



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:01 AM UTC

PDB ID : 7EAV / pdb_00007eav
Title : The X-ray crystallographic structure of glycogen debranching enzyme from *Sulfolobus solfataricus* STB09
Authors : Li, Z.F.; Ban, X.F.; Tian, Y.X.; Li, C.M.; Cheng, L.; Hong, Y.; Gu, Z.B.
Deposited on : 2021-03-08
Resolution : 2.80 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

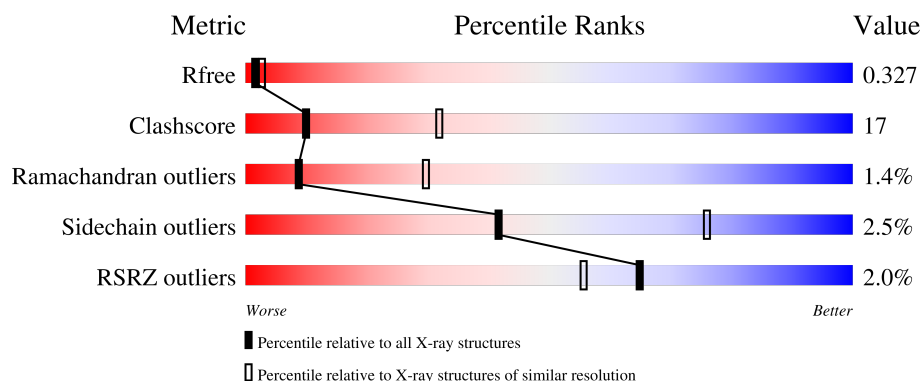
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

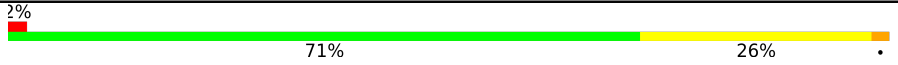
The reported resolution of this entry is 2.80 Å.

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	718	
1	B	718	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11872 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 Glycogen debranching enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5848	3753	985	1091	19			
1	B	714	Total	C	N	O	S	0	0	0
			5844	3749	985	1091	19			

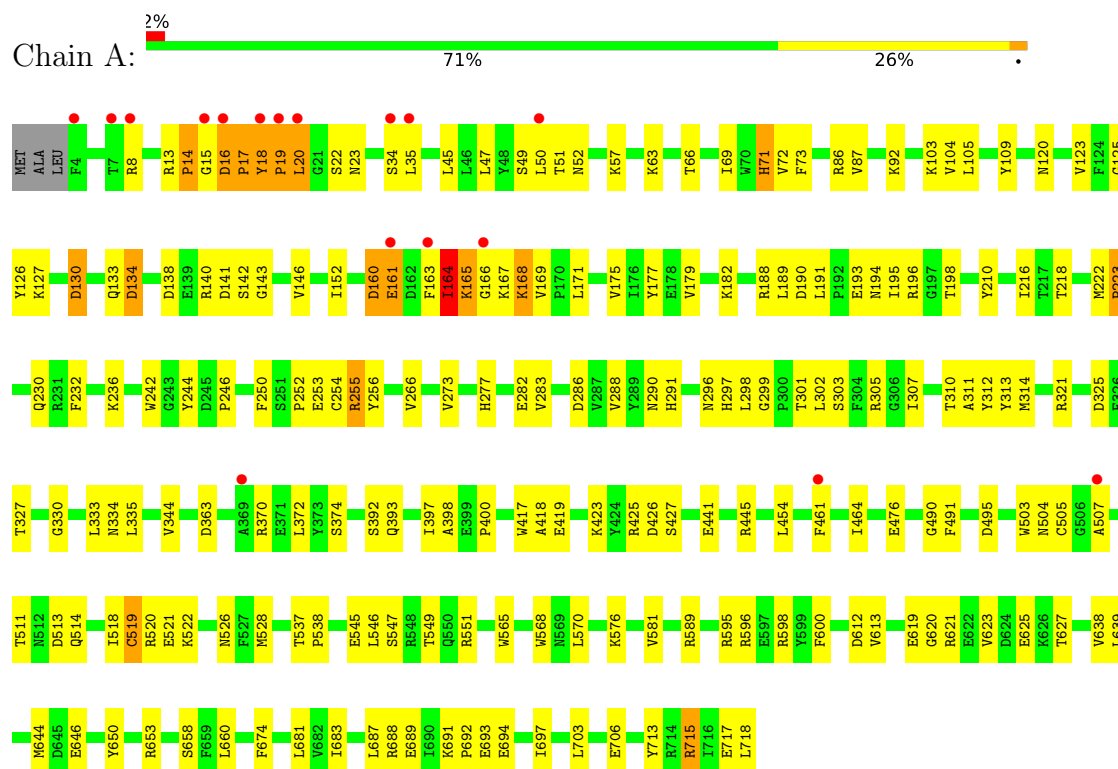
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	90	Total	O	0	0
			90	90		

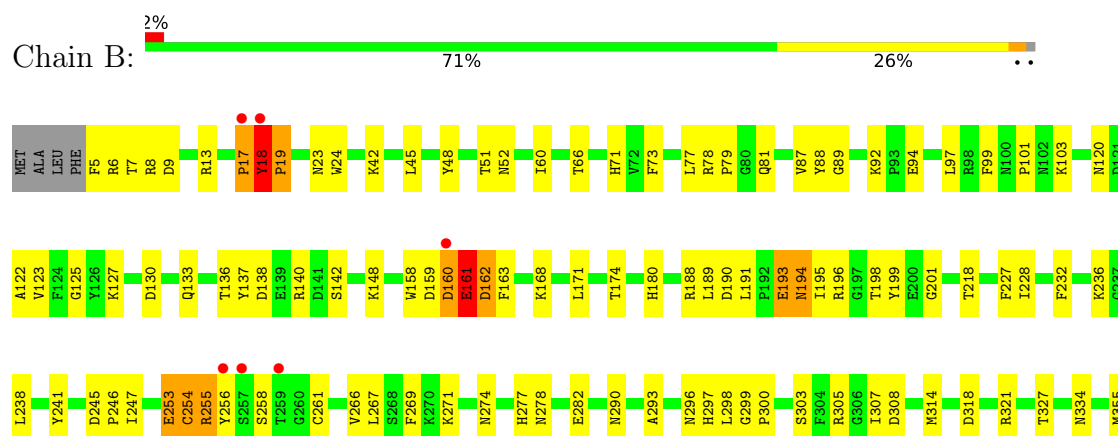
3 Residue-property plots

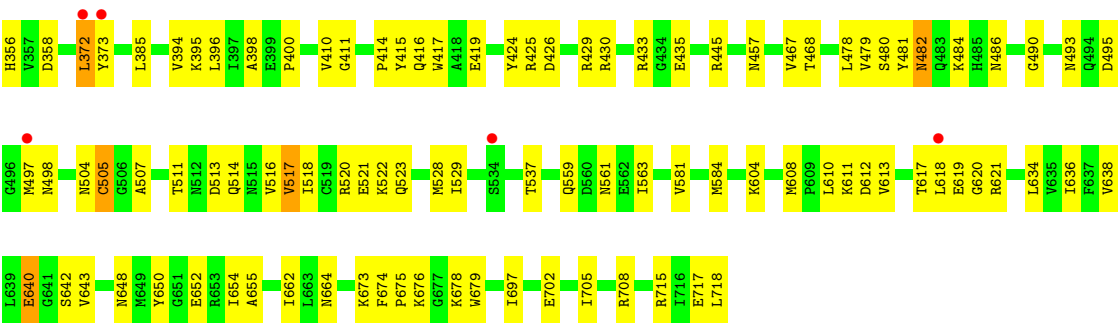
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycogen debranching enzyme



• Molecule 1: Glycogen debranching enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.54Å 203.54Å 89.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.11 – 2.80 49.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.11-2.80) 98.9 (49.11-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.264 , 0.325 0.272 , 0.327	Depositor DCC
R_{free} test set	2605 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11872	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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

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	0.33	0/6002	0.50	3/8136 (0.0%)
1	B	0.25	0/5997	0.45	2/8130 (0.0%)
All	All	0.29	0/11999	0.47	5/16266 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	ILE	N-CA-C	6.70	117.49	110.72
1	A	160	ASP	N-CA-C	6.06	119.99	112.47
1	A	514	GLN	N-CA-C	5.63	118.14	111.33
1	B	161	GLU	N-CA-C	-5.40	107.06	113.97
1	A	255	ARG	N-CA-C	5.15	119.05	112.87

There are no chirality outliers.

There are no planarity outliers.

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	5848	0	5662	218	0
1	B	5844	0	5671	190	0
2	A	90	0	0	5	0
2	B	90	0	0	4	0
All	All	11872	0	11333	399	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 17.

All (399) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HB3	1:A:109:TYR:CD2	1.37	1.59
1:B:254:CYS:HB2	1:B:261:CYS:SG	1.59	1.41
1:B:18:TYR:HB3	1:B:19:PRO:CD	1.53	1.38
1:A:20:LEU:HB3	1:A:109:TYR:CE2	1.66	1.28
1:A:20:LEU:HG	1:A:109:TYR:CZ	1.78	1.17
1:A:505:CYS:HB3	1:A:519:CYS:SG	1.85	1.16
1:A:164:ILE:HD13	1:A:277:HIS:HD2	1.10	1.15
1:A:20:LEU:HB3	1:A:109:TYR:CG	1.81	1.15
1:A:20:LEU:CB	1:A:109:TYR:CD2	2.32	1.13
1:A:17:PRO:HG3	1:A:71:HIS:ND1	1.63	1.11
1:A:505:CYS:CB	1:A:519:CYS:SG	2.40	1.10
1:A:19:PRO:C	1:A:20:LEU:HD13	1.76	1.10
1:B:254:CYS:CB	1:B:261:CYS:SG	2.40	1.09
1:A:504:ASN:HB2	1:A:507:ALA:O	1.51	1.08
1:B:18:TYR:HB3	1:B:19:PRO:HD3	1.24	1.07
1:A:393:GLN:HG2	1:B:18:TYR:CZ	1.89	1.06
1:A:393:GLN:HG2	1:B:18:TYR:OH	1.54	1.05
1:B:17:PRO:HG3	1:B:66:THR:OG1	1.56	1.04
1:B:290:ASN:HD22	1:B:327:THR:CG2	1.75	0.99
1:B:18:TYR:CB	1:B:19:PRO:CD	2.42	0.98
1:A:164:ILE:HD13	1:A:277:HIS:CD2	2.00	0.96
1:A:20:LEU:CB	1:A:109:TYR:CG	2.47	0.96
1:B:18:TYR:HB3	1:B:19:PRO:HD2	1.45	0.95
1:A:164:ILE:HG21	1:A:277:HIS:CD2	2.03	0.93
1:A:715:ARG:HH11	1:A:715:ARG:HB3	1.33	0.93
1:A:164:ILE:CD1	1:A:277:HIS:HD2	1.80	0.92
1:A:17:PRO:CG	1:A:71:HIS:CE1	2.53	0.91
1:B:198:THR:HG21	1:B:258:SER:HB3	1.52	0.90
1:A:20:LEU:CB	1:A:109:TYR:CE2	2.51	0.89
1:A:715:ARG:HE	1:A:718:LEU:HD22	1.36	0.89
1:A:17:PRO:HG3	1:A:71:HIS:CE1	2.08	0.89
1:B:198:THR:CG2	1:B:258:SER:HB3	2.02	0.89
1:A:715:ARG:HH21	1:A:718:LEU:CD2	1.85	0.88
1:A:20:LEU:CG	1:A:109:TYR:CZ	2.57	0.87
1:B:504:ASN:HB2	1:B:507:ALA:O	1.75	0.86
1:B:6:ARG:HH21	1:B:8:ARG:HB3	1.41	0.85
1:B:198:THR:HG21	1:B:258:SER:CB	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ARG:HH21	1:A:718:LEU:HD22	1.40	0.84
1:A:17:PRO:CG	1:A:71:HIS:ND1	2.41	0.82
1:A:8:ARG:HH12	1:A:63:LYS:HZ3	1.22	0.82
1:B:290:ASN:HD22	1:B:327:THR:HG22	1.43	0.82
1:A:18:TYR:HB3	1:A:19:PRO:HD3	1.61	0.81
1:B:290:ASN:HD22	1:B:327:THR:HG21	1.43	0.81
1:B:504:ASN:CB	1:B:507:ALA:O	2.28	0.81
1:A:17:PRO:HD3	1:A:71:HIS:CE1	2.16	0.81
1:A:715:ARG:NE	1:A:718:LEU:HD22	1.95	0.81
1:A:8:ARG:HH12	1:A:63:LYS:NZ	1.79	0.80
1:A:715:ARG:NH2	1:A:718:LEU:HD22	1.96	0.80
1:A:19:PRO:HB3	1:A:23:ASN:ND2	1.98	0.77
1:A:19:PRO:C	1:A:20:LEU:CD1	2.55	0.77
1:A:161:GLU:OE1	1:A:277:HIS:CG	2.36	0.77
1:A:193:GLU:O	1:A:194:ASN:ND2	2.18	0.76
1:A:19:PRO:O	1:A:20:LEU:CD1	2.33	0.76
1:B:640:GLU:HB3	1:B:643:VAL:HG22	1.68	0.76
1:A:8:ARG:NH1	1:A:63:LYS:HZ3	1.85	0.75
1:A:17:PRO:CD	1:A:71:HIS:CE1	2.70	0.75
1:A:14:PRO:O	1:A:72:VAL:HA	1.86	0.75
1:A:715:ARG:HH11	1:A:715:ARG:CB	1.99	0.74
1:A:161:GLU:O	1:A:161:GLU:HG3	1.88	0.74
1:A:393:GLN:CG	1:B:18:TYR:OH	2.34	0.74
1:B:619:GLU:OE2	1:B:619:GLU:N	2.17	0.73
1:A:236:LYS:NZ	1:A:490:GLY:O	2.21	0.73
1:A:290:ASN:ND2	1:A:363:ASP:O	2.22	0.72
1:A:20:LEU:HB3	1:A:109:TYR:CZ	2.23	0.72
1:A:13:ARG:HD3	1:B:650:TYR:HA	1.72	0.72
1:A:17:PRO:HB3	1:A:69:ILE:HG21	1.70	0.72
1:A:504:ASN:CB	1:A:507:ALA:O	2.34	0.72
1:A:198:THR:HB	1:A:256:TYR:O	1.90	0.72
1:B:482:ASN:HD21	1:B:504:ASN:CG	1.98	0.71
1:B:18:TYR:CB	1:B:19:PRO:HD3	2.14	0.71
1:B:198:THR:CB	1:B:258:SER:HB3	2.20	0.71
1:B:159:ASP:O	1:B:160:ASP:C	2.33	0.71
1:B:193:GLU:HA	1:B:196:ARG:HG3	1.71	0.71
1:B:522:LYS:NZ	1:B:708:ARG:O	2.24	0.70
1:B:618:LEU:HG	1:B:619:GLU:OE2	1.91	0.70
1:A:19:PRO:HB3	1:A:23:ASN:HD21	1.54	0.70
1:A:193:GLU:HA	1:A:196:ARG:HG3	1.73	0.70
1:B:236:LYS:NZ	1:B:490:GLY:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HB3	1:A:303:SER:HA	1.74	0.69
1:B:662:ILE:HG21	1:B:705:ILE:HD13	1.75	0.69
1:A:19:PRO:O	1:A:20:LEU:HD13	1.91	0.69
1:A:715:ARG:CZ	1:A:718:LEU:HD22	2.23	0.69
1:A:715:ARG:NH2	1:A:718:LEU:CD2	2.54	0.69
1:A:660:LEU:HB3	1:A:713:TYR:HB2	1.75	0.68
1:A:301:THR:HG23	1:A:305:ARG:HB3	1.75	0.68
1:A:109:TYR:CE1	1:A:250:PHE:CZ	2.82	0.68
1:A:8:ARG:HH22	1:A:63:LYS:HZ3	1.42	0.68
1:A:20:LEU:CB	1:A:109:TYR:CD1	2.77	0.67
1:B:429:ARG:HH21	1:B:478:LEU:HD13	1.58	0.67
1:A:164:ILE:CD1	1:A:277:HIS:CD2	2.70	0.67
1:B:504:ASN:O	1:B:505:CYS:HB2	1.95	0.67
1:A:20:LEU:HG	1:A:109:TYR:CE1	2.29	0.67
1:A:20:LEU:CG	1:A:109:TYR:CE1	2.79	0.66
1:A:20:LEU:HD13	1:A:20:LEU:N	2.09	0.66
1:B:520:ARG:O	1:B:523:GLN:N	2.28	0.66
1:B:253:GLU:OE1	1:B:255:ARG:HB3	1.96	0.66
1:B:296:ASN:ND2	1:B:297:HIS:O	2.29	0.65
1:A:20:LEU:HB2	1:A:109:TYR:CG	2.31	0.65
1:B:254:CYS:CB	1:B:261:CYS:HG	2.01	0.65
1:B:199:TYR:CE1	1:B:256:TYR:HB3	2.32	0.65
1:A:164:ILE:CG2	1:A:277:HIS:CD2	2.79	0.64
1:B:504:ASN:ND2	1:B:507:ALA:O	2.30	0.64
1:A:20:LEU:CB	1:A:109:TYR:CZ	2.81	0.64
1:A:134:ASP:OD2	1:A:321:ARG:NH2	2.27	0.64
1:A:188:ARG:HG3	1:A:190:ASP:HB3	1.81	0.63
1:A:20:LEU:HB3	1:A:109:TYR:CD1	2.33	0.63
1:A:123:VAL:HG12	1:A:142:SER:HB2	1.80	0.63
1:B:89:GLY:HA3	1:B:99:PHE:HD2	1.62	0.63
1:B:529:ILE:HA	1:B:584:MET:HE2	1.80	0.63
1:B:247:ILE:HG23	1:B:293:ALA:HB3	1.81	0.63
1:B:94:GLU:HA	1:B:321:ARG:HB2	1.80	0.63
1:A:393:GLN:HG2	1:B:18:TYR:CE2	2.33	0.63
1:B:619:GLU:HA	1:B:673:LYS:HD3	1.81	0.62
1:A:522:LYS:O	1:A:526:ASN:ND2	2.32	0.62
1:B:198:THR:HB	1:B:258:SER:HB3	1.81	0.62
1:B:195:ILE:HD12	1:B:201:GLY:HA2	1.80	0.61
1:A:109:TYR:CD1	1:A:250:PHE:CZ	2.88	0.61
1:A:296:ASN:ND2	1:A:297:HIS:O	2.33	0.61
1:A:20:LEU:HG	1:A:109:TYR:CE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:NZ	1:B:122:ALA:O	2.33	0.61
1:B:300:PRO:O	1:B:305:ARG:NH1	2.34	0.61
1:A:20:LEU:HD23	1:A:109:TYR:CE1	2.35	0.61
1:A:19:PRO:O	1:A:20:LEU:HD12	1.99	0.60
1:A:549:THR:HG22	1:A:551:ARG:H	1.65	0.60
1:A:505:CYS:CB	1:A:519:CYS:HG	1.99	0.60
1:B:18:TYR:CB	1:B:19:PRO:HD2	2.24	0.60
1:B:480:SER:HA	1:B:520:ARG:NH2	2.17	0.60
1:B:497:MET:HE3	1:B:498:ASN:H	1.67	0.60
1:B:127:LYS:HB3	1:B:130:ASP:HB2	1.84	0.60
1:B:123:VAL:HG12	1:B:142:SER:HB2	1.83	0.59
1:A:218:THR:HG22	1:A:282:GLU:HB2	1.84	0.59
1:B:24:TRP:CD2	1:B:79:PRO:HD3	2.37	0.59
1:A:8:ARG:NH2	1:A:63:LYS:HZ3	1.98	0.59
1:B:481:TYR:C	1:B:482:ASN:OD1	2.45	0.59
1:B:161:GLU:OE1	1:B:356:HIS:ND1	2.33	0.59
1:B:168:LYS:NZ	2:B:814:HOH:O	2.36	0.59
1:A:19:PRO:HG3	1:A:23:ASN:ND2	2.18	0.59
1:B:193:GLU:C	1:B:195:ILE:H	2.11	0.59
1:B:520:ARG:O	1:B:521:GLU:C	2.40	0.59
1:A:8:ARG:HH22	1:A:63:LYS:NZ	2.00	0.58
1:A:691:LYS:HD2	1:A:693:GLU:HB2	1.83	0.58
1:B:189:LEU:HD12	1:B:189:LEU:H	1.68	0.58
1:A:18:TYR:HB3	1:A:19:PRO:CD	2.31	0.58
1:A:105:LEU:HD12	1:A:302:LEU:C	2.29	0.58
1:A:311:ALA:O	1:A:313:TYR:N	2.37	0.58
1:A:193:GLU:HG2	1:A:194:ASN:N	2.19	0.58
1:B:636:ILE:HD12	1:B:662:ILE:HD12	1.86	0.58
1:B:162:ASP:OD1	1:B:162:ASP:N	2.34	0.57
1:B:158:TRP:HB3	1:B:161:GLU:HG2	1.85	0.57
1:B:513:ASP:HB3	1:B:516:VAL:HG23	1.87	0.57
1:B:290:ASN:ND2	1:B:327:THR:HG21	2.17	0.57
1:A:16:ASP:C	1:A:18:TYR:H	2.13	0.56
1:B:92:LYS:NZ	2:B:819:HOH:O	2.38	0.56
1:A:161:GLU:OE1	1:A:277:HIS:CB	2.54	0.56
1:B:482:ASN:OD1	1:B:504:ASN:HB3	2.05	0.56
1:A:19:PRO:CB	1:A:23:ASN:ND2	2.67	0.55
1:A:253:GLU:CG	1:A:255:ARG:HG2	2.36	0.55
1:B:290:ASN:ND2	1:B:327:THR:CG2	2.59	0.55
1:A:688:ARG:NH2	1:A:706:GLU:OE2	2.39	0.55
1:A:16:ASP:O	1:A:18:TYR:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TRP:HB3	1:A:244:TYR:HD1	1.71	0.55
1:B:559:GLN:HG2	1:B:563:ILE:HD12	1.88	0.55
1:A:650:TYR:HA	1:B:13:ARG:HD3	1.88	0.55
1:A:17:PRO:HD3	1:A:71:HIS:ND1	2.22	0.55
1:A:522:LYS:NZ	2:A:814:HOH:O	2.39	0.54
1:B:415:TYR:O	1:B:416:GLN:HB3	2.06	0.54
1:A:17:PRO:CD	1:A:71:HIS:ND1	2.70	0.54
1:A:51:THR:OG1	1:A:52:ASN:N	2.40	0.54
1:A:193:GLU:HG2	1:A:194:ASN:H	1.71	0.54
1:A:528:MET:HG2	1:A:581:VAL:HG22	1.89	0.54
1:A:425:ARG:NH1	1:A:426:ASP:OD1	2.41	0.54
1:A:596:ARG:NE	1:A:646:GLU:HG2	2.23	0.53
1:A:8:ARG:CZ	1:A:63:LYS:HZ3	2.21	0.53
1:A:161:GLU:OE1	1:A:277:HIS:ND1	2.40	0.53
1:A:619:GLU:O	1:A:621:ARG:N	2.42	0.53
1:A:503:TRP:CZ3	1:A:505:CYS:HA	2.42	0.53
1:B:636:ILE:HD12	1:B:662:ILE:CD1	2.39	0.53
1:A:66:THR:HB	1:A:71:HIS:HE1	1.73	0.53
1:A:242:TRP:HB3	1:A:244:TYR:CD1	2.43	0.53
1:A:17:PRO:CB	1:A:69:ILE:HG21	2.37	0.53
1:B:6:ARG:HG2	1:B:7:THR:H	1.72	0.53
1:B:372:LEU:HG	1:B:373:TYR:HD1	1.73	0.53
1:A:400:PRO:HG3	1:A:419:GLU:HB3	1.91	0.53
1:B:198:THR:HG21	1:B:258:SER:HB2	1.89	0.53
1:A:20:LEU:CG	1:A:109:TYR:CE2	2.87	0.52
1:A:596:ARG:HD3	1:A:600:PHE:CE1	2.43	0.52
1:B:171:LEU:HG	1:B:537:THR:HG21	1.90	0.52
1:A:18:TYR:CB	1:A:19:PRO:CD	2.87	0.52
1:A:103:LYS:HE3	1:A:125:GLY:H	1.75	0.52
1:B:282:GLU:CD	1:B:395:LYS:HZ1	2.18	0.52
1:A:20:LEU:CD1	1:A:20:LEU:N	2.73	0.52
1:B:414:PRO:O	1:B:417:TRP:HB2	2.09	0.52
1:A:223:PRO:HD3	1:A:286:ASP:HB3	1.92	0.52
1:B:191:LEU:O	1:B:196:ARG:NH1	2.42	0.52
1:B:87:VAL:HG21	1:B:307:ILE:HD13	1.92	0.51
1:A:694:GLU:HG2	1:A:703:LEU:HD21	1.91	0.51
1:B:610:LEU:HB3	1:B:640:GLU:HG2	1.91	0.51
1:A:17:PRO:HG3	1:A:69:ILE:CG2	2.40	0.51
1:A:20:LEU:CB	1:A:109:TYR:CE1	2.94	0.51
1:A:546:LEU:HD22	1:A:570:LEU:HD21	1.93	0.51
1:B:290:ASN:ND2	1:B:327:THR:HG22	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:GLU:C	1:B:621:ARG:H	2.17	0.51
1:B:640:GLU:HB3	1:B:643:VAL:CG2	2.38	0.51
1:B:218:THR:HG22	1:B:282:GLU:HB2	1.92	0.51
1:A:86:ARG:NH2	1:A:141:ASP:OD2	2.40	0.51
1:A:50:LEU:HD23	1:A:50:LEU:H	1.76	0.51
1:B:648:ASN:HD21	1:B:652:GLU:HB2	1.76	0.51
1:A:109:TYR:HE1	1:A:250:PHE:CZ	2.29	0.51
1:A:370:ARG:HA	1:A:374:SER:O	2.11	0.51
1:A:393:GLN:CG	1:B:18:TYR:CZ	2.81	0.50
1:B:486:ASN:ND2	1:B:495:ASP:O	2.42	0.50
1:A:177:TYR:HB2	1:A:216:ILE:HG21	1.92	0.50
1:B:133:GLN:O	1:B:136:THR:OG1	2.28	0.50
1:A:8:ARG:HH11	1:A:8:ARG:HG3	1.76	0.50
1:A:688:ARG:HG2	1:A:689:GLU:N	2.26	0.50
1:A:691:LYS:HD3	1:A:692:PRO:HD2	1.93	0.50
1:B:193:GLU:O	1:B:195:ILE:N	2.40	0.50
1:B:193:GLU:CD	1:B:194:ASN:H	2.20	0.50
1:A:623:VAL:HG13	1:A:627:THR:HG23	1.94	0.50
1:A:681:LEU:HD23	1:A:713:TYR:CZ	2.47	0.50
1:B:48:TYR:CZ	1:B:148:LYS:HE2	2.46	0.50
1:B:679:TRP:CZ3	1:B:715:ARG:HB2	2.46	0.50
1:A:392:SER:HB2	1:B:18:TYR:HE1	1.77	0.50
1:A:521:GLU:HB3	1:A:687:LEU:HD21	1.93	0.50
1:A:312:TYR:O	1:A:333:LEU:HD12	2.12	0.50
1:A:674:PHE:CG	1:A:697:ILE:HG21	2.47	0.50
1:A:120:ASN:O	1:A:123:VAL:HG22	2.12	0.49
1:B:19:PRO:HB2	1:B:23:ASN:OD1	2.12	0.49
1:A:182:LYS:HD3	1:A:565:TRP:CH2	2.46	0.49
1:B:103:LYS:HE3	1:B:125:GLY:HA2	1.94	0.49
1:A:311:ALA:C	1:A:313:TYR:H	2.20	0.49
1:A:17:PRO:HG3	1:A:69:ILE:HG22	1.95	0.49
1:B:45:LEU:N	1:B:60:ILE:O	2.38	0.49
1:B:398:ALA:HB2	1:B:417:TRP:CE3	2.48	0.49
1:A:20:LEU:CD2	1:A:109:TYR:CE1	2.95	0.49
1:A:398:ALA:HB2	1:A:417:TRP:CZ3	2.48	0.49
1:A:715:ARG:HD3	1:A:717:GLU:O	2.11	0.49
1:B:457:ASN:ND2	2:B:822:HOH:O	2.45	0.49
1:A:127:LYS:HE2	1:A:130:ASP:OD1	2.12	0.49
1:B:480:SER:HA	1:B:520:ARG:HH21	1.77	0.49
1:A:20:LEU:HG	1:A:109:TYR:OH	2.11	0.48
1:B:528:MET:HG2	1:B:581:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:OH	1:A:545:GLU:OE1	2.28	0.48
1:B:77:LEU:HD13	1:B:81:GLN:HG2	1.95	0.48
1:A:393:GLN:CG	1:B:18:TYR:CE2	2.96	0.48
1:B:676:LYS:HE2	1:B:676:LYS:H	1.77	0.48
1:A:152:ILE:O	2:A:801:HOH:O	2.20	0.48
1:B:17:PRO:HG3	1:B:66:THR:HG1	1.73	0.48
1:B:199:TYR:CZ	1:B:256:TYR:HB2	2.47	0.48
1:B:482:ASN:OD1	1:B:482:ASN:N	2.45	0.48
1:A:17:PRO:CG	1:A:69:ILE:HG21	2.44	0.48
1:A:20:LEU:HB2	1:A:109:TYR:CD1	2.48	0.48
1:A:163:PHE:C	1:A:165:LYS:H	2.21	0.48
1:A:166:GLY:O	1:A:168:LYS:N	2.46	0.48
1:A:335:LEU:HD21	1:A:344:VAL:HG21	1.95	0.48
1:A:18:TYR:CB	1:A:19:PRO:HD3	2.36	0.48
1:B:189:LEU:HA	1:B:196:ARG:NH1	2.29	0.48
1:A:19:PRO:CG	1:A:23:ASN:ND2	2.76	0.47
1:A:191:LEU:HB3	1:A:195:ILE:HD11	1.95	0.47
1:B:17:PRO:HB3	1:B:71:HIS:CD2	2.49	0.47
1:B:673:LYS:HG3	1:B:702:GLU:HG2	1.96	0.47
1:A:87:VAL:HG21	1:A:307:ILE:HA	1.94	0.47
1:B:278:ASN:O	2:B:801:HOH:O	2.20	0.47
1:A:491:PHE:HB2	1:A:495:ASP:OD2	2.15	0.47
1:A:291:HIS:HB3	1:A:327:THR:HG21	1.96	0.47
1:B:159:ASP:O	1:B:161:GLU:N	2.48	0.47
1:B:433:ARG:NH1	1:B:435:GLU:OE1	2.41	0.47
1:A:22:SER:O	1:A:23:ASN:OD1	2.32	0.47
1:A:246:PRO:HG3	1:A:288:VAL:HB	1.97	0.47
1:A:505:CYS:SG	1:A:520:ARG:HG2	2.55	0.47
1:B:715:ARG:HD3	1:B:718:LEU:HB2	1.97	0.47
1:B:120:ASN:O	1:B:123:VAL:HG22	2.14	0.47
1:B:103:LYS:NZ	1:B:125:GLY:H	2.13	0.47
1:B:517:VAL:O	1:B:520:ARG:HB2	2.15	0.47
1:A:464:ILE:HD13	1:A:537:THR:HB	1.96	0.46
1:A:715:ARG:CB	1:A:715:ARG:NH1	2.74	0.46
1:B:642:SER:HA	1:B:655:ALA:HB1	1.97	0.46
1:A:104:VAL:HG21	1:A:143:GLY:HA2	1.96	0.46
1:B:604:LYS:HA	1:B:611:LYS:HA	1.97	0.46
1:A:164:ILE:O	1:A:164:ILE:HG23	2.15	0.46
1:B:171:LEU:HA	1:B:174:THR:OG1	2.16	0.46
1:A:314:MET:HG3	1:A:334:ASN:HA	1.97	0.46
1:B:429:ARG:O	1:B:433:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:NH2	1:B:8:ARG:HE	2.14	0.46
1:B:619:GLU:O	1:B:621:ARG:N	2.47	0.46
1:B:400:PRO:HG2	1:B:410:VAL:HG22	1.98	0.46
1:A:175:VAL:HG13	1:A:538:PRO:HG2	1.98	0.45
1:A:397:ILE:HG12	1:A:418:ALA:HB3	1.99	0.45
1:A:546:LEU:HD11	1:A:568:TRP:CZ3	2.51	0.45
1:A:596:ARG:HH21	1:A:598:ARG:HB2	1.81	0.45
1:A:619:GLU:HG2	1:A:621:ARG:HG3	1.98	0.45
1:A:639:LEU:O	1:A:658:SER:HA	2.17	0.45
1:B:227:PHE:CE1	1:B:255:ARG:CZ	3.00	0.45
1:A:253:GLU:OE1	1:A:255:ARG:HG2	2.16	0.45
1:A:20:LEU:HB3	1:A:109:TYR:CE1	2.52	0.45
1:A:612:ASP:OD1	1:A:613:VAL:N	2.49	0.45
1:B:227:PHE:HA	1:B:246:PRO:HA	1.99	0.45
1:A:252:PRO:HD2	1:A:266:VAL:HG12	1.99	0.45
1:B:424:TYR:HA	1:B:445:ARG:HD3	1.97	0.45
1:A:297:HIS:C	1:A:299:GLY:H	2.24	0.45
1:B:42:LYS:HB3	1:B:88:TYR:HB2	1.99	0.45
1:B:180:HIS:NE2	1:B:241:TYR:O	2.33	0.45
1:A:8:ARG:CZ	1:A:8:ARG:HB2	2.46	0.45
1:A:230:GLN:NE2	1:A:230:GLN:HA	2.31	0.45
1:B:51:THR:OG1	1:B:52:ASN:N	2.50	0.45
1:B:159:ASP:CG	1:B:274:ASN:HD21	2.25	0.45
1:B:648:ASN:ND2	1:B:652:GLU:HB2	2.32	0.45
1:A:193:GLU:C	1:A:195:ILE:H	2.25	0.44
1:B:648:ASN:HB3	1:B:654:ILE:HD11	1.99	0.44
1:B:78:ARG:HB3	1:B:79:PRO:HD2	2.00	0.44
1:B:314:MET:HG3	1:B:334:ASN:HA	2.00	0.44
1:A:109:TYR:CE1	1:A:250:PHE:HZ	2.34	0.44
1:B:266:VAL:HG23	1:B:355:MET:HE1	1.99	0.44
1:B:608:MET:HG3	1:B:643:VAL:HG12	1.99	0.44
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.76	0.44
1:B:120:ASN:C	1:B:122:ALA:H	2.26	0.44
1:B:13:ARG:HB2	1:B:73:PHE:HD2	1.83	0.44
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.74	0.44
1:B:621:ARG:HD2	1:B:621:ARG:HA	1.82	0.44
1:B:358:ASP:O	1:B:394:VAL:HB	2.17	0.44
1:B:174:THR:HG23	1:B:218:THR:HG23	1.99	0.44
1:B:479:VAL:O	1:B:520:ARG:HG2	2.18	0.44
1:B:87:VAL:HG21	1:B:307:ILE:HA	2.00	0.44
1:B:426:ASP:O	1:B:430:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ARG:NH1	1:B:467:VAL:O	2.51	0.43
1:B:612:ASP:N	1:B:612:ASP:OD1	2.50	0.43
1:B:678:LYS:HB3	1:B:717:GLU:HB3	1.99	0.43
1:A:92:LYS:NZ	2:A:824:HOH:O	2.52	0.43
1:B:269:PHE:CD1	1:B:355:MET:HE3	2.54	0.43
1:A:273:VAL:HG23	1:A:283:VAL:HG21	2.01	0.43
1:A:14:PRO:HB2	1:A:15:GLY:H	1.64	0.43
1:A:687:LEU:N	2:A:814:HOH:O	2.46	0.43
1:B:228:ILE:HD11	1:B:247:ILE:HD13	2.01	0.43
1:A:109:TYR:HE1	1:A:250:PHE:HZ	1.66	0.43
1:A:253:GLU:HG3	1:A:255:ARG:HG2	1.99	0.43
1:B:103:LYS:HZ1	1:B:125:GLY:H	1.67	0.43
1:B:675:PRO:HG2	1:B:679:TRP:CZ2	2.53	0.43
1:A:576:LYS:HD3	1:A:576:LYS:HA	1.67	0.43
1:B:92:LYS:N	1:B:97:LEU:O	2.49	0.43
1:B:613:VAL:HA	1:B:638:VAL:O	2.19	0.43
1:B:425:ARG:NH1	1:B:426:ASP:OD1	2.46	0.43
1:B:160:ASP:OD1	1:B:163:PHE:HB2	2.19	0.43
1:A:476:GLU:OE1	1:A:547:SER:HB3	2.20	0.42
1:B:13:ARG:HB2	1:B:73:PHE:CD2	2.55	0.42
1:A:133:GLN:HB2	1:A:298:LEU:CD2	2.50	0.42
1:B:297:HIS:ND1	1:B:298:LEU:HG	2.33	0.42
1:B:634:LEU:HD12	1:B:664:ASN:HB2	2.01	0.42
1:B:267:LEU:HG	1:B:271:LYS:HE2	2.01	0.42
1:B:415:TYR:C	1:B:417:TRP:H	2.27	0.42
1:A:325:ASP:OD2	1:A:330:GLY:N	2.53	0.42
1:B:297:HIS:C	1:B:299:GLY:H	2.26	0.42
1:B:484:LYS:HG3	1:B:493:ASN:HD21	1.84	0.42
1:B:559:GLN:HG3	1:B:561:ASN:HD21	1.83	0.42
1:A:311:ALA:O	1:A:312:TYR:HB2	2.19	0.42
1:B:484:LYS:HG3	1:B:493:ASN:ND2	2.34	0.42
1:B:199:TYR:CE1	1:B:256:TYR:CB	3.01	0.42
1:B:617:THR:OG1	1:B:618:LEU:N	2.52	0.42
1:A:13:ARG:HB2	1:A:73:PHE:HB3	2.02	0.42
1:B:411:GLY:H	1:B:419:GLU:CD	2.27	0.42
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.87	0.42
1:B:127:LYS:HD3	1:B:136:THR:HB	2.02	0.42
1:B:199:TYR:CZ	1:B:256:TYR:CB	3.03	0.42
1:B:467:VAL:HG23	1:B:468:THR:HG23	2.02	0.42
1:B:514:GLN:HA	1:B:517:VAL:HG12	2.02	0.42
1:A:189:LEU:HA	1:A:196:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ASP:OD1	1:B:318:ASP:N	2.44	0.41
1:B:516:VAL:O	1:B:520:ARG:HD2	2.19	0.41
1:A:138:ASP:OD1	1:A:140:ARG:HB2	2.20	0.41
1:A:694:GLU:HG2	1:A:703:LEU:HD11	2.02	0.41
1:B:5:PHE:HB3	1:B:9:ASP:HB2	2.02	0.41
1:B:188:ARG:NH1	1:B:190:ASP:OD2	2.52	0.41
1:B:188:ARG:O	1:B:196:ARG:HD3	2.20	0.41
1:A:126:TYR:HB2	2:A:820:HOH:O	2.20	0.41
1:A:45:LEU:HD21	1:A:47:LEU:HD21	2.02	0.41
1:A:49:SER:HB2	1:A:57:LYS:HD3	2.03	0.41
1:A:104:VAL:CG2	1:A:143:GLY:HA2	2.50	0.41
1:A:232:PHE:O	1:A:236:LYS:HD2	2.20	0.41
1:B:161:GLU:OE2	1:B:277:HIS:ND1	2.52	0.41
1:A:423:LYS:O	1:A:427:SER:OG	2.36	0.41
1:A:13:ARG:O	1:A:14:PRO:C	2.64	0.41
1:B:253:GLU:OE2	1:B:253:GLU:HA	2.21	0.41
1:B:385:LEU:HD21	1:B:396:LEU:HD13	2.03	0.41
1:B:504:ASN:O	1:B:505:CYS:CB	2.63	0.41
1:B:674:PHE:CZ	1:B:697:ILE:HG13	2.56	0.41
1:A:142:SER:O	1:A:146:VAL:HG23	2.20	0.41
1:A:179:VAL:O	1:A:222:MET:HG3	2.20	0.41
1:B:101:PRO:HD2	1:B:137:TYR:OH	2.21	0.41
1:B:194:ASN:O	1:B:258:SER:HB2	2.21	0.41
1:B:232:PHE:O	1:B:236:LYS:HD2	2.21	0.41
1:A:171:LEU:HD13	1:A:461:PHE:HB3	2.01	0.41
1:A:19:PRO:HB2	1:A:20:LEU:H	1.69	0.40
1:A:441:GLU:O	1:A:445:ARG:HG2	2.21	0.40
1:A:589:ARG:HA	1:A:595:ARG:HE	1.86	0.40
1:A:644:MET:O	1:A:653:ARG:HD2	2.21	0.40
1:B:138:ASP:OD1	1:B:140:ARG:HB2	2.21	0.40
1:A:398:ALA:HB2	1:A:417:TRP:CE3	2.57	0.40
1:A:613:VAL:HA	1:A:638:VAL:O	2.21	0.40
1:B:198:THR:HA	1:B:256:TYR:O	2.22	0.40
1:B:513:ASP:HB3	1:B:516:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	713/718 (99%)	649 (91%)	54 (8%)	10 (1%)	9	30
1	B	712/718 (99%)	651 (91%)	51 (7%)	10 (1%)	9	30
All	All	1425/1436 (99%)	1300 (91%)	105 (7%)	20 (1%)	9	30

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	620	GLY
1	A	683	ILE
1	B	18	TYR
1	B	160	ASP
1	B	193	GLU
1	B	194	ASN
1	A	19	PRO
1	B	303	SER
1	B	372	LEU
1	B	620	GLY
1	A	160	ASP
1	A	168	LYS
1	A	513	ASP
1	B	308	ASP
1	A	164	ILE
1	B	17	PRO
1	A	17	PRO
1	B	19	PRO
1	A	223	PRO

5.3.2 Protein sidechains [i](#)

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	631/636 (99%)	611 (97%)	20 (3%)	34	70
1	B	633/636 (100%)	621 (98%)	12 (2%)	50	81
All	All	1264/1272 (99%)	1232 (98%)	32 (2%)	42	76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	18	TYR
1	A	20	LEU
1	A	34	SER
1	A	35	LEU
1	A	71	HIS
1	A	130	ASP
1	A	134	ASP
1	A	161	GLU
1	A	164	ILE
1	A	165	LYS
1	A	167	LYS
1	A	169	VAL
1	A	254	CYS
1	A	310	THR
1	A	511	THR
1	A	518	ILE
1	A	519	CYS
1	A	625	GLU
1	A	715	ARG
1	B	18	TYR
1	B	161	GLU
1	B	162	ASP
1	B	245	ASP
1	B	253	GLU
1	B	254	CYS
1	B	255	ARG
1	B	482	ASN
1	B	505	CYS
1	B	511	THR
1	B	517	VAL

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Mol	Chain	Res	Type
1	B	640	GLU

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

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	ASN
1	A	52	ASN
1	A	114	ASN
1	A	226	HIS
1	A	230	GLN
1	A	274	ASN
1	A	277	HIS
1	A	319	ASN
1	A	416	GLN
1	A	421	ASN
1	A	526	ASN
1	A	553	ASN
1	A	555	ASN
1	B	23	ASN
1	B	102	ASN
1	B	274	ASN
1	B	290	ASN
1	B	376	ASN
1	B	498	ASN
1	B	535	GLN
1	B	555	ASN
1	B	561	ASN
1	B	591	HIS
1	B	633	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	715/718 (99%)	0.27	17 (2%)	59 49	30, 62, 81, 101	0
1	B	714/718 (99%)	0.13	11 (1%)	72 63	37, 58, 81, 103	0
All	All	1429/1436 (99%)	0.20	28 (1%)	65 56	30, 60, 81, 103	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	TYR	5.0
1	A	4	PHE	3.9
1	A	166	GLY	3.8
1	B	259	THR	3.8
1	A	18	TYR	3.6
1	A	19	PRO	3.3
1	A	20	LEU	3.3
1	A	35	LEU	3.0
1	A	7	THR	2.9
1	B	534	SER	2.7
1	A	50	LEU	2.6
1	B	256	TYR	2.6
1	A	8	ARG	2.6
1	B	17	PRO	2.5
1	B	618	LEU	2.5
1	A	163	PHE	2.5
1	A	15	GLY	2.4
1	A	16	ASP	2.4
1	A	34	SER	2.3
1	B	372	LEU	2.3
1	A	507	ALA	2.2
1	A	369	ALA	2.2
1	B	373	TYR	2.1
1	B	497	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	461	PHE	2.1
1	B	257	SER	2.0
1	B	160	ASP	2.0
1	A	161	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.