



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:14 AM UTC

PDB ID : 7CLG / pdb_00007clg
Title : Crystal structure of the ATP-dependent restriction endonuclease SauUSI
Authors : Saikrishnan, K.; Tumuluri, V.S.
Deposited on : 2020-07-21
Resolution : 3.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

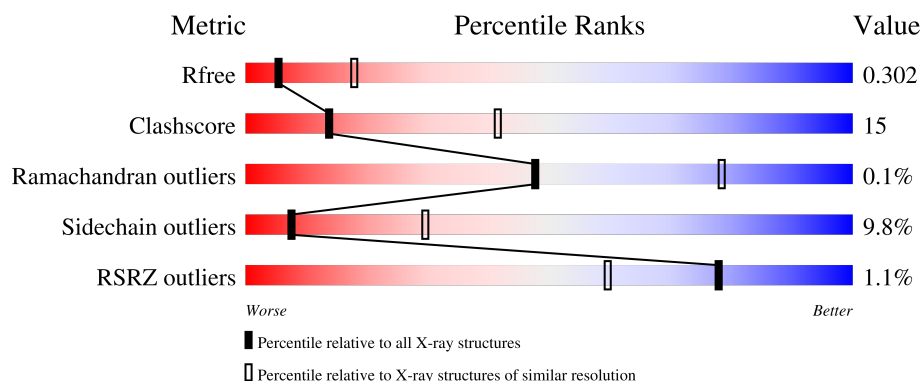
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	953	
1	B	953	

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	SO4	B	1003	-	-	X	-

2 Entry composition [i](#)

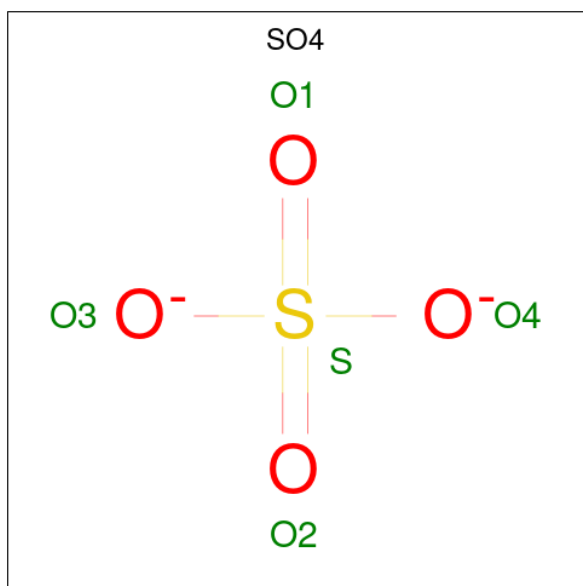
There are 3 unique types of molecules in this entry. The entry contains 12328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative helicase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	838	Total	C	N	O	S	Se	0	0	0
			6233	3976	1028	1211	3	15			
1	B	806	Total	C	N	O	S	Se	0	0	0
			6042	3872	992	1162	3	13			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

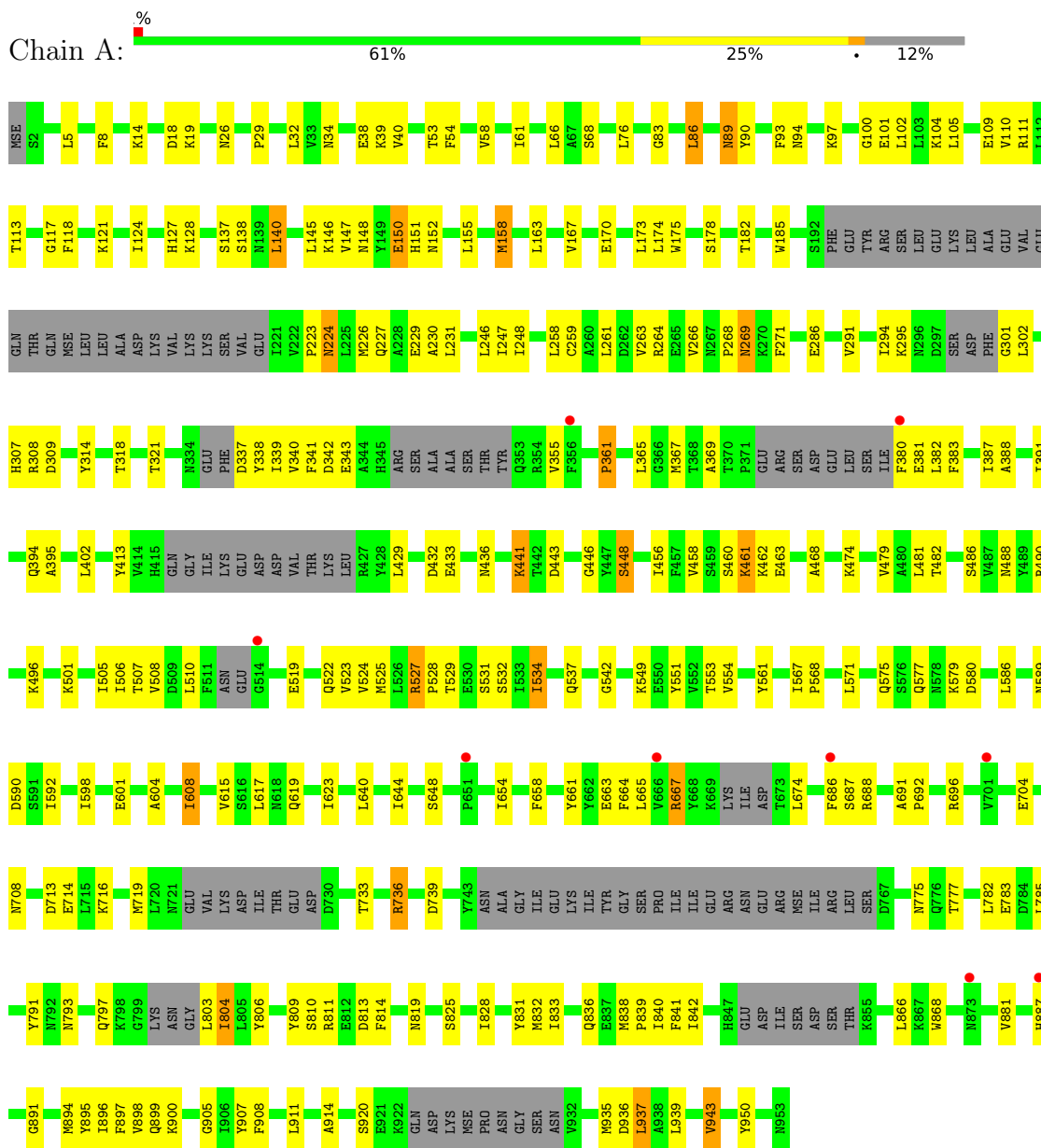
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total 15	O 15	0	0
3	B	18	Total 18	O 18	0	0

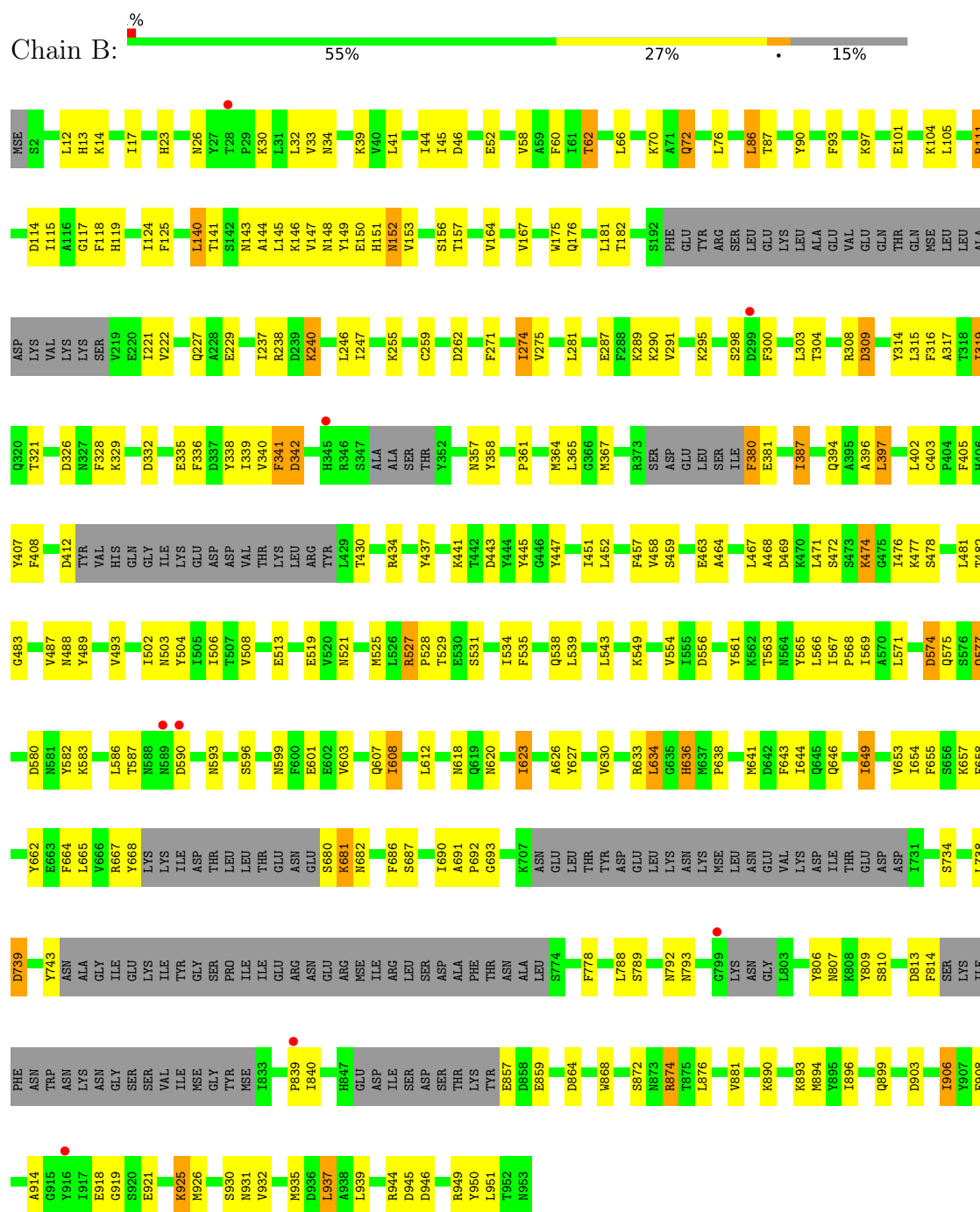
3 Residue-property plots [i](#)

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: Putative helicase



• Molecule 1: Putative helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.58Å 175.68Å 89.38Å 90.00° 115.68° 90.00°	Depositor
Resolution (Å)	56.79 – 3.10 56.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (56.79-3.10) 99.6 (56.79-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.245 , 0.297 0.253 , 0.302	Depositor DCC
R_{free} test set	2025 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 141.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12328	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.24	0/6320	0.46	1/8556 (0.0%)
1	B	0.22	0/6135	0.44	1/8306 (0.0%)
All	All	0.23	0/12455	0.45	2/16862 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	906	ILE	N-CA-C	-5.65	105.92	112.98
1	A	94	ASN	N-CA-C	-5.35	99.40	110.80

There are no chirality outliers.

There are no planarity outliers.

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	6233	0	5647	155	0
1	B	6042	0	5559	195	0
2	A	5	0	0	0	0
2	B	15	0	0	4	0
3	A	15	0	0	1	0
3	B	18	0	0	0	0
All	All	12328	0	11206	341	0

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

All (341) 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:567:ILE:HG13	1:B:568:PRO:HD3	1.46	0.97
1:B:481:LEU:HD21	1:B:493:VAL:HG21	1.57	0.86
1:B:403:CYS:SG	1:B:549:LYS:NZ	2.55	0.80
1:B:86:LEU:HD22	1:B:175:TRP:HE3	1.47	0.80
1:A:268:PRO:HG2	1:A:338:TYR:HB2	1.64	0.80
1:B:531:SER:HB3	1:B:534:ILE:HD13	1.64	0.79
1:A:246:LEU:HD23	1:A:380:PHE:N	1.99	0.77
1:B:925:LYS:HG2	1:B:932:VAL:HG22	1.69	0.74
1:B:925:LYS:HD3	1:B:926:MSE:H	1.52	0.74
1:B:806:TYR:CE1	1:B:944:ARG:HB2	2.23	0.73
1:B:97:LYS:NZ	1:B:447:TYR:O	2.21	0.73
1:B:531:SER:HA	1:B:566:LEU:HD21	1.70	0.72
1:A:89:ASN:ND2	3:A:1101:HOH:O	2.23	0.71
1:B:328:PHE:HD1	1:B:358:TYR:HE2	1.37	0.70
1:A:914:ALA:HB2	1:A:939:LEU:HD23	1.73	0.69
1:B:925:LYS:HB2	1:B:931:ASN:HA	1.72	0.69
1:A:868:TRP:HD1	1:A:935:MSE:HE2	1.56	0.69
1:A:713:ASP:HA	1:A:716:LYS:HB3	1.75	0.67
1:B:271:PHE:HB3	1:B:314:TYR:HD1	1.59	0.67
1:A:733:THR:HA	1:A:819:ASN:OD1	1.93	0.67
1:B:275:VAL:HG11	1:B:281:LEU:HB2	1.75	0.67
1:B:70:LYS:NZ	1:B:101:GLU:OE1	2.24	0.67
1:B:568:PRO:HG2	1:B:608:ILE:HG21	1.77	0.67
1:A:441:LYS:NZ	1:A:601:GLU:OE2	2.28	0.66
1:A:104:LYS:NZ	1:A:443:ASP:O	2.22	0.66
1:B:115:ILE:HD11	1:B:118:PHE:HD1	1.61	0.66
1:B:86:LEU:HD22	1:B:175:TRP:CE3	2.30	0.66
1:A:263:VAL:HA	1:A:338:TYR:HE2	1.61	0.66
1:B:810:SER:HB2	1:B:906:ILE:HA	1.78	0.65
1:A:736:ARG:NH1	1:A:739:ASP:OD1	2.30	0.65
1:A:369:ALA:O	1:A:537:GLN:NE2	2.30	0.65
1:A:579:LYS:NZ	1:A:615:VAL:O	2.25	0.65
1:B:238:ARG:NH2	1:B:262:ASP:OD2	2.27	0.65
1:A:456:ILE:HG12	1:A:524:VAL:HB	1.80	0.64
1:A:247:ILE:HG12	1:A:367:MSE:HG2	1.80	0.64
1:A:571:LEU:HD13	1:A:598:ILE:HD13	1.81	0.63
1:B:303:LEU:HB3	1:B:317:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:GLN:H	1:B:653:VAL:HG21	1.63	0.63
1:B:259:CYS:HB2	1:B:367:MSE:HE1	1.81	0.63
1:B:477:LYS:CB	1:B:503:ASN:H	2.11	0.63
1:B:872:SER:HA	1:B:932:VAL:HG12	1.80	0.63
1:A:170:GLU:HG2	1:B:34:ASN:ND2	2.14	0.62
1:A:814:PHE:CE2	1:A:839:PRO:HG3	2.34	0.62
1:A:525:MSE:HE3	1:A:527:ARG:HH11	1.64	0.62
1:B:309:ASP:N	1:B:309:ASP:OD1	2.31	0.62
1:A:118:PHE:HA	1:B:149:TYR:HB3	1.82	0.61
1:B:441:LYS:NZ	1:B:601:GLU:OE2	2.33	0.61
1:B:644:ILE:HD11	1:B:788:LEU:HD13	1.80	0.61
1:A:577:GLN:HB3	1:A:617:LEU:HD23	1.81	0.61
1:B:124:ILE:HD11	1:B:167:VAL:HG11	1.82	0.61
1:A:337:ASP:HA	1:A:361:PRO:HB2	1.81	0.61
1:A:271:PHE:HD2	1:A:338:TYR:HB3	1.66	0.61
1:B:246:LEU:HD12	1:B:247:ILE:H	1.66	0.61
1:A:896:ILE:HD11	1:A:911:LEU:HB2	1.82	0.60
1:B:101:GLU:HA	1:B:104:LYS:HD2	1.83	0.60
1:A:674:LEU:CB	1:A:775:ASN:HD21	2.15	0.60
1:B:525:MSE:HE3	1:B:556:ASP:HB2	1.82	0.60
1:A:381:GLU:HG3	1:A:382:LEU:HD12	1.83	0.59
1:B:332:ASP:HB3	1:B:335:GLU:HB3	1.82	0.59
1:B:289:LYS:HG3	1:B:300:PHE:CE1	2.36	0.59
1:B:119:HIS:NE2	2:B:1001:SO4:O1	2.34	0.59
1:B:342:ASP:OD2	1:B:342:ASP:N	2.34	0.59
1:B:328:PHE:HD1	1:B:358:TYR:CE2	2.19	0.58
1:A:227:GLN:O	1:A:231:LEU:HG	2.01	0.58
1:A:833:ILE:HB	1:A:838:MSE:HG3	1.84	0.58
1:B:687:SER:O	1:B:691:ALA:N	2.28	0.58
1:A:542:GLY:O	1:A:549:LYS:NZ	2.37	0.57
1:B:430:THR:O	1:B:434:ARG:HB2	2.04	0.57
1:A:90:TYR:CD1	1:A:117:GLY:HA2	2.40	0.57
1:B:14:LYS:NZ	1:B:864:ASP:OD2	2.31	0.57
1:B:662:TYR:HA	1:B:665:LEU:HD12	1.87	0.57
1:A:301:GLY:N	1:A:314:TYR:O	2.37	0.57
1:A:137:SER:OG	1:A:150:GLU:HG3	2.04	0.57
1:A:318:THR:HG23	1:A:321:THR:H	1.68	0.57
1:B:582:TYR:O	1:B:586:LEU:HB2	2.04	0.57
1:B:840:ILE:HD12	1:B:894:MSE:HE3	1.86	0.57
1:B:643:PHE:HB3	1:B:649:ILE:O	2.05	0.56
1:B:471:LEU:O	1:B:476:ILE:HB	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:TYR:HE1	1:B:944:ARG:HB2	1.70	0.56
1:B:104:LYS:NZ	1:B:443:ASP:O	2.36	0.56
1:A:686:PHE:CE1	1:A:782:LEU:HD13	2.40	0.56
1:A:831:TYR:HB3	1:A:868:TRP:HZ2	1.70	0.56
1:B:271:PHE:HB3	1:B:314:TYR:CD1	2.40	0.56
1:B:693:GLY:HA3	1:B:793:ASN:HB2	1.87	0.56
1:A:448:SER:HB3	1:A:551:TYR:CE1	2.41	0.55
1:A:887:HIS:O	1:A:891:GLY:N	2.39	0.55
1:A:461:LYS:HB3	1:A:482:THR:HG21	1.89	0.55
1:A:806:TYR:OH	1:A:943:VAL:HA	2.06	0.55
1:B:381:GLU:CD	1:B:381:GLU:H	2.14	0.55
1:B:394:GLN:NE2	1:B:571:LEU:O	2.40	0.55
1:A:432:ASP:O	1:A:436:ASN:ND2	2.33	0.54
1:A:446:GLY:O	1:A:553:THR:HG21	2.07	0.54
1:A:247:ILE:HG22	1:A:388:ALA:HB3	1.88	0.54
1:A:458:VAL:HB	1:A:463:GLU:CD	2.32	0.54
1:B:45:ILE:HD12	1:B:72:GLN:HG3	1.90	0.54
1:A:14:LYS:NZ	1:A:19:LYS:O	2.41	0.54
1:A:294:ILE:HG22	1:A:295:LYS:H	1.72	0.54
1:B:580:ASP:OD1	1:B:950:TYR:OH	2.23	0.54
1:A:263:VAL:HA	1:A:338:TYR:CE2	2.42	0.54
1:B:60:PHE:HD1	1:B:93:PHE:CD2	2.26	0.54
1:B:66:LEU:HD11	1:B:105:LEU:HD11	1.90	0.54
1:B:238:ARG:HH22	1:B:262:ASP:CG	2.16	0.54
1:A:907:TYR:C	1:A:908:PHE:HD1	2.15	0.53
1:A:719:MSE:HA	1:A:719:MSE:HE2	1.91	0.53
1:B:407:TYR:OH	1:B:556:ASP:OD2	2.24	0.53
1:A:811:ARG:HD3	1:A:841:PHE:CD1	2.42	0.53
1:A:833:ILE:HA	1:A:838:MSE:HA	1.90	0.53
1:B:262:ASP:OD2	1:B:338:TYR:OH	2.24	0.53
1:B:814:PHE:HE1	1:B:839:PRO:HG3	1.73	0.53
1:A:97:LYS:NZ	1:A:101:GLU:OE2	2.40	0.53
1:B:634:LEU:HD12	1:B:636:HIS:H	1.74	0.53
1:A:522:GLN:HG2	1:A:553:THR:HG23	1.90	0.53
1:B:489:TYR:O	1:B:493:VAL:HG22	2.09	0.53
1:A:167:VAL:HG22	1:B:32:LEU:HD22	1.90	0.53
1:A:86:LEU:HD21	1:A:174:LEU:HD12	1.91	0.53
1:A:868:TRP:CD1	1:A:935:MSE:HE2	2.41	0.52
1:B:472:SER:HA	1:B:476:ILE:O	2.09	0.52
1:B:925:LYS:HG3	1:B:930:SER:O	2.09	0.52
1:A:519:GLU:N	1:A:519:GLU:OE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ILE:HD13	1:A:791:TYR:CE1	2.44	0.52
1:B:459:SER:OG	1:B:463:GLU:OE2	2.27	0.52
1:A:704:GLU:O	1:A:708:ASN:N	2.42	0.52
1:A:113:THR:HB	1:A:178:SER:HB3	1.90	0.52
1:B:143:ASN:ND2	2:B:1003:SO4:O3	2.43	0.52
1:A:223:PRO:HB3	1:A:261:LEU:HD21	1.90	0.52
1:A:170:GLU:HG2	1:B:34:ASN:HD22	1.74	0.52
1:B:734:SER:O	1:B:738:LEU:HD12	2.10	0.52
1:B:281:LEU:HD11	1:B:316:PHE:HB3	1.91	0.51
1:B:295:LYS:HD2	1:B:298:SER:H	1.75	0.51
1:A:138:SER:CB	1:A:152:ASN:HD21	2.23	0.51
1:B:303:LEU:HB2	1:B:315:LEU:HD11	1.93	0.51
1:A:797:GLN:OE1	1:A:809:TYR:OH	2.26	0.51
1:B:481:LEU:HD21	1:B:493:VAL:CG2	2.34	0.51
1:B:574:ASP:HB3	1:B:582:TYR:CE1	2.45	0.51
1:A:5:LEU:HG	1:A:158:MSE:HE1	1.91	0.51
1:B:810:SER:O	1:B:813:ASP:N	2.45	0.50
1:B:274:ILE:HG22	1:B:319:ILE:HG12	1.94	0.50
1:A:259:CYS:O	1:A:263:VAL:HG23	2.11	0.50
1:B:452:LEU:HD21	1:B:504:TYR:CZ	2.46	0.50
1:B:471:LEU:HD13	1:B:476:ILE:HG21	1.92	0.50
1:B:874:ARG:N	1:B:931:ASN:O	2.45	0.50
1:A:413:TYR:CZ	1:A:433:GLU:HB3	2.46	0.50
1:B:894:MSE:HE1	1:B:937:LEU:HG	1.94	0.50
1:B:58:VAL:HG21	1:B:140:LEU:HB2	1.94	0.49
1:A:394:GLN:NE2	1:A:571:LEU:O	2.45	0.49
1:B:633:ARG:HG2	1:B:646:GLN:HG3	1.94	0.49
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.94	0.49
1:B:577:GLN:H	1:B:653:VAL:CG2	2.24	0.49
1:A:486:SER:O	1:A:490:ARG:HG3	2.12	0.49
1:A:686:PHE:HE1	1:A:782:LEU:HD13	1.76	0.49
1:B:921:GLU:H	1:B:921:GLU:CD	2.20	0.49
1:A:525:MSE:HE3	1:A:527:ARG:NH1	2.26	0.49
1:A:589:ASN:O	1:A:592:ILE:HG22	2.12	0.49
1:B:690:ILE:O	1:B:789:SER:HB2	2.12	0.49
1:A:836:GLN:NE2	1:A:891:GLY:O	2.45	0.49
1:B:682:ASN:O	1:B:686:PHE:HB2	2.13	0.49
1:B:41:LEU:O	1:B:45:ILE:HG12	2.13	0.49
1:A:663:GLU:O	1:A:667:ARG:HB2	2.12	0.49
1:B:451:ILE:O	1:B:521:ASN:ND2	2.46	0.49
1:B:634:LEU:HD13	1:B:636:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HD2	1:A:462:LYS:H	1.77	0.49
1:B:682:ASN:HB2	1:B:778:PHE:HZ	1.77	0.49
1:B:919:GLY:N	1:B:921:GLU:OE1	2.46	0.49
1:A:507:THR:HG21	1:A:510:LEU:HB2	1.95	0.48
1:A:733:THR:HA	1:A:819:ASN:CG	2.37	0.48
1:B:39:LYS:HD3	1:B:146:LYS:O	2.13	0.48
1:B:539:LEU:O	1:B:543:LEU:HG	2.13	0.48
1:B:13:HIS:HA	1:B:17:ILE:HD12	1.95	0.48
1:B:140:LEU:HD12	1:B:145:LEU:HD11	1.95	0.48
1:B:246:LEU:CD2	1:B:380:PHE:HB2	2.43	0.48
1:B:921:GLU:HB2	1:B:935:MSE:HA	1.95	0.48
1:A:828:ILE:HG23	1:A:832:MSE:HB3	1.94	0.48
1:A:163:LEU:HD21	1:B:153:VAL:HG21	1.95	0.48
1:A:266:VAL:O	1:A:268:PRO:HD3	2.13	0.48
1:A:481:LEU:O	1:A:507:THR:HG23	2.13	0.48
1:B:287:GLU:OE2	1:B:290:LYS:NZ	2.30	0.48
1:A:97:LYS:O	1:A:100:GLY:N	2.47	0.48
1:A:696:ARG:CB	1:A:793:ASN:HD21	2.27	0.48
1:B:563:THR:HA	1:B:565:TYR:CE1	2.49	0.48
1:B:574:ASP:HB3	1:B:582:TYR:HE1	1.79	0.48
1:B:247:ILE:HB	1:B:367:MSE:HG2	1.95	0.48
1:B:468:ALA:O	1:B:478:SER:OG	2.30	0.48
1:A:34:ASN:ND2	1:A:148:ASN:O	2.39	0.47
1:A:460:SER:C	1:A:508:VAL:HG21	2.40	0.47
1:A:736:ARG:HG2	1:A:819:ASN:HA	1.97	0.47
1:B:527:ARG:NH1	1:B:529:THR:OG1	2.47	0.47
1:B:341:PHE:HZ	1:B:364:MSE:SE	2.48	0.47
1:B:937:LEU:HD13	1:B:937:LEU:H	1.80	0.47
1:B:944:ARG:HD2	1:B:946:ASP:OD1	2.14	0.47
1:A:340:VAL:HA	1:A:365:LEU:O	2.14	0.47
1:A:920:SER:HB2	1:A:936:ASP:H	1.79	0.47
1:B:328:PHE:CD1	1:B:358:TYR:CE2	3.02	0.47
1:B:658:PHE:CD1	1:B:664:PHE:HB2	2.50	0.47
1:B:90:TYR:CE2	1:B:117:GLY:HA2	2.50	0.47
1:B:474:LYS:HA	1:B:474:LYS:HD3	1.59	0.47
1:B:259:CYS:SG	1:B:340:VAL:HG21	2.55	0.47
1:A:124:ILE:HD11	1:A:167:VAL:CG1	2.45	0.47
1:B:255:LYS:HE3	1:B:255:LYS:HB2	1.58	0.47
1:A:124:ILE:HD11	1:A:167:VAL:HG11	1.96	0.46
1:B:412:ASP:HB3	1:B:437:TYR:CE1	2.50	0.46
1:A:226:MSE:HE1	1:A:395:ALA:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:PRO:HA	1:B:792:ASN:HD22	1.80	0.46
1:B:387:ILE:H	1:B:387:ILE:HG13	1.55	0.46
1:A:528:PRO:HB3	1:A:561:TYR:CG	2.50	0.46
1:B:899:GLN:HG2	1:B:903:ASP:HB3	1.96	0.46
1:B:914:ALA:HB2	1:B:939:LEU:HD23	1.97	0.46
1:A:468:ALA:HB2	1:A:506:ILE:HD13	1.96	0.46
1:A:897:PHE:HB3	1:A:908:PHE:HB2	1.98	0.46
1:B:397:LEU:HD21	1:B:405:PHE:HE1	1.80	0.46
1:A:224:ASN:OD1	1:A:227:GLN:N	2.49	0.46
1:B:478:SER:OG	1:B:478:SER:O	2.34	0.46
1:B:874:ARG:HD2	1:B:874:ARG:HA	1.65	0.46
1:A:61:ILE:HG23	1:A:140:LEU:HG	1.97	0.45
1:B:945:ASP:O	1:B:949:ARG:HG3	2.16	0.45
1:A:32:LEU:HB2	1:A:152:ASN:HB2	1.96	0.45
1:A:138:SER:OG	1:A:152:ASN:ND2	2.46	0.45
1:B:361:PRO:HG2	1:B:364:MSE:HG2	1.98	0.45
1:B:583:LYS:O	1:B:587:THR:HG22	2.17	0.45
1:A:246:LEU:HD12	1:A:247:ILE:N	2.31	0.45
1:A:937:LEU:HD13	1:A:937:LEU:H	1.82	0.45
1:B:115:ILE:HD11	1:B:118:PHE:CD1	2.47	0.45
1:B:574:ASP:O	1:B:582:TYR:OH	2.30	0.45
1:A:39:LYS:HE2	1:A:146:LYS:O	2.16	0.45
1:B:44:ILE:HG13	1:B:125:PHE:HZ	1.81	0.45
1:B:304:THR:C	1:B:321:THR:HG21	2.42	0.45
1:A:29:PRO:HB3	1:A:155:LEU:HD23	1.99	0.45
1:A:580:ASP:OD1	1:A:950:TYR:OH	2.23	0.45
1:A:271:PHE:CD2	1:A:338:TYR:HB3	2.50	0.44
1:A:531:SER:HB3	1:A:534:ILE:HD13	1.99	0.44
1:B:944:ARG:NH1	1:B:946:ASP:OD2	2.50	0.44
1:A:640:LEU:HD11	1:A:661:TYR:CG	2.51	0.44
1:B:445:TYR:OH	1:B:601:GLU:OE2	2.27	0.44
1:A:661:TYR:CE1	1:A:665:LEU:HD11	2.52	0.44
1:A:86:LEU:HD21	1:A:174:LEU:CD1	2.47	0.44
1:A:109:GLU:HB3	1:A:175:TRP:HH2	1.82	0.44
1:B:655:PHE:CE1	1:B:687:SER:HB2	2.53	0.44
1:A:163:LEU:HD13	1:B:30:LYS:O	2.18	0.44
1:A:658:PHE:CE2	1:A:664:PHE:HD2	2.35	0.44
1:A:842:ILE:HD11	1:A:898:VAL:HG22	2.00	0.44
1:B:157:THR:HG21	1:B:164:VAL:CG2	2.48	0.44
1:A:174:LEU:HD21	1:B:149:TYR:CZ	2.53	0.44
1:A:341:PHE:HB3	1:A:342:ASP:H	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PHE:CZ	1:A:83:GLY:HA3	2.53	0.43
1:A:496:LYS:HG2	1:A:501:LYS:HB3	2.00	0.43
1:B:627:TYR:CE2	1:B:638:PRO:HD2	2.53	0.43
1:B:58:VAL:O	1:B:87:THR:HG22	2.18	0.43
1:B:340:VAL:HA	1:B:365:LEU:O	2.18	0.43
1:B:519:GLU:OE2	1:B:519:GLU:N	2.51	0.43
1:A:810:SER:H	1:A:813:ASP:HB2	1.82	0.43
1:B:246:LEU:HD12	1:B:247:ILE:N	2.30	0.43
1:B:565:TYR:HB3	1:B:612:LEU:HA	2.00	0.43
1:B:739:ASP:OD1	1:B:739:ASP:N	2.51	0.43
1:B:14:LYS:HD2	1:B:23:HIS:ND1	2.33	0.43
1:B:62:THR:HG21	2:B:1003:SO4:O1	2.19	0.43
1:B:72:GLN:O	1:B:76:LEU:HD13	2.19	0.43
1:B:26:ASN:OD1	1:B:26:ASN:N	2.52	0.43
1:B:565:TYR:O	1:B:569:ILE:HG13	2.18	0.43
1:B:876:LEU:HA	1:B:881:VAL:HG21	2.01	0.43
1:A:686:PHE:HB3	1:A:785:LEU:HD13	1.99	0.43
1:A:145:LEU:O	1:A:146:LYS:HG2	2.18	0.43
1:A:687:SER:O	1:A:692:PRO:HD3	2.18	0.43
1:A:246:LEU:HD12	1:A:247:ILE:H	1.83	0.43
1:A:246:LEU:HB2	1:A:383:PHE:CD1	2.54	0.43
1:A:528:PRO:HD3	1:A:561:TYR:CZ	2.54	0.43
1:B:221:ILE:HG21	1:B:291:VAL:HG22	2.01	0.43
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.90	0.42
1:A:269:ASN:O	1:A:269:ASN:ND2	2.53	0.42
1:B:397:LEU:HD21	1:B:405:PHE:CE1	2.53	0.42
1:B:868:TRP:CD1	1:B:935:MSE:HE2	2.53	0.42
1:A:905:GLY:C	1:A:907:TYR:H	2.25	0.42
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.88	0.42
1:B:111:ARG:HG3	1:B:175:TRP:CH2	2.54	0.42
1:A:158:MSE:HG3	1:B:17:ILE:HA	2.01	0.42
1:A:840:ILE:N	1:A:895:TYR:O	2.47	0.42
1:B:336:PHE:HB2	1:B:339:ILE:HD11	2.01	0.42
1:B:458:VAL:HG21	1:B:464:ALA:HB2	2.00	0.42
1:A:527:ARG:NH2	1:A:529:THR:HA	2.35	0.42
1:A:797:GLN:O	1:A:804:ILE:HD11	2.20	0.42
1:B:341:PHE:CD1	1:B:341:PHE:N	2.87	0.42
1:B:529:THR:HG23	1:B:535:PHE:HB2	2.01	0.42
1:A:182:THR:HG23	1:A:185:TRP:H	1.85	0.42
1:A:248:ILE:O	1:A:391:ILE:N	2.43	0.42
1:A:687:SER:O	1:A:691:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:PRO:HD3	1:B:561:TYR:CZ	2.55	0.42
1:B:593:ASN:OD1	1:B:593:ASN:N	2.53	0.42
1:A:523:VAL:HB	1:A:554:VAL:HG22	2.01	0.42
1:B:539:LEU:HG	1:B:543:LEU:HD11	2.02	0.42
1:B:620:ASN:HA	1:B:623:ILE:HG22	2.00	0.42
1:A:623:ILE:HG23	1:A:654:ILE:HG13	2.02	0.42
1:B:289:LYS:HB2	1:B:289:LYS:HE3	1.64	0.42
1:B:408:PHE:CD1	1:B:599:ASN:HB2	2.55	0.42
1:B:339:ILE:HG13	1:B:361:PRO:HG3	2.02	0.41
1:B:72:GLN:OE1	1:B:599:ASN:ND2	2.43	0.41
1:B:326:ASP:HB3	1:B:329:LYS:HG3	2.01	0.41
1:B:342:ASP:HA	1:B:367:MSE:O	2.20	0.41
1:B:237:ILE:HA	1:B:240:LYS:HG2	2.02	0.41
1:A:14:LYS:HA	1:A:18:ASP:O	2.20	0.41
1:A:158:MSE:HE3	1:B:17:ILE:HG23	2.02	0.41
1:A:102:LEU:HD13	1:A:110:VAL:HG11	2.01	0.41
1:A:146:LYS:HE3	1:A:146:LYS:HB3	1.70	0.41
1:A:894:MSE:HE2	1:A:937:LEU:HG	2.03	0.41
1:B:114:ASP:N	1:B:114:ASP:OD1	2.53	0.41
1:B:141:THR:HG23	1:B:144:ALA:H	1.86	0.41
1:B:397:LEU:HD12	1:B:397:LEU:HA	1.82	0.41
1:B:618:ASN:HB3	1:B:657:LYS:HD3	2.02	0.41
1:B:626:ALA:O	1:B:630:VAL:HG23	2.20	0.41
1:B:181:LEU:HD12	1:B:181:LEU:HA	1.93	0.41
1:B:451:ILE:HD12	1:B:451:ILE:HA	1.87	0.41
1:B:569:ILE:HG12	1:B:582:TYR:CE2	2.56	0.41
1:A:842:ILE:HG22	1:A:868:TRP:CZ3	2.55	0.41
1:B:457:PHE:CE1	1:B:538:GLN:HG2	2.56	0.41
1:A:34:ASN:OD1	1:A:40:VAL:HG23	2.20	0.41
1:A:230:ALA:HB1	1:A:258:LEU:HD21	2.03	0.41
1:A:339:ILE:O	1:A:365:LEU:N	2.48	0.41
1:A:488:ASN:OD1	1:A:488:ASN:N	2.49	0.41
1:A:604:ALA:O	1:A:608:ILE:HD12	2.21	0.41
1:B:809:TYR:O	1:B:908:PHE:HB2	2.20	0.41
1:B:899:GLN:CG	1:B:903:ASP:HB3	2.50	0.41
1:A:127:HIS:ND1	1:A:127:HIS:N	2.69	0.41
1:A:907:TYR:N	1:A:907:TYR:CD2	2.89	0.41
1:B:467:LEU:HD12	1:B:506:ILE:HD13	2.03	0.41
1:B:482:THR:HG22	1:B:483:GLY:N	2.36	0.41
1:A:302:LEU:H	1:A:309:ASP:HB2	1.86	0.40
1:A:567:ILE:HB	1:A:568:PRO:HD3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HA	1:A:590:ASP:OD2	2.20	0.40
1:B:148:ASN:HB3	1:B:150:GLU:HG2	2.02	0.40
1:B:567:ILE:HD13	1:B:567:ILE:HG21	1.90	0.40
1:B:914:ALA:HB1	1:B:937:LEU:HD23	2.02	0.40
1:A:531:SER:OG	1:A:532:SER:N	2.54	0.40
1:A:575:GLN:HG2	1:A:648:SER:C	2.46	0.40
1:A:842:ILE:HG22	1:A:868:TRP:HZ3	1.86	0.40
1:B:303:LEU:HD13	1:B:308:ARG:HA	2.03	0.40
1:A:899:GLN:HB2	1:A:908:PHE:CG	2.57	0.40
1:B:46:ASP:OD1	1:B:949:ARG:HD3	2.21	0.40
1:B:396:ALA:HB1	1:B:402:LEU:HD13	2.03	0.40
1:A:479:VAL:O	1:A:505:ILE:HA	2.21	0.40
1:B:33:VAL:CG2	1:B:152:ASN:HB2	2.51	0.40
1:B:141:THR:OG1	2:B:1003:SO4:O1	2.38	0.40
1:B:143:ASN:O	1:B:148:ASN:HB2	2.21	0.40
1:B:623:ILE:HD11	1:B:654:ILE:HG12	2.03	0.40
1:B:680:SER:OG	1:B:681:LYS:N	2.55	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	810/953 (85%)	743 (92%)	66 (8%)	1 (0%)	48	78
1	B	784/953 (82%)	729 (93%)	55 (7%)	0	100	100
All	All	1594/1906 (84%)	1472 (92%)	121 (8%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	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	605/848 (71%)	550 (91%)	55 (9%)	9	32
1	B	600/848 (71%)	537 (90%)	63 (10%)	6	26
All	All	1205/1696 (71%)	1087 (90%)	118 (10%)	7	29

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	26	ASN
1	A	53	THR
1	A	58	VAL
1	A	68	SER
1	A	76	LEU
1	A	86	LEU
1	A	89	ASN
1	A	93	PHE
1	A	105	LEU
1	A	111	ARG
1	A	121	LYS
1	A	128	LYS
1	A	140	LEU
1	A	147	VAL
1	A	150	GLU
1	A	151	HIS
1	A	158	MSE
1	A	173	LEU
1	A	224	ASN
1	A	229	GLU
1	A	264	ARG
1	A	269	ASN
1	A	286	GLU
1	A	291	VAL
1	A	307	HIS
1	A	308	ARG

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Mol	Chain	Res	Type
1	A	343	GLU
1	A	355	VAL
1	A	387	ILE
1	A	402	LEU
1	A	429	LEU
1	A	441	LYS
1	A	448	SER
1	A	461	LYS
1	A	474	LYS
1	A	527	ARG
1	A	534	ILE
1	A	586	LEU
1	A	608	ILE
1	A	619	GLN
1	A	667	ARG
1	A	688	ARG
1	A	714	GLU
1	A	736	ARG
1	A	777	THR
1	A	783	GLU
1	A	803	LEU
1	A	804	ILE
1	A	825	SER
1	A	866	LEU
1	A	881	VAL
1	A	900	LYS
1	A	937	LEU
1	A	943	VAL
1	B	52	GLU
1	B	62	THR
1	B	72	GLN
1	B	86	LEU
1	B	111	ARG
1	B	140	LEU
1	B	147	VAL
1	B	151	HIS
1	B	152	ASN
1	B	156	SER
1	B	176	GLN
1	B	182	THR
1	B	222	VAL
1	B	227	GLN

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Mol	Chain	Res	Type
1	B	229	GLU
1	B	240	LYS
1	B	274	ILE
1	B	309	ASP
1	B	319	ILE
1	B	341	PHE
1	B	342	ASP
1	B	357	ASN
1	B	380	PHE
1	B	387	ILE
1	B	397	LEU
1	B	469	ASP
1	B	474	LYS
1	B	487	VAL
1	B	488	ASN
1	B	502	ILE
1	B	508	VAL
1	B	513	GLU
1	B	527	ARG
1	B	554	VAL
1	B	574	ASP
1	B	575	GLN
1	B	577	GLN
1	B	590	ASP
1	B	596	SER
1	B	603	VAL
1	B	607	GLN
1	B	608	ILE
1	B	623	ILE
1	B	634	LEU
1	B	636	HIS
1	B	641	MSE
1	B	649	ILE
1	B	667	ARG
1	B	668	TYR
1	B	681	LYS
1	B	739	ASP
1	B	743	TYR
1	B	807	ASN
1	B	857	GLU
1	B	859	GLU
1	B	874	ARG

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Mol	Chain	Res	Type
1	B	890	LYS
1	B	893	LYS
1	B	896	ILE
1	B	918	GLU
1	B	925	LYS
1	B	937	LEU
1	B	951	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	HIS
1	A	607	GLN
1	A	647	HIS
1	B	127	HIS
1	B	357	ASN
1	B	503	ASN
1	B	792	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
2	SO4	A	1001	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	B	1001	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	B	1002	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	B	1003	-	4,4,4	0.24	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SO4	1	0
2	B	1003	SO4	3	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	822/953 (86%)	-0.07	9 (1%) 78 59	62, 128, 221, 288	0
1	B	792/953 (83%)	-0.08	8 (1%) 79 61	59, 119, 196, 286	0
All	All	1614/1906 (84%)	-0.07	17 (1%) 78 59	59, 124, 211, 288	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	ASN	3.4
1	A	666	VAL	3.0
1	B	799	GLY	2.9
1	A	356	PHE	2.9
1	A	686	PHE	2.9
1	A	514	GLY	2.7
1	B	299	ASP	2.6
1	A	380	PHE	2.5
1	B	28	THR	2.4
1	A	701	VAL	2.4
1	A	887	HIS	2.3
1	A	651	PRO	2.3
1	B	839	PRO	2.2
1	B	916	TYR	2.1
1	A	873	ASN	2.0
1	B	590	ASP	2.0
1	B	345	HIS	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](#)

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($\text{\AA}^2$)	Q<0.9
2	SO4	B	1001	5/5	0.83	0.08	102,127,135,139	0
2	SO4	B	1002	5/5	0.88	0.07	140,141,142,152	0
2	SO4	A	1001	5/5	0.93	0.11	72,78,94,94	0
2	SO4	B	1003	5/5	0.95	0.08	54,85,88,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.