:227:GLY:HA2	1:A:384:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:GLU:O	1:B:843:GLU:HB2	2.10	0.52
1:B:680:MET:HE2	1:B:751:TYR:CE1	2.43	0.52
1:B:698:ALA:O	1:B:701:GLU:HG3	2.09	0.52
1:B:182:SER:HB3	1:B:195:SER:HB3	1.91	0.52
1:B:627:PHE:CZ	1:B:669:ALA:HB1	2.45	0.52
1:B:602:LYS:HG3	1:B:605:ASP:OD2	2.10	0.52
1:B:683:LEU:HA	1:B:686:GLU:OE1	2.10	0.52
1:B:137:ILE:HG22	1:B:138:ASP:O	2.11	0.51
1:B:472:VAL:HG11	1:B:502:LEU:HG	1.92	0.51
1:A:29:GLU:HB2	1:A:292:ARG:NH2	2.26	0.51
1:A:79:HIS:CD2	1:A:81:ASP:H	2.29	0.51
1:B:711:SER:HB3	1:B:724:SER:CA	2.36	0.51
1:A:683:LEU:HD11	1:A:761:VAL:HG11	1.92	0.51
1:B:299:ASP:CB	1:B:309:SER:HB3	2.40	0.51
1:B:153:VAL:HG12	1:B:154:ALA:N	2.26	0.51
1:B:250:ASP:HB3	1:B:252:ARG:H	1.76	0.51
1:B:637:TRP:CZ3	1:B:871:MET:HG2	2.45	0.51
1:A:205:SER:OG	1:A:380:ALA:O	2.26	0.51
1:A:412:VAL:CG1	1:A:413:ASP:N	2.73	0.51
1:A:846:ASP:HB2	5:A:1027:HOH:O	2.10	0.51
1:A:152:GLY:HA2	1:A:198:VAL:O	2.10	0.50
1:A:895:LEU:HB3	1:A:896:PRO:CD	2.41	0.50
1:B:500:ALA:HB3	1:B:893:PHE:HE1	1.73	0.50
1:B:573:MET:HE3	1:B:626:LEU:HD11	1.91	0.50
1:B:82:PRO:HG2	1:B:245:ARG:NH1	2.26	0.50
1:B:444:ILE:O	1:B:444:ILE:HG12	2.08	0.50
1:A:587:LYS:HE2	1:A:631:VAL:CG1	2.40	0.50
1:B:707:GLN:C	1:B:709:ARG:N	2.65	0.50
1:A:158:TYR:CE2	1:A:907:LEU:HD12	2.47	0.50
1:A:252:ARG:NH1	1:A:252:ARG:CG	2.74	0.49
1:A:360:ARG:HD2	1:A:365:PRO:HA	1.92	0.49
1:A:487:GLN:O	1:A:491:ILE:HG12	2.11	0.49
1:B:364:ARG:CZ	1:B:433:ARG:HE	2.25	0.49
1:A:387:LEU:C	1:A:387:LEU:HD23	2.32	0.49
1:A:676:ARG:NH2	1:A:803:ASN:OD1	2.40	0.49
1:B:570:TRP:CZ3	1:B:572:GLY:HA3	2.47	0.49
1:A:734:SER:OG	1:A:744:VAL:HG21	2.12	0.49
1:A:738:ALA:O	1:A:739:ALA:CB	2.61	0.49
1:A:765:LEU:O	1:A:769:THR:CG2	2.61	0.49
1:B:308:PRO:HG2	1:B:347:ILE:CD1	2.41	0.49
1:B:467:HIS:CD2	1:B:468:ASP:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:CG1	1:A:154:ALA:N	2.75	0.49
1:A:174:THR:HG23	5:A:1044:HOH:O	2.11	0.49
1:A:574:GLY:H	1:A:607:LEU:HD22	1.78	0.49
1:A:637:TRP:CZ3	1:A:871:MET:HG2	2.48	0.49
1:B:332:ASP:OD2	1:B:433:ARG:NH1	2.45	0.49
1:B:573:MET:HE1	1:B:626:LEU:CD1	2.41	0.49
1:B:829:SER:CB	1:B:830:PRO:CD	2.77	0.49
1:B:399:LEU:O	1:B:425:ASN:HA	2.12	0.49
1:B:831:HIS:HD2	1:B:859:ARG:H	1.60	0.49
1:A:162:THR:O	1:A:163:ALA:CB	2.60	0.48
1:B:475:VAL:CG1	1:B:515:ARG:NH1	2.76	0.48
1:A:341:THR:HG22	1:A:344:GLY:H	1.77	0.48
1:A:118:ASP:OD2	1:A:120:GLN:HB2	2.13	0.48
1:A:709:ARG:HH11	1:A:709:ARG:HB3	1.72	0.48
1:A:763:GLU:HG2	1:A:764:GLU:H	1.71	0.48
1:A:210:HIS:HE1	1:B:220:GLU:OE2	1.96	0.48
1:B:120:GLN:NE2	1:B:231:VAL:H	2.11	0.48
1:A:515:ARG:NH1	1:A:875:HIS:CE1	2.82	0.48
1:A:738:ALA:O	1:A:739:ALA:HB3	2.13	0.48
1:B:369:GLY:CA	1:B:402:THR:CG2	2.92	0.48
1:B:831:HIS:CD2	1:B:859:ARG:HG3	2.48	0.48
1:A:428:TRP:O	1:A:435:ARG:NH1	2.45	0.48
1:A:507:LEU:HD22	1:A:890:ALA:HB3	1.96	0.48
1:A:80:PRO:O	1:A:82:PRO:HD3	2.14	0.48
1:A:250:ASP:OD1	1:A:252:ARG:HD2	2.14	0.48
1:A:373:SER:HB2	1:A:403:LEU:HB2	1.96	0.48
1:A:480:SER:HB2	5:A:1019:HOH:O	2.13	0.48
1:B:259:GLY:O	1:B:260:ALA:C	2.51	0.47
1:B:345:ASP:HB2	1:B:346:PRO:HD3	1.96	0.47
1:B:515:ARG:NH2	5:B:1049:HOH:O	2.39	0.47
1:B:703:LEU:HD22	1:B:709:ARG:NH2	2.24	0.47
1:B:709:ARG:HA	1:B:725:GLY:HA3	1.96	0.47
1:B:737:CYS:HA	1:B:739:ALA:O	2.13	0.47
1:A:330:ASP:HB3	1:A:436:ARG:NH1	2.28	0.47
1:A:758:ILE:C	1:A:760:ARG:H	2.16	0.47
1:A:372:LYS:HD3	1:A:377:HIS:HA	1.95	0.47
1:A:544:ALA:CB	5:A:996:HOH:O	2.60	0.47
1:A:369:GLY:CA	1:A:402:THR:OG1	2.63	0.47
1:A:708:ASP:N	1:A:708:ASP:OD2	2.47	0.47
1:A:440:SER:HB3	1:A:450:HIS:ND1	2.29	0.47
1:B:79:HIS:CD2	1:B:81:ASP:H	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:LEU:CD2	1:B:772:ILE:HD11	2.42	0.47
1:B:713:ALA:HB2	1:B:724:SER:HB2	1.97	0.47
1:A:199:ASP:CG	1:B:179:ALA:HB2	2.35	0.47
1:A:772:ILE:HG12	1:A:774:PRO:HD3	1.96	0.47
1:B:564:PRO:HD2	1:B:630:MET:SD	2.54	0.47
1:A:807:THR:HG23	5:A:985:HOH:O	2.15	0.47
1:A:872:ALA:O	1:A:876:VAL:HB	2.15	0.47
1:B:601:TRP:CG	1:B:614:PRO:HG2	2.50	0.47
1:A:588:ILE:HD13	1:A:588:ILE:HA	1.85	0.47
1:A:648:VAL:CG2	1:A:817:LEU:HD11	2.45	0.47
1:B:494:LEU:HD21	1:B:893:PHE:CE2	2.49	0.47
1:B:134:ASN:HD22	1:B:134:ASN:HA	1.58	0.47
1:B:834:VAL:O	1:B:838:VAL:HG23	2.15	0.47
1:A:770:GLY:C	1:A:772:ILE:H	2.18	0.46
1:B:45:GLY:N	1:B:97:ASP:OD2	2.49	0.46
1:A:580:SER:O	1:A:581:SER:C	2.51	0.46
1:A:807:THR:HG22	5:A:964:HOH:O	2.15	0.46
1:B:335:GLU:OE2	1:B:371:VAL:HG22	2.15	0.46
1:A:769:THR:O	1:A:772:ILE:HG22	2.14	0.46
1:B:200:THR:CG2	1:B:203:SER:OG	2.64	0.46
1:B:768:THR:HG22	1:B:768:THR:O	2.15	0.46
1:B:898:TYR:HA	1:B:899:PRO:HD3	1.69	0.46
1:A:102:PHE:CD1	1:A:122:ARG:HB3	2.50	0.46
1:A:407:GLU:HA	1:A:408:PRO:HD2	1.82	0.46
1:B:413:ASP:CG	1:B:413:ASP:O	2.54	0.46
1:A:689:MET:HG2	1:A:724:SER:OG	2.15	0.46
1:B:353:LEU:CD2	1:B:419:VAL:HB	2.46	0.46
1:B:169:GLU:N	1:B:169:GLU:OE1	2.49	0.46
1:A:91:ASP:C	1:A:91:ASP:OD2	2.54	0.46
1:A:250:ASP:OD1	1:A:252:ARG:CB	2.63	0.46
1:A:353:LEU:HD23	1:A:419:VAL:HG23	1.97	0.46
1:A:650:HIS:CE1	1:A:716:ASN:OD1	2.60	0.46
1:A:831:HIS:CD2	1:A:859:ARG:HG3	2.51	0.46
1:B:351:ALA:HA	5:B:1020:HOH:O	2.16	0.46
1:B:476:VAL:HG23	1:B:484:LEU:HD21	1.98	0.46
1:B:791:ASP:OD1	1:B:791:ASP:N	2.44	0.46
1:B:168:VAL:HG12	1:B:168:VAL:O	2.16	0.45
1:A:390:VAL:HG21	1:A:439:VAL:HG22	1.98	0.45
1:A:663:ALA:HA	1:A:775:ARG:O	2.15	0.45
1:B:232:MET:SD	1:B:237:VAL:CG2	3.04	0.45
1:B:618:ARG:HB2	1:B:620:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:HG3	1:A:292:ARG:NH2	2.31	0.45
1:A:200:THR:O	1:A:200:THR:HG22	2.15	0.45
1:A:94:GLY:O	1:A:266:SER:HA	2.17	0.45
1:A:152:GLY:HA3	1:A:204:SER:HB3	1.98	0.45
1:A:578:LEU:HD21	1:A:588:ILE:HG21	1.99	0.45
1:A:731:ARG:HG3	1:A:731:ARG:HH11	1.82	0.45
1:B:430:ARG:NH2	1:B:455:GLU:OE2	2.48	0.45
1:B:335:GLU:OE1	1:B:389:LYS:HD3	2.15	0.45
1:B:778:ARG:HE	1:B:778:ARG:HB3	1.52	0.45
1:B:842:VAL:CG1	1:B:843:GLU:N	2.80	0.45
1:A:524:ALA:HB1	1:A:529:GLU:HG3	1.99	0.45
1:A:812:ASP:CA	1:A:815:THR:HG22	2.35	0.45
1:A:106:PHE:CD2	1:A:479:ARG:HG3	2.52	0.45
1:A:217:ARG:HG3	1:A:217:ARG:NH1	2.32	0.45
1:A:113:GLU:O	1:A:117:MET:HG3	2.17	0.45
1:B:369:GLY:CA	1:B:402:THR:HG21	2.46	0.45
1:B:528:GLU:O	1:B:532:ARG:HB2	2.16	0.45
1:B:573:MET:CE	1:B:830:PRO:HG3	2.47	0.45
1:B:587:LYS:NZ	1:B:659:HIS:NE2	2.63	0.45
1:A:333:ALA:HA	1:A:367:TRP:O	2.17	0.45
1:A:676:ARG:O	1:A:680:MET:HG2	2.17	0.45
1:A:766:LEU:HA	1:A:769:THR:HG22	1.99	0.45
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.79	0.44
1:A:147:THR:HG23	1:A:223:MET:HB2	1.99	0.44
1:A:244:GLN:HE21	1:A:244:GLN:HB2	1.61	0.44
1:A:210:HIS:CE1	1:B:220:GLU:OE2	2.70	0.44
1:B:29:GLU:O	1:B:29:GLU:HG2	2.16	0.44
1:B:48:THR:HG23	1:B:50:GLN:H	1.81	0.44
1:A:573:MET:HB3	1:A:607:LEU:HD22	1.98	0.44
1:A:788:ARG:O	1:A:789:SER:C	2.56	0.44
1:B:495:LEU:HD13	1:B:505:VAL:HG21	1.99	0.44
1:A:353:LEU:HD23	1:A:419:VAL:CG2	2.47	0.44
1:A:711:SER:O	1:A:712:VAL:HB	2.17	0.44
1:A:865:SER:O	1:A:869:ARG:HG2	2.17	0.44
1:A:500:ALA:HB3	1:A:527:ARG:HD2	1.98	0.44
1:B:573:MET:CE	1:B:626:LEU:HD13	2.44	0.44
1:B:710:LEU:HD11	5:B:1006:HOH:O	2.17	0.44
1:B:880:ASP:OD1	1:B:880:ASP:N	2.45	0.44
1:A:138:ASP:OD1	1:A:140:HIS:HB2	2.18	0.44
1:B:106:PHE:CD1	1:B:900:PHE:HE1	2.36	0.44
1:B:510:ALA:HA	1:B:515:ARG:HH22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:PHE:CE2	1:B:656:ALA:HA	2.52	0.44
1:B:875:HIS:HD2	1:B:879:VAL:O	2.01	0.44
1:A:205:SER:OG	1:A:384:VAL:HG22	2.18	0.44
1:B:758:ILE:HD13	1:B:758:ILE:HA	1.78	0.44
1:B:765:LEU:HD23	1:B:769:THR:HG21	2.00	0.44
1:A:38:MET:CE	1:A:391:VAL:CG1	2.95	0.44
1:B:563:PHE:HA	1:B:564:PRO:HD3	1.72	0.44
1:B:299:ASP:HB2	1:B:309:SER:CB	2.46	0.43
1:A:148:GLY:O	1:A:224:ALA:HA	2.17	0.43
1:B:570:TRP:CE3	1:B:572:GLY:HA3	2.52	0.43
1:B:558:ASN:HB2	1:B:822:TYR:HA	2.00	0.43
1:A:680:MET:CE	1:A:751:TYR:HB2	2.48	0.43
1:A:710:LEU:HB2	1:A:756:PRO:HG3	2.00	0.43
1:A:745:ARG:HA	5:A:1020:HOH:O	2.18	0.43
1:B:852:VAL:HG22	1:B:877:SER:HB3	2.00	0.43
1:A:34:ALA:N	1:A:275:GLU:O	2.52	0.43
1:A:41:ARG:HH21	1:A:902:ARG:HH21	1.66	0.43
1:A:317:ILE:O	1:A:320:ALA:HB3	2.18	0.43
1:A:409:THR:OG1	1:A:411:HIS:ND1	2.43	0.43
1:A:409:THR:HG1	1:A:411:HIS:HD1	1.62	0.43
1:A:710:LEU:N	5:A:1023:HOH:O	2.51	0.43
1:B:825:PHE:O	1:B:853:VAL:HA	2.18	0.43
1:A:70:ARG:NH1	1:A:267:GLU:OE1	2.41	0.43
1:A:412:VAL:CG1	1:A:413:ASP:H	2.32	0.43
1:A:703:LEU:HD11	1:A:711:SER:HG	1.83	0.43
1:A:432:GLU:H	1:A:432:GLU:HG3	1.59	0.43
1:A:785:VAL:HG21	1:A:803:ASN:HA	2.00	0.43
1:A:706:TRP:C	1:A:708:ASP:H	2.21	0.43
1:B:353:LEU:HD21	1:B:419:VAL:HB	2.01	0.43
1:B:106:PHE:CE2	1:B:898:TYR:CZ	3.06	0.43
1:B:298:GLN:HA	1:B:446:GLY:O	2.18	0.43
1:B:785:VAL:HG21	1:B:803:ASN:HA	2.01	0.43
1:A:637:TRP:CH2	1:A:871:MET:HG2	2.54	0.43
1:B:326:LEU:HD23	1:B:326:LEU:HA	1.86	0.43
1:B:623:GLN:NE2	1:B:652:GLN:OE1	2.52	0.43
1:B:756:PRO:C	1:B:758:ILE:H	2.22	0.43
1:A:200:THR:HG22	1:A:203:SER:OG	2.19	0.42
1:A:254:LYS:NZ	1:A:261:ASP:HB2	2.33	0.42
1:A:573:MET:HE3	1:A:830:PRO:HG2	2.01	0.42
1:B:668:ASP:CB	1:B:772:ILE:HG13	2.36	0.42
1:A:200:THR:O	1:A:200:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:HB2	1:A:433:ARG:H	1.64	0.42
1:B:709:ARG:NH1	1:B:729:ALA:O	2.51	0.42
1:A:41:ARG:HH21	1:A:902:ARG:NH2	2.17	0.42
1:B:206:LEU:HD13	1:B:383:GLY:HA3	2.01	0.42
1:B:299:ASP:CB	1:B:312:ALA:HB2	2.49	0.42
1:B:513:ARG:HA	1:B:513:ARG:HD2	1.70	0.42
1:A:48:THR:HG22	1:A:51:ARG:N	2.17	0.42
1:A:115:ALA:HA	1:A:905:TYR:HB3	2.00	0.42
1:A:276:ARG:O	1:A:277:LEU:C	2.58	0.42
1:A:601:TRP:CG	1:A:614:PRO:HG2	2.54	0.42
1:B:153:VAL:CG1	1:B:154:ALA:N	2.83	0.42
1:B:299:ASP:HB3	1:B:312:ALA:HB3	1.99	0.42
1:B:569:GLN:H	1:B:569:GLN:HG3	1.24	0.42
1:A:515:ARG:HD2	5:A:1022:HOH:O	2.19	0.42
1:B:206:LEU:HD12	1:B:206:LEU:HA	1.79	0.42
1:B:468:ASP:C	1:B:469:GLY:O	2.58	0.42
1:A:209:LEU:HA	1:A:226:VAL:HG11	2.01	0.42
1:B:413:ASP:OD1	1:B:416:SER:O	2.38	0.42
1:B:478:ALA:O	1:B:518:HIS:HB2	2.20	0.42
1:B:492:ALA:O	1:B:496:GLU:HG2	2.19	0.42
1:B:891:ALA:HA	1:B:892:PRO:HD3	1.93	0.42
1:A:601:TRP:CH2	1:A:621:VAL:HA	2.55	0.42
1:A:714:ALA:HB3	1:A:722:VAL:HB	2.01	0.42
1:B:79:HIS:HD2	1:B:81:ASP:H	1.68	0.42
1:B:361:ASP:C	1:B:363:ASP:N	2.72	0.42
1:B:470:ARG:HA	1:B:471:PRO:HD3	1.81	0.42
1:A:142:LEU:O	1:A:145:THR:HB	2.19	0.42
1:A:799:TYR:CD1	1:A:799:TYR:C	2.93	0.42
1:B:543:THR:HB	5:B:1036:HOH:O	2.20	0.42
1:A:244:GLN:OE1	1:B:170:GLY:HA3	2.20	0.42
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.89	0.42
1:A:79:HIS:HD2	1:A:81:ASP:H	1.67	0.42
1:A:601:TRP:CB	1:A:614:PRO:HG2	2.50	0.42
1:B:230:ALA:N	1:B:268:GLY:O	2.41	0.42
1:B:683:LEU:CD1	1:B:761:VAL:HG11	2.38	0.42
1:A:867:PHE:O	1:A:870:SER:HB2	2.20	0.41
1:B:313:GLN:OE1	1:B:348:GLU:HA	2.20	0.41
1:A:413:ASP:N	1:A:413:ASP:OD2	2.52	0.41
1:B:209:LEU:HD22	1:B:274:LEU:HD11	2.02	0.41
1:B:358:ARG:C	1:B:359:ASP:O	2.57	0.41
1:B:543:THR:O	1:B:544:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLN:HG2	1:B:181:ALA:HA	2.02	0.41
1:B:375:ILE:O	1:B:375:ILE:HG13	2.19	0.41
1:B:694:LEU:HD22	1:B:742:ILE:HD13	2.03	0.41
1:A:774:PRO:HB2	1:A:793:THR:HA	2.02	0.41
1:A:341:THR:HG22	1:A:343:LEU:N	2.36	0.41
1:A:581:SER:HA	1:A:582:PRO:HD2	1.89	0.41
1:A:735:GLU:O	1:A:738:ALA:O	2.39	0.41
1:B:355:THR:OG1	1:B:356:TYR:N	2.54	0.41
1:A:196:ILE:HG22	1:A:198:VAL:HG23	2.03	0.41
1:A:703:LEU:CD2	1:A:709:ARG:NH1	2.78	0.41
1:B:369:GLY:HA2	1:B:402:THR:CG2	2.51	0.41
1:A:173:VAL:HG21	1:B:240:ASP:HB3	2.03	0.41
1:A:329:GLY:O	1:A:433:ARG:NH2	2.34	0.41
1:B:161:ASP:O	1:B:162:THR:OG1	2.33	0.41
1:B:719:ARG:HD3	1:B:719:ARG:HA	1.83	0.41
1:B:310:GLY:N	1:B:311:PRO:CD	2.84	0.41
1:A:718:PRO:HD2	5:A:967:HOH:O	2.20	0.41
1:A:760:ARG:O	1:A:763:GLU:OE2	2.39	0.41
1:A:827:GLU:OE2	1:A:832:PRO:HA	2.21	0.41
1:B:120:GLN:HE21	1:B:231:VAL:N	2.18	0.41
1:B:760:ARG:CB	5:B:1044:HOH:O	2.58	0.41
1:B:366:LEU:CD2	1:B:419:VAL:HG22	2.49	0.41
1:B:500:ALA:HB3	1:B:893:PHE:CZ	2.56	0.40
1:A:73:ASP:O	1:A:77:LEU:HB2	2.21	0.40
1:A:200:THR:O	1:A:201:ALA:CB	2.69	0.40
1:A:512:THR:O	1:A:513:ARG:HD3	2.21	0.40
1:B:709:ARG:HD2	1:B:730:LEU:HD12	2.03	0.40
1:B:248:ALA:HA	1:B:261:ASP:HB3	2.04	0.40
1:B:487:GLN:HB2	1:B:899:PRO:HG2	2.01	0.40
1:A:515:ARG:HH12	1:A:875:HIS:CE1	2.39	0.40
1:A:700:ARG:HH11	1:A:700:ARG:HD3	1.66	0.40
1:B:120:GLN:HE21	1:B:230:ALA:CA	2.27	0.40
1:B:484:LEU:HD12	1:B:518:HIS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	863/915 (94%)	779 (90%)	64 (7%)	20 (2%)	5	10
1	B	867/915 (95%)	781 (90%)	62 (7%)	24 (3%)	4	7
All	All	1730/1830 (94%)	1560 (90%)	126 (7%)	44 (2%)	4	8

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	358	ARG
1	A	415	SER
1	A	432	GLU
1	A	470	ARG
1	A	499	ASP
1	A	573	MET
1	A	707	GLN
1	A	711	SER
1	B	162	THR
1	B	360	ARG
1	B	465	THR
1	B	499	ASP
1	B	544	ALA
1	B	796	ASP
1	B	863	ASP
1	A	338	GLY
1	A	363	ASP
1	A	379	GLN
1	A	739	ALA
1	B	338	GLY
1	B	467	HIS
1	B	709	ARG
1	B	711	SER
1	A	201	ALA

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Mol	Chain	Res	Type
1	A	501	ASP
1	A	575	ALA
1	A	763	GLU
1	B	161	ASP
1	B	303	ASN
1	B	470	ARG
1	B	707	GLN
1	B	757	GLN
1	A	771	ASP
1	B	362	ALA
1	B	542	ALA
1	A	581	SER
1	B	466	ALA
1	B	710	LEU
1	A	469	GLY
1	B	236	GLY
1	B	469	GLY
1	B	619	VAL
1	B	712	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	654/688 (95%)	592 (90%)	62 (10%)	7	14
1	B	657/688 (96%)	579 (88%)	78 (12%)	4	8
All	All	1311/1376 (95%)	1171 (89%)	140 (11%)	5	11

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	31	ASP
1	A	48	THR
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	54	GLU
1	A	77	LEU
1	A	112	ARG
1	A	160	GLU
1	A	161	ASP
1	A	162	THR
1	A	182	SER
1	A	198	VAL
1	A	200	THR
1	A	206	LEU
1	A	243	ARG
1	A	290	VAL
1	A	327	GLU
1	A	358	ARG
1	A	360	ARG
1	A	361	ASP
1	A	371	VAL
1	A	384	VAL
1	A	413	ASP
1	A	421	LEU
1	A	432	GLU
1	A	433	ARG
1	A	468	ASP
1	A	481	THR
1	A	495	LEU
1	A	496	GLU
1	A	543	THR
1	A	548	VAL
1	A	566	GLN
1	A	569	GLN
1	A	573	MET
1	A	579	SER
1	A	589	ARG
1	A	614	PRO
1	A	616	LEU
1	A	617	ASP
1	A	619	VAL
1	A	631	VAL
1	A	636	LEU
1	A	639	SER
1	A	673	VAL
1	A	676	ARG

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Mol	Chain	Res	Type
1	A	708	ASP
1	A	710	LEU
1	A	744	VAL
1	A	746	ASP
1	A	749	VAL
1	A	750	ASP
1	A	767	GLU
1	A	772	ILE
1	A	788	ARG
1	A	789	SER
1	A	807	THR
1	A	820	SER
1	A	846	ASP
1	A	863	ASP
1	A	870	SER
1	A	876	VAL
1	B	30	SER
1	B	48	THR
1	B	98	ASP
1	B	112	ARG
1	B	160	GLU
1	B	162	THR
1	B	174	THR
1	B	196	ILE
1	B	200	THR
1	B	202	CYS
1	B	206	LEU
1	B	209	LEU
1	B	218	LYS
1	B	250	ASP
1	B	276	ARG
1	B	341	THR
1	B	358	ARG
1	B	359	ASP
1	B	360	ARG
1	B	368	LEU
1	B	371	VAL
1	B	375	ILE
1	B	402	THR
1	B	413	ASP
1	B	416	SER
1	B	430	ARG

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Mol	Chain	Res	Type
1	B	433	ARG
1	B	444	ILE
1	B	455	GLU
1	B	465	THR
1	B	467	HIS
1	B	472	VAL
1	B	484	LEU
1	B	495	LEU
1	B	512	THR
1	B	513	ARG
1	B	526	THR
1	B	527	ARG
1	B	528	GLU
1	B	531	VAL
1	B	543	THR
1	B	557	ARG
1	B	566	GLN
1	B	569	GLN
1	B	573	MET
1	B	577	LEU
1	B	602	LYS
1	B	604	SER
1	B	626	LEU
1	B	631	VAL
1	B	652	GLN
1	B	701	GLU
1	B	707	GLN
1	B	709	ARG
1	B	710	LEU
1	B	711	SER
1	B	731	ARG
1	B	733	PHE
1	B	745	ARG
1	B	749	VAL
1	B	758	ILE
1	B	769	THR
1	B	772	ILE
1	B	775	ARG
1	B	778	ARG
1	B	790	MET
1	B	791	ASP
1	B	793	THR

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Mol	Chain	Res	Type
1	B	808	VAL
1	B	823	ASP
1	B	836	GLN
1	B	854	VAL
1	B	856	SER
1	B	864	LEU
1	B	865	SER
1	B	876	VAL
1	B	904	ARG
1	B	908	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	120	GLN
1	A	134	ASN
1	A	140	HIS
1	A	210	HIS
1	A	285	HIS
1	A	516	HIS
1	A	650	HIS
1	A	782	HIS
1	A	831	HIS
1	A	875	HIS
1	B	79	HIS
1	B	120	GLN
1	B	134	ASN
1	B	210	HIS
1	B	285	HIS
1	B	404	HIS
1	B	467	HIS
1	B	490	GLN
1	B	650	HIS
1	B	707	GLN
1	B	831	HIS
1	B	875	HIS
1	B	908	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	B	950	-	3,3,3	0.77	0	3,3,3	1.38	0
4	CER	B	960	1	6,7,15	0.59	0	5,8,17	0.55	0
4	CER	A	960	1	6,7,15	0.60	0	5,8,17	0.59	0
2	ACT	A	950	-	3,3,3	0.90	0	3,3,3	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CER	A	960	1	-	0/5/6/16	-
4	CER	B	960	1	-	2/5/6/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	960	CER	C2-C3-C4-O1
4	B	960	CER	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	960	CER	2	0
4	A	960	CER	1	0
2	A	950	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	869/915 (94%)	-0.09	15 (1%) 69 64	7, 20, 38, 50	0
1	B	873/915 (95%)	-0.06	21 (2%) 59 54	7, 19, 40, 61	0
All	All	1742/1830 (95%)	-0.08	36 (2%) 63 58	7, 20, 39, 61	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	LEU	5.1
1	A	499	ASP	4.3
1	B	771	ASP	4.2
1	B	710	LEU	3.8
1	A	860	ASP	3.5
1	A	849	GLU	3.2
1	B	555	ASP	3.1
1	B	162	THR	3.0
1	B	467	HIS	3.0
1	B	415	SER	2.9
1	B	772	ILE	2.9
1	A	469	GLY	2.9
1	B	417	GLY	2.9
1	A	500	ALA	2.7
1	B	600	ASP	2.7
1	A	746	ASP	2.6
1	B	465	THR	2.5
1	B	163	ALA	2.4
1	B	464	THR	2.4
1	A	417	GLY	2.4
1	B	708	ASP	2.3
1	B	161	ASP	2.3
1	B	709	ARG	2.3
1	B	413	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	2.3
1	B	542	ALA	2.3
1	A	361	ASP	2.2
1	B	501	ASP	2.2
1	A	415	SER	2.1
1	B	359	ASP	2.1
1	A	709	ARG	2.1
1	A	701	GLU	2.1
1	B	541	ALA	2.1
1	B	543	THR	2.1
1	A	359	ASP	2.1
1	A	553	GLU	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, 95th 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(\AA^2)	Q<0.9
4	CER	A	960	8/16	0.81	0.16	38,40,42,43	0
2	ACT	B	950	4/4	0.84	0.20	37,37,37,37	0
2	ACT	A	950	4/4	0.84	0.15	30,30,31,31	0
4	CER	B	960	8/16	0.91	0.15	40,42,47,49	0
3	CL	A	2	1/1	0.95	0.08	36,36,36,36	0
3	CL	B	1	1/1	0.95	0.08	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.