



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:32 pm GMT

PDB ID : 5B86
Title : Crystal structure of M-Sec
Authors : Yamashita, M.; Sato, Y.; Yamagata, A.; Fukai, S.
Deposited on : 2016-06-12
Resolution : 3.02 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

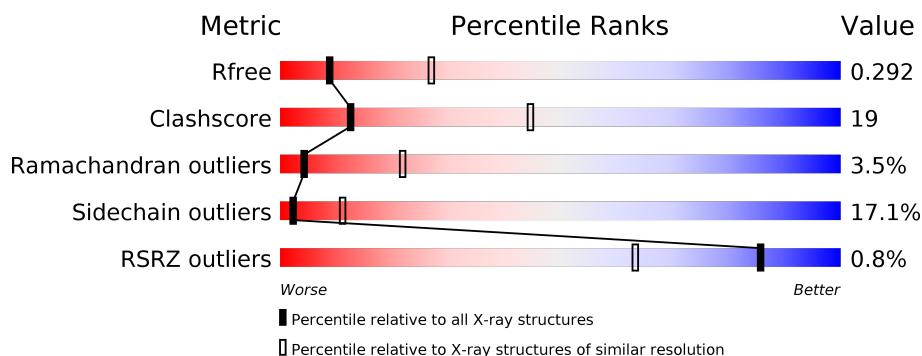
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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}	100719	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	600	<div> <div></div> <div>52% 38% 6% . .</div> </div>
1	B	600	<div> <div></div> <div>49% 39% 9% . .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9312 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 Tumor necrosis factor alpha-induced protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	Se	0	0	0
			4638	2948	814	859	8	9			
1	B	578	Total	C	N	O	S	Se	0	0	0
			4628	2942	811	858	8	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP Q61333
A	52	PRO	-	expression tag	UNP Q61333
B	51	GLY	-	expression tag	UNP Q61333
B	52	PRO	-	expression tag	UNP Q61333

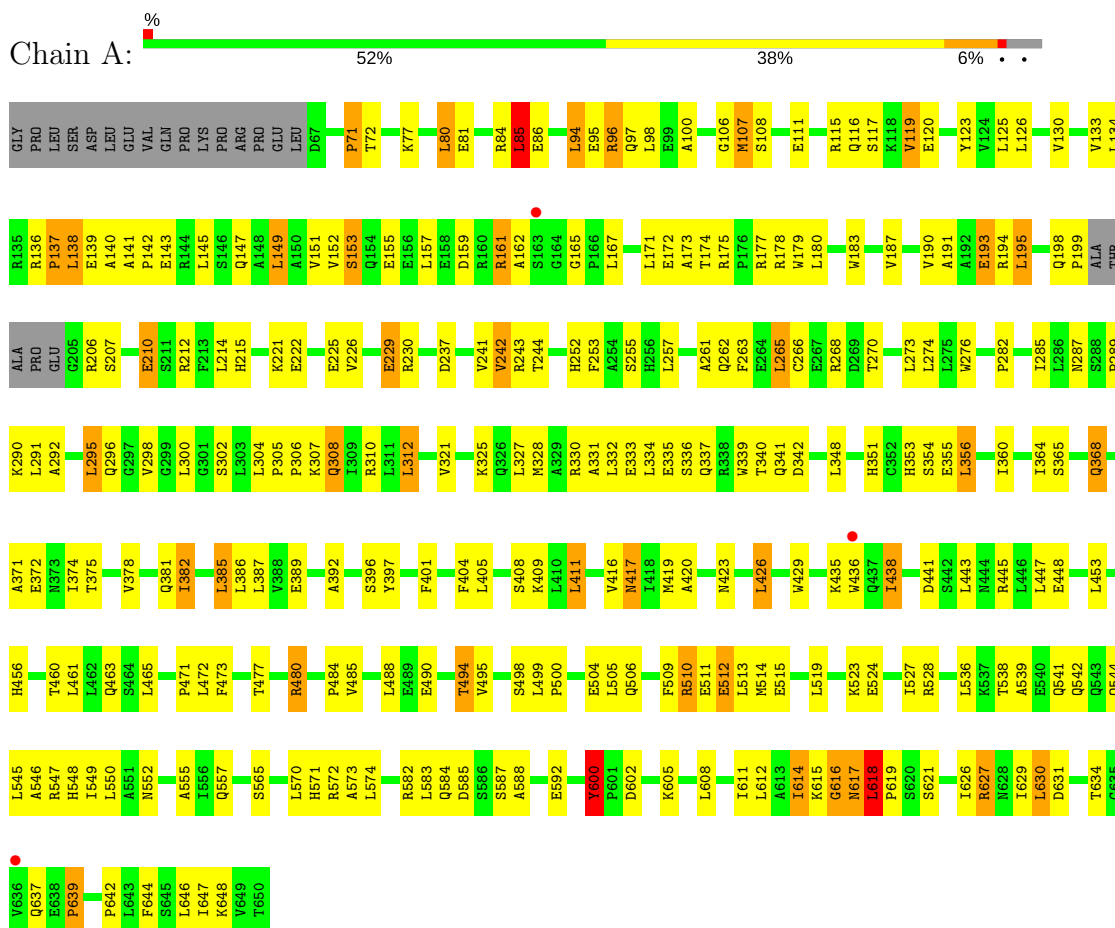
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	30	Total	O	0	0
			30	30		

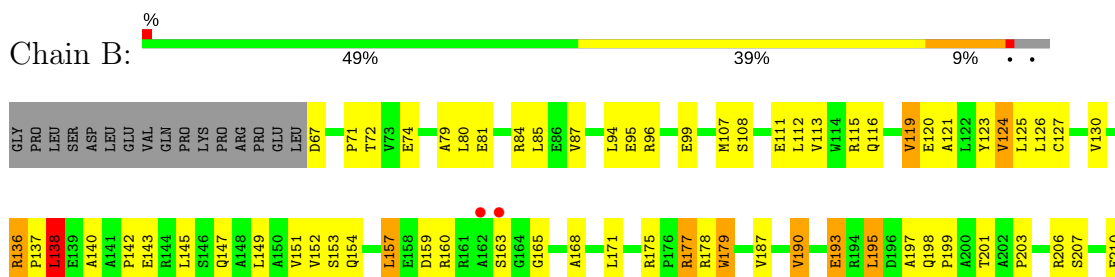
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Tumor necrosis factor alpha-induced protein 2



• Molecule 1: Tumor necrosis factor alpha-induced protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.41 Å 107.83 Å 229.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 3.02 46.44 – 3.02	Depositor EDS
% Data completeness (in resolution range)	86.1 (46.44-3.02) 87.3 (46.44-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.229 , 0.292 0.225 , 0.292	Depositor DCC
R_{free} test set	3717 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9312	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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](#)

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	0.50	0/4717	0.71	2/6380 (0.0%)
1	B	0.46	0/4708	0.69	2/6369 (0.0%)
All	All	0.48	0/9425	0.70	4/12749 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	7.45	132.44	115.30
1	B	265	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	618	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	85	LEU	CA-CB-CG	5.41	127.74	115.30

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	4638	0	4693	166	1
1	B	4628	0	4679	183	1
2	A	16	0	0	3	0
2	B	30	0	0	9	0
All	All	9312	0	9372	349	1

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 19.

All (349) 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:605:LYS:HE3	1:B:630:LEU:HB2	1.52	0.92
1:B:179:TRP:NE1	2:B:701:HOH:O	2.00	0.91
1:A:608:LEU:HD23	1:A:626:ILE:HG12	1.51	0.91
1:A:328:MSE:HE2	1:A:360:ILE:HG23	1.53	0.90
1:B:615:LYS:HB3	1:B:618:LEU:HD21	1.55	0.89
1:B:157:LEU:HD11	1:B:177:ARG:HB2	1.53	0.88
1:B:353:HIS:HB2	1:B:420:ALA:HB1	1.55	0.86
1:B:157:LEU:HD21	1:B:178:ARG:H	1.41	0.85
1:A:157:LEU:HD21	1:A:178:ARG:H	1.42	0.84
1:A:291:LEU:HB3	1:A:295:LEU:HD11	1.60	0.84
1:B:538:THR:HB	1:B:541:GLN:HG2	1.58	0.82
1:B:503:SER:HA	1:B:510:ARG:HH21	1.44	0.81
1:B:197:ALA:O	1:B:212:ARG:NH2	2.17	0.77
1:B:335:GLU:OE1	1:B:353:HIS:NE2	2.18	0.76
1:B:351:HIS:HD2	1:B:419:MSE:HB2	1.50	0.75
1:A:472:LEU:HD13	1:A:490:GLU:HG2	1.68	0.74
1:A:130:VAL:HG21	1:A:149:LEU:HD11	1.69	0.73
1:A:642:PRO:HB3	1:A:646:LEU:HD21	1.71	0.72
1:B:195:LEU:HG	1:B:216:MSE:HG2	1.70	0.72
1:B:536:LEU:HD23	1:B:542:GLN:HA	1.71	0.72
1:B:426:LEU:HB2	1:B:509:PHE:HE1	1.55	0.71
1:A:328:MSE:HG2	1:A:360:ILE:HD12	1.73	0.70
1:B:317:LEU:HB3	1:B:382:ILE:HD11	1.71	0.70
1:A:335:GLU:HG3	1:A:356:LEU:HG	1.72	0.70
1:B:215:HIS:O	1:B:219:THR:OG1	2.09	0.70
1:A:130:VAL:HG22	1:A:149:LEU:HD21	1.72	0.70
1:A:544:GLN:OE1	1:A:547:ARG:NH2	2.25	0.70
1:A:615:LYS:O	1:A:617:ASN:N	2.24	0.69
1:B:442:SER:HA	1:B:445:ARG:HE	1.58	0.69
1:B:328:MSE:HE2	1:B:360:ILE:HG23	1.74	0.69
1:B:335:GLU:HG3	1:B:356:LEU:HD23	1.74	0.69
1:A:484:PRO:HB3	1:A:552:ASN:HD21	1.58	0.69
1:B:474:LYS:HG2	1:B:528:ARG:NH2	2.08	0.69
1:B:318:SER:O	1:B:322:THR:OG1	2.11	0.68
1:A:465:LEU:HD21	1:A:495:VAL:HG23	1.74	0.67
1:A:157:LEU:HD11	1:A:177:ARG:HB2	1.77	0.67
1:B:216:MSE:HE1	1:B:256:HIS:CD2	2.30	0.67
1:A:335:GLU:HB3	1:A:353:HIS:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:HIS:O	1:A:460:THR:OG1	2.12	0.66
1:B:274:LEU:HD11	1:B:313:GLU:HA	1.75	0.66
1:A:157:LEU:HD21	1:A:178:ARG:N	2.10	0.66
1:B:489:GLU:O	1:B:493:THR:OG1	2.13	0.65
1:B:289:PRO:HA	2:B:706:HOH:O	1.96	0.65
1:A:408:SER:HB3	1:A:411:LEU:HG	1.79	0.65
1:A:557:GLN:HG3	1:A:571:HIS:CE1	2.31	0.65
1:B:642:PRO:HB2	1:B:646:LEU:HD21	1.77	0.65
1:A:335:GLU:HB3	1:A:353:HIS:NE2	2.12	0.65
1:B:602:ASP:OD2	1:B:644:PHE:N	2.30	0.64
1:A:371:ALA:HB1	1:A:378:VAL:HG12	1.80	0.64
1:A:321:VAL:HG21	1:A:385:LEU:HD22	1.80	0.64
1:B:96:ARG:NH1	1:B:159:ASP:OD1	2.30	0.64
1:B:364:ILE:HG23	1:B:386:LEU:HD13	1.81	0.63
1:B:168:ALA:HB3	1:B:171:LEU:HG	1.80	0.62
1:A:108:SER:HB3	1:A:111:GLU:HB2	1.81	0.62
1:A:426:LEU:HD13	1:A:506:GLN:HG2	1.80	0.62
1:B:153:SER:O	1:B:157:LEU:HD13	2.00	0.62
1:B:142:PRO:HA	1:B:145:LEU:HD12	1.80	0.62
1:B:615:LYS:HD2	1:B:618:LEU:HD11	1.81	0.61
1:B:207:SER:HB3	1:B:210:GLU:H	1.65	0.60
1:B:67:ASP:N	1:B:67:ASP:OD2	2.34	0.60
1:B:375:THR:HB	1:B:378:VAL:H	1.66	0.60
1:A:126:LEU:O	1:A:130:VAL:HG23	2.02	0.60
1:A:302:SER:OG	1:A:304:LEU:O	2.09	0.60
1:A:140:ALA:HB3	1:A:142:PRO:HD3	1.82	0.60
1:A:510:ARG:HH12	1:A:514:MSE:HE3	1.67	0.60
1:B:538:THR:HG22	1:B:540:GLU:H	1.66	0.59
1:B:72:THR:HG22	1:B:74:GLU:H	1.67	0.59
1:A:157:LEU:HD11	1:A:177:ARG:H	1.66	0.59
1:A:356:LEU:HD22	1:A:360:ILE:HG12	1.84	0.59
1:B:429:TRP:HZ3	1:B:443:LEU:HD13	1.67	0.59
1:A:307:LYS:HA	1:A:310:ARG:HH11	1.68	0.58
1:B:475:LYS:HA	1:B:478:GLN:HB2	1.85	0.58
1:B:510:ARG:NH1	2:B:702:HOH:O	2.16	0.58
1:B:276:TRP:HZ3	1:B:285:ILE:HD11	1.69	0.58
1:A:602:ASP:OD1	1:A:644:PHE:N	2.33	0.57
1:B:321:VAL:HG21	1:B:385:LEU:HD13	1.86	0.57
1:A:527:ILE:HG12	1:A:647:ILE:HG23	1.86	0.57
1:B:157:LEU:HD21	1:B:178:ARG:N	2.17	0.57
1:A:300:LEU:HD12	1:A:300:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HG3	1:A:647:ILE:HG12	1.85	0.57
1:B:288:SER:OG	1:B:289:PRO:HD3	2.05	0.57
1:B:121:ALA:O	1:B:124:VAL:HG13	2.05	0.57
1:B:335:GLU:CD	1:B:353:HIS:HE2	2.07	0.57
1:A:605:LYS:HE2	1:A:630:LEU:HA	1.87	0.56
1:A:538:THR:O	1:A:541:GLN:HG2	2.05	0.56
1:A:265:LEU:HD22	1:A:265:LEU:H	1.70	0.56
1:A:147:GLN:O	1:A:151:VAL:HG23	2.04	0.56
1:A:351:HIS:CE1	1:A:416:VAL:HG13	2.41	0.56
1:B:203:PRO:HD2	1:B:206:ARG:NE	2.20	0.56
1:B:289:PRO:HD2	1:B:291:LEU:HB2	1.88	0.56
1:A:546:ALA:CB	1:A:582:ARG:HB2	2.37	0.55
1:A:332:LEU:HD11	1:A:397:TYR:HA	1.88	0.55
1:B:207:SER:HB3	1:B:210:GLU:HB2	1.88	0.55
1:B:147:GLN:O	1:B:151:VAL:HG23	2.06	0.55
1:B:408:SER:HB3	1:B:411:LEU:HD12	1.88	0.55
1:A:342:ASP:HB2	1:A:411:LEU:HD13	1.89	0.55
1:B:465:LEU:HD11	1:B:495:VAL:HA	1.88	0.55
1:A:484:PRO:HG2	1:A:548:HIS:CG	2.42	0.54
1:B:177:ARG:HG2	1:B:179:TRP:CZ3	2.42	0.54
1:B:625:SER:O	1:B:628:ASN:HB2	2.07	0.54
1:A:401:PHE:O	1:A:404:PHE:HB3	2.08	0.54
1:B:615:LYS:HD2	1:B:618:LEU:HD21	1.89	0.54
1:A:420:ALA:O	1:A:423:ASN:HB2	2.08	0.54
1:B:175:ARG:O	1:B:177:ARG:N	2.41	0.54
1:B:534:LEU:O	1:B:614:ILE:HG22	2.08	0.53
1:B:157:LEU:HG	1:B:177:ARG:H	1.73	0.53
1:B:419:MSE:O	1:B:423:ASN:ND2	2.41	0.53
1:B:426:LEU:HB2	1:B:509:PHE:CE1	2.41	0.53
1:A:542:GLN:OE1	1:A:584:GLN:NE2	2.41	0.53
1:B:274:LEU:HD13	1:B:374:ILE:HD13	1.89	0.53
1:A:473:PHE:CE2	1:A:524:GLU:HB3	2.44	0.53
1:B:617:ASN:H	1:B:618:LEU:HD22	1.74	0.53
1:A:96:ARG:NE	2:A:702:HOH:O	2.42	0.53
1:A:167:LEU:HD22	1:A:173:ALA:HA	1.90	0.52
1:B:108:SER:HB2	1:B:111:GLU:HB2	1.91	0.52
1:B:608:LEU:O	1:B:612:LEU:HG	2.09	0.52
1:B:615:LYS:HB3	1:B:618:LEU:CD2	2.35	0.52
1:B:115:ARG:O	1:B:119:VAL:HG12	2.09	0.52
1:A:583:LEU:HD22	1:A:588:ALA:HB1	1.90	0.52
1:B:462:LEU:HD21	1:B:513:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG12	1:A:134:LEU:HD23	1.90	0.52
1:B:157:LEU:HD11	1:B:177:ARG:CB	2.35	0.52
1:B:583:LEU:HD13	1:B:588:ALA:HB1	1.91	0.52
1:B:353:HIS:O	1:B:355:GLU:N	2.42	0.52
1:A:95:GLU:OE2	1:A:175:ARG:NH1	2.43	0.52
1:B:81:GLU:HG3	1:B:125:LEU:HD21	1.91	0.52
1:B:95:GLU:OE1	1:B:175:ARG:NH1	2.43	0.52
1:A:261:ALA:HB2	1:A:304:LEU:HD11	1.92	0.51
1:B:263:PHE:O	1:B:265:LEU:HD22	2.10	0.51
1:A:96:ARG:NH1	1:A:159:ASP:OD2	2.42	0.51
1:A:337:GLN:HA	1:A:340:THR:HB	1.92	0.51
1:A:546:ALA:HB2	1:A:582:ARG:HB2	1.93	0.51
1:A:84:ARG:CD	1:A:86:GLU:H	2.23	0.51
1:B:354:SER:O	1:B:358:ILE:HG12	2.10	0.51
1:B:515:GLU:HG2	1:B:567:ALA:HB2	1.93	0.51
1:B:126:LEU:O	1:B:130:VAL:HG23	2.10	0.51
1:B:224:LEU:O	1:B:228:VAL:HG23	2.11	0.51
1:A:222:GLU:O	1:A:226:VAL:HG23	2.11	0.51
1:A:509:PHE:HA	1:A:512:GLU:HB2	1.92	0.51
1:B:154:GLN:HA	1:B:157:LEU:HD22	1.91	0.51
1:A:339:TRP:HA	1:A:417:ASN:OD1	2.10	0.51
1:B:542:GLN:NE2	1:B:615:LYS:O	2.44	0.51
1:B:187:VAL:HG11	1:B:244:THR:HG22	1.92	0.50
1:B:607:HIS:HE2	1:B:647:ILE:HG22	1.76	0.50
1:A:96:ARG:NH2	1:A:159:ASP:OD2	2.44	0.50
1:B:523:LYS:O	1:B:527:ILE:HG13	2.11	0.50
1:A:295:LEU:HA	1:A:298:VAL:HG23	1.93	0.50
1:B:519:LEU:O	1:B:523:LYS:HB2	2.12	0.50
1:A:605:LYS:NZ	1:A:630:LEU:HD13	2.26	0.50
1:A:221:LYS:HE3	1:A:225:GLU:OE2	2.11	0.49
1:B:120:GLU:O	1:B:124:VAL:HG12	2.12	0.49
1:B:429:TRP:NE1	2:B:703:HOH:O	2.34	0.49
1:A:153:SER:O	1:A:157:LEU:HD13	2.12	0.49
1:B:279:ASN:O	1:B:283:ASN:HB2	2.12	0.49
1:A:180:LEU:O	1:A:183:TRP:HB3	2.12	0.49
1:B:351:HIS:CD2	1:B:419:MSE:HB2	2.40	0.49
1:A:365:SER:HB3	1:A:435:LYS:NZ	2.27	0.49
1:A:573:ALA:HA	1:A:600:TYR:CE1	2.48	0.49
1:B:136:ARG:HH11	1:B:136:ARG:HB2	1.78	0.49
1:B:190:VAL:HA	1:B:193:GLU:HG2	1.95	0.49
1:B:214:LEU:HD22	1:B:276:TRP:HZ2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:VAL:HG11	1:B:294:GLU:HG3	1.95	0.49
1:B:543:GLN:HG3	1:B:582:ARG:HG2	1.95	0.49
1:A:193:GLU:HG3	1:A:194:ARG:N	2.29	0.48
1:A:536:LEU:O	1:A:616:GLY:HA3	2.13	0.48
1:B:126:LEU:HD23	2:B:701:HOH:O	2.14	0.48
1:B:328:MSE:HB3	1:B:393:LEU:HD13	1.94	0.48
1:A:206:ARG:HD2	1:A:206:ARG:H	1.78	0.48
1:A:229:GLU:HB3	1:A:230:ARG:HG3	1.96	0.48
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.65	0.48
1:B:623:VAL:HA	1:B:626:ILE:HB	1.96	0.48
1:A:524:GLU:HA	1:A:527:ILE:HD12	1.96	0.48
1:A:133:VAL:HA	1:A:139:GLU:OE1	2.14	0.48
1:B:257:LEU:HB3	1:B:304:LEU:HD21	1.96	0.48
1:A:107:MSE:HE1	1:A:115:ARG:CZ	2.44	0.48
1:A:519:LEU:HD13	1:A:570:LEU:HD21	1.96	0.47
1:B:281:TYR:CE1	1:B:286:LEU:HD13	2.48	0.47
1:A:207:SER:HB3	1:A:210:GLU:H	1.79	0.47
1:A:488:LEU:HD21	1:A:555:ALA:HB3	1.96	0.47
1:B:354:SER:HA	1:B:424:ASN:OD1	2.14	0.47
1:B:199:PRO:HB3	1:B:215:HIS:HB2	1.96	0.47
1:B:351:HIS:NE2	1:B:416:VAL:HG12	2.28	0.47
1:A:331:ALA:O	1:A:335:GLU:HG2	2.13	0.47
1:B:476:PHE:CE2	1:B:487:THR:HB	2.49	0.47
1:A:85:LEU:HD12	1:A:145:LEU:HB2	1.97	0.47
1:A:270:THR:O	1:A:274:LEU:HB2	2.15	0.47
1:A:514:MSE:HG3	1:A:565:SER:HB2	1.96	0.47
1:B:528:ARG:HA	1:B:528:ARG:HD3	1.60	0.47
1:A:419:MSE:HG2	1:A:505:LEU:HD13	1.96	0.47
1:A:353:HIS:C	1:A:355:GLU:N	2.68	0.47
1:B:454:LYS:HD3	1:B:509:PHE:HE2	1.79	0.47
1:A:225:GLU:N	1:A:291:LEU:HD21	2.30	0.46
1:B:236:PRO:HG2	1:B:239:PHE:CD2	2.50	0.46
1:B:618:LEU:HD22	1:B:618:LEU:N	2.31	0.46
1:A:545:LEU:O	1:A:548:HIS:HB2	2.16	0.46
1:A:195:LEU:HD23	1:A:252:HIS:HB3	1.98	0.46
1:A:257:LEU:HB3	1:A:304:LEU:CD2	2.45	0.46
1:B:605:LYS:HE2	1:B:626:ILE:HG22	1.97	0.46
1:B:618:LEU:HD22	1:B:618:LEU:H	1.81	0.46
1:B:606:GLY:HA3	1:B:649:VAL:HG11	1.96	0.46
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.65	0.46
1:B:221:LYS:HB3	1:B:221:LYS:HE2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:VAL:HG21	1:B:385:LEU:HD22	1.98	0.46
1:B:342:ASP:HB3	1:B:411:LEU:HD13	1.98	0.46
1:B:619:PRO:HG2	1:B:621:SER:HB2	1.98	0.46
1:A:149:LEU:CD1	1:A:179:TRP:HZ3	2.29	0.46
1:B:269:ASP:HA	1:B:272:LEU:HG	1.98	0.46
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.81	0.45
1:A:510:ARG:NH1	1:A:514:MSE:HE3	2.30	0.45
1:A:282:PRO:O	1:A:287:ASN:HB2	2.15	0.45
1:B:343:VAL:O	1:B:345:PRO:HD3	2.16	0.45
1:B:345:PRO:HB2	1:B:351:HIS:CE1	2.51	0.45
1:B:429:TRP:CD2	1:B:447:LEU:HD12	2.51	0.45
1:A:276:TRP:HZ3	1:A:285:ILE:HD11	1.81	0.45
1:A:490:GLU:O	1:A:494:THR:OG1	2.34	0.45
1:A:506:GLN:HB3	1:A:509:PHE:HD1	1.82	0.45
1:B:438:ILE:HG22	1:B:439:SER:H	1.81	0.45
1:B:450:LEU:HA	1:B:450:LEU:HD23	1.77	0.45
1:B:473:PHE:CE1	1:B:491:ILE:HD13	2.52	0.45
1:B:507:ASP:HA	1:B:510:ARG:HG2	1.96	0.45
1:B:470:LYS:HB2	1:B:471:PRO:HD3	1.99	0.45
1:B:590:LYS:HZ3	1:B:624:ARG:HB3	1.81	0.45
1:A:142:PRO:HB2	1:A:145:LEU:HD12	1.99	0.45
1:A:167:LEU:HD13	1:A:173:ALA:HB2	1.99	0.45
1:B:203:PRO:HD2	1:B:206:ARG:HE	1.81	0.45
1:B:280:LEU:O	1:B:284:ASP:HB2	2.16	0.45
1:B:289:PRO:HB2	1:B:290:LYS:H	1.58	0.45
1:B:607:HIS:NE2	1:B:647:ILE:HG22	2.32	0.45
1:B:605:LYS:HG2	1:B:626:ILE:HG23	1.99	0.45
1:A:137:PRO:HB3	1:A:143:GLU:OE1	2.16	0.45
1:A:263:PHE:O	1:A:265:LEU:HD13	2.16	0.45
1:B:272:LEU:HA	1:B:275:LEU:HB3	1.99	0.45
1:A:140:ALA:HB3	1:A:142:PRO:CD	2.47	0.45
1:A:353:HIS:HB2	1:A:420:ALA:HB1	1.98	0.45
1:B:231:LEU:HD22	1:B:231:LEU:HA	1.77	0.44
1:A:221:LYS:HB2	1:A:285:ILE:HG23	1.99	0.44
1:A:165:GLY:O	1:A:167:LEU:HD12	2.17	0.44
1:B:627:ARG:HA	1:B:627:ARG:HD3	1.64	0.44
1:A:84:ARG:HD3	1:A:86:GLU:H	1.82	0.44
1:B:136:ARG:NH1	1:B:136:ARG:HB2	2.32	0.44
1:B:163:SER:C	1:B:165:GLY:H	2.20	0.44
1:B:488:LEU:HD22	1:B:552:ASN:HB3	2.00	0.44
1:A:536:LEU:HD23	1:A:542:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ARG:HA	1:A:572:ARG:HD3	1.64	0.44
1:A:583:LEU:HD11	1:A:592:GLU:HG3	1.99	0.44
1:B:442:SER:HA	1:B:445:ARG:NE	2.29	0.44
1:A:330:ARG:NH1	1:A:333:GLU:OE1	2.51	0.44
1:A:401:PHE:CD2	1:A:453:LEU:HG	2.53	0.44
1:B:398:GLN:NE2	2:B:707:HOH:O	2.41	0.44
1:B:79:ALA:O	1:B:84:ARG:HG3	2.16	0.44
1:A:305:PRO:HG2	1:A:308:GLN:HB2	1.98	0.44
1:A:98:LEU:HD21	1:A:171:LEU:HD21	1.99	0.44
1:B:127:CYS:HA	2:B:701:HOH:O	2.18	0.44
1:B:136:ARG:HH11	1:B:138:LEU:HD22	1.83	0.44
1:B:175:ARG:CZ	1:B:177:ARG:HD2	2.48	0.44
1:B:481:TRP:CZ2	1:B:529:LEU:HD12	2.53	0.44
1:A:438:ILE:H	1:A:438:ILE:HG13	1.58	0.44
1:A:488:LEU:HD22	1:A:552:ASN:OD1	2.18	0.44
1:A:190:VAL:HA	1:A:193:GLU:HG2	1.98	0.43
1:B:157:LEU:CD2	1:B:178:ARG:H	2.22	0.43
1:A:375:THR:HB	1:A:378:VAL:HG23	2.00	0.43
1:B:415:ARG:HD3	1:B:501:GLU:OE2	2.17	0.43
1:A:242:VAL:HG23	1:A:243:ARG:H	1.83	0.43
1:A:389:GLU:O	1:A:392:ALA:HB3	2.19	0.43
1:A:648:LYS:HA	1:A:648:LYS:HD3	1.56	0.43
1:A:151:VAL:O	1:A:155:GLU:HG2	2.19	0.43
1:A:557:GLN:HG3	1:A:571:HIS:ND1	2.33	0.43
1:A:136:ARG:HB3	1:A:138:LEU:HD23	2.01	0.43
1:A:545:LEU:O	1:A:549:ILE:HG12	2.17	0.43
1:A:81:GLU:HG2	1:A:125:LEU:HD21	2.01	0.43
1:B:458:PHE:HA	1:B:461:LEU:HD11	2.01	0.43
1:B:623:VAL:O	1:B:627:ARG:HG2	2.19	0.43
1:B:468:ASP:O	1:B:472:LEU:HG	2.18	0.43
1:B:473:PHE:CE2	1:B:524:GLU:HB3	2.54	0.43
1:A:199:PRO:HB3	1:A:215:HIS:HB2	2.00	0.42
1:B:227:VAL:O	1:B:231:LEU:HB2	2.19	0.42
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.71	0.42
1:A:637:GLN:C	1:A:639:PRO:HD3	2.40	0.42
1:B:237:ASP:N	1:B:237:ASP:OD2	2.50	0.42
1:B:398:GLN:HA	1:B:453:LEU:HD12	2.01	0.42
1:B:467:LEU:HA	1:B:470:LYS:HG3	2.00	0.42
1:B:480:ARG:NH2	2:B:704:HOH:O	2.37	0.42
1:B:212:ARG:HD2	2:B:729:HOH:O	2.19	0.42
1:A:351:HIS:CE1	1:A:504:GLU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD12	1:B:175:ARG:HE	1.85	0.42
1:B:357:ALA:HA	1:B:428:PHE:CE1	2.54	0.42
1:B:559:PHE:HA	1:B:562:GLU:OE2	2.20	0.42
1:B:602:ASP:N	1:B:602:ASP:OD1	2.39	0.42
1:B:615:LYS:O	1:B:617:ASN:N	2.53	0.42
1:A:157:LEU:CD1	1:A:177:ARG:H	2.29	0.42
1:B:254:ALA:O	1:B:258:CYS:HB2	2.20	0.42
1:B:281:TYR:CE1	1:B:303:LEU:HD21	2.55	0.42
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.88	0.42
1:B:140:ALA:H	1:B:142:PRO:HD2	1.84	0.42
1:A:71:PRO:HD3	2:A:704:HOH:O	2.20	0.42
1:B:247:GLU:HB3	1:B:251:TYR:CE2	2.54	0.42
1:A:328:MSE:HE3	1:A:364:ILE:HG13	2.02	0.42
1:A:97:GLN:O	1:A:100:ALA:HB3	2.19	0.41
1:A:515:GLU:HB2	2:A:710:HOH:O	2.19	0.41
1:A:574:LEU:HD23	1:A:574:LEU:HA	1.78	0.41
1:B:330:ARG:O	1:B:334:LEU:HB2	2.20	0.41
1:A:611:ILE:O	1:A:614:ILE:HG12	2.20	0.41
1:B:527:ILE:HG12	1:B:647:ILE:HG12	2.02	0.41
1:A:274:LEU:HD11	1:A:312:LEU:HB3	2.03	0.41
1:A:523:LYS:HG2	1:A:527:ILE:HD11	2.02	0.41
1:B:160:ARG:HB2	1:B:175:ARG:HG2	2.01	0.41
1:B:420:ALA:HA	1:B:423:ASN:HD22	1.85	0.41
1:A:187:VAL:HG11	1:A:244:THR:HG22	2.03	0.41
1:A:416:VAL:H	1:A:416:VAL:HG23	1.64	0.41
1:A:441:ASP:O	1:A:445:ARG:HB2	2.20	0.41
1:A:506:GLN:HB3	1:A:509:PHE:CD1	2.55	0.41
1:B:168:ALA:O	1:B:171:LEU:HB2	2.21	0.41
1:A:191:ALA:O	1:A:195:LEU:HB2	2.21	0.41
1:A:353:HIS:CB	1:A:420:ALA:HB1	2.51	0.41
1:A:360:ILE:HD13	1:A:360:ILE:HA	1.76	0.41
1:A:84:ARG:HD3	1:A:85:LEU:N	2.36	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.84	0.41
1:B:441:ASP:O	1:B:445:ARG:HG3	2.21	0.41
1:B:618:LEU:HA	1:B:619:PRO:HD2	1.73	0.41
1:A:368:GLN:O	1:A:372:GLU:HB2	2.20	0.41
1:A:435:LYS:HB3	1:A:436:TRP:CE3	2.56	0.41
1:B:252:HIS:O	1:B:255:SER:HB3	2.20	0.41
1:B:353:HIS:C	1:B:355:GLU:N	2.74	0.41
1:B:381:GLN:O	1:B:385:LEU:HB2	2.21	0.41
1:A:119:VAL:HG12	1:A:120:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HB3	1:A:162:ALA:H	1.74	0.41
1:A:617:ASN:O	1:A:618:LEU:HD23	2.21	0.41
1:A:583:LEU:CD1	1:A:592:GLU:HG3	2.51	0.41
1:B:576:MSE:O	1:B:580:ILE:HG13	2.20	0.41
1:B:501:GLU:HG2	1:B:502:PHE:CD1	2.56	0.40
1:A:602:ASP:N	1:A:602:ASP:OD2	2.46	0.40
1:A:612:LEU:O	1:A:615:LYS:HB2	2.21	0.40
1:A:84:ARG:HD2	1:A:86:GLU:H	1.84	0.40
1:B:358:ILE:O	1:B:362:GLN:HB2	2.21	0.40
1:A:327:LEU:HD23	1:A:327:LEU:HA	1.93	0.40
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.77	0.40
1:A:77:LYS:O	1:A:81:GLU:HG3	2.20	0.40
1:B:305:PRO:HG2	1:B:308:GLN:HB2	2.03	0.40
1:B:316:PHE:O	1:B:319:ASN:HB2	2.21	0.40
1:B:324:VAL:HG21	1:B:386:LEU:CD2	2.51	0.40
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.67	0.40
1:B:358:ILE:HG22	1:B:427:PHE:CZ	2.56	0.40
1:A:157:LEU:HD12	1:A:175:ARG:HE	1.86	0.40
1:A:381:GLN:O	1:A:385:LEU:HB2	2.22	0.40
1:A:382:ILE:O	1:A:386:LEU:HG	2.21	0.40
1:A:471:PRO:O	1:A:473:PHE:N	2.54	0.40
1:B:228:VAL:CG1	1:B:294:GLU:HG3	2.51	0.40
1:B:393:LEU:HG	1:B:393:LEU:O	2.14	0.40
1:B:85:LEU:HD23	1:B:145:LEU:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ARG:NH1	1:B:264:GLU:OE2[4_455]	2.17	0.03

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	575/600 (96%)	483 (84%)	67 (12%)	25 (4%)	3	17
1	B	574/600 (96%)	496 (86%)	63 (11%)	15 (3%)	6	29
All	All	1149/1200 (96%)	979 (85%)	130 (11%)	40 (4%)	4	22

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	463	GLN
1	A	639	PRO
1	B	286	LEU
1	B	616	GLY
1	B	619	PRO
1	A	292	ALA
1	A	480	ARG
1	A	500	PRO
1	A	616	GLY
1	A	627	ARG
1	A	629	ILE
1	B	113	VAL
1	B	201	THR
1	B	288	SER
1	B	289	PRO
1	A	161	ARG
1	A	172	GLU
1	A	306	PRO
1	A	409	LYS
1	A	619	PRO
1	A	630	LEU
1	A	634	THR
1	B	112	LEU
1	B	639	PRO
1	A	106	GLY
1	A	289	PRO
1	A	618	LEU
1	A	137	PRO
1	A	539	ALA
1	B	71	PRO
1	B	306	PRO
1	B	137	PRO
1	B	350	GLY

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Mol	Chain	Res	Type
1	B	354	SER
1	A	141	ALA
1	B	374	ILE
1	A	374	ILE
1	A	600	TYR
1	A	614	ILE

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	504/513 (98%)	429 (85%)	75 (15%)	3 16
1	B	502/513 (98%)	405 (81%)	97 (19%)	1 8
All	All	1006/1026 (98%)	834 (83%)	172 (17%)	2 11

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	80	LEU
1	A	85	LEU
1	A	94	LEU
1	A	96	ARG
1	A	107	MSE
1	A	116	GLN
1	A	117	SER
1	A	119	VAL
1	A	123	TYR
1	A	138	LEU
1	A	149	LEU
1	A	152	VAL
1	A	153	SER
1	A	174	THR
1	A	193	GLU
1	A	195	LEU

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Mol	Chain	Res	Type
1	A	198	GLN
1	A	210	GLU
1	A	212	ARG
1	A	229	GLU
1	A	237	ASP
1	A	241	VAL
1	A	242	VAL
1	A	253	PHE
1	A	255	SER
1	A	262	GLN
1	A	265	LEU
1	A	266	CYS
1	A	268	ARG
1	A	273	LEU
1	A	290	LYS
1	A	295	LEU
1	A	296	GLN
1	A	308	GLN
1	A	312	LEU
1	A	325	LYS
1	A	334	LEU
1	A	336	SER
1	A	341	GLN
1	A	348	LEU
1	A	354	SER
1	A	356	LEU
1	A	368	GLN
1	A	382	ILE
1	A	385	LEU
1	A	396	SER
1	A	411	LEU
1	A	417	ASN
1	A	426	LEU
1	A	429	TRP
1	A	438	ILE
1	A	443	LEU
1	A	447	LEU
1	A	448	GLU
1	A	461	LEU
1	A	477	THR
1	A	485	VAL
1	A	494	THR

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Mol	Chain	Res	Type
1	A	498	SER
1	A	499	LEU
1	A	510	ARG
1	A	511	GLU
1	A	512	GLU
1	A	513	LEU
1	A	528	ARG
1	A	550	LEU
1	A	585	ASP
1	A	587	SER
1	A	600	TYR
1	A	617	ASN
1	A	618	LEU
1	A	621	SER
1	A	627	ARG
1	A	631	ASP
1	B	80	LEU
1	B	87	VAL
1	B	94	LEU
1	B	99	GLU
1	B	107	MSE
1	B	116	GLN
1	B	119	VAL
1	B	123	TYR
1	B	124	VAL
1	B	136	ARG
1	B	138	LEU
1	B	143	GLU
1	B	149	LEU
1	B	152	VAL
1	B	157	LEU
1	B	177	ARG
1	B	179	TRP
1	B	190	VAL
1	B	193	GLU
1	B	195	LEU
1	B	198	GLN
1	B	212	ARG
1	B	218	ARG
1	B	219	THR
1	B	229	GLU
1	B	231	LEU

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Mol	Chain	Res	Type
1	B	234	LEU
1	B	241	VAL
1	B	242	VAL
1	B	253	PHE
1	B	257	LEU
1	B	258	CYS
1	B	260	LEU
1	B	264	GLU
1	B	265	LEU
1	B	266	CYS
1	B	274	LEU
1	B	284	ASP
1	B	290	LYS
1	B	308	GLN
1	B	309	ILE
1	B	311	LEU
1	B	312	LEU
1	B	316	PHE
1	B	322	THR
1	B	323	SER
1	B	326	GLN
1	B	339	TRP
1	B	342	ASP
1	B	351	HIS
1	B	354	SER
1	B	361	LEU
1	B	368	GLN
1	B	372	GLU
1	B	375	THR
1	B	376	SER
1	B	383	LYS
1	B	385	LEU
1	B	394	LEU
1	B	395	ARG
1	B	398	GLN
1	B	409	LYS
1	B	410	LEU
1	B	415	ARG
1	B	416	VAL
1	B	436	TRP
1	B	443	LEU
1	B	447	LEU

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Mol	Chain	Res	Type
1	B	448	GLU
1	B	453	LEU
1	B	461	LEU
1	B	462	LEU
1	B	463	GLN
1	B	464	SER
1	B	465	LEU
1	B	489	GLU
1	B	493	THR
1	B	495	VAL
1	B	496	SER
1	B	505	LEU
1	B	510	ARG
1	B	533	ARG
1	B	536	LEU
1	B	543	GLN
1	B	544	GLN
1	B	550	LEU
1	B	557	GLN
1	B	568	THR
1	B	579	GLU
1	B	593	VAL
1	B	605	LYS
1	B	614	ILE
1	B	615	LYS
1	B	618	LEU
1	B	621	SER
1	B	623	VAL
1	B	646	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	ASN
1	A	417	ASN
1	A	520	HIS
1	A	552	ASN
1	B	250	HIS
1	B	256	HIS
1	B	518	HIS
1	B	541	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [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	570/600 (95%)	-0.06	3 (0%)	90 73	28, 74, 126, 185	0
1	B	569/600 (94%)	-0.05	6 (1%)	80 54	36, 77, 132, 184	0
All	All	1139/1200 (94%)	-0.06	9 (0%)	86 63	28, 76, 130, 185	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	636	VAL	7.0
1	B	162	ALA	4.4
1	B	415	ARG	3.6
1	B	354	SER	3.1
1	A	163	SER	3.1
1	A	436	TRP	2.8
1	B	163	SER	2.6
1	B	631	ASP	2.0
1	B	628	ASN	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 carbohydrates 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.