



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:36 AM UTC

PDB ID : 6LYR / pdb_00006lyr
Title : Structure of the BAM complex
Authors : Xiao, L.; Huang, Y.
Deposited on : 2020-02-15
Resolution : 3.28 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

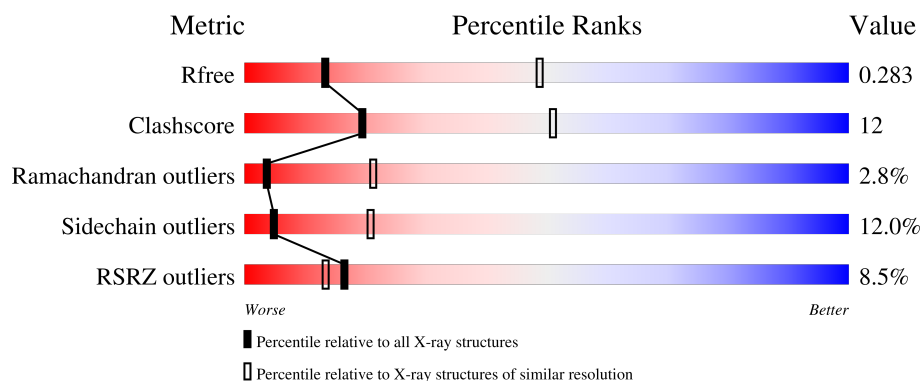
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	810	8% 69% 23% 5% .
2	B	400	8% 55% 30% 5% 11%
3	C	344	2% 11% 5% 84%
4	D	245	6% 61% 23% . 15%
5	E	119	3% 39% 27% 8% 26%

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Mol	Chain	Length	Quality of chain
6	P	9	11% 22% 33% 44%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11439 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	0	0
			6074	3826	1022	1210	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	760	TRP	TYR	conflict	UNP P0A940

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2629	1652	449	522	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	393	TRP	-	expression tag	UNP P77774
B	394	SER	-	expression tag	UNP P77774
B	395	HIS	-	expression tag	UNP P77774
B	396	PRO	-	expression tag	UNP P77774
B	397	GLN	-	expression tag	UNP P77774
B	398	PHE	-	expression tag	UNP P77774
B	399	GLU	-	expression tag	UNP P77774
B	400	LYS	-	expression tag	UNP P77774

- Molecule 3 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	56	Total	C	N	O	S	0	0	0
			378	239	63	75	1			

- Molecule 4 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1642	1035	286	314	7			

- Molecule 5 is a protein called Outer membrane protein assembly factor BamE.

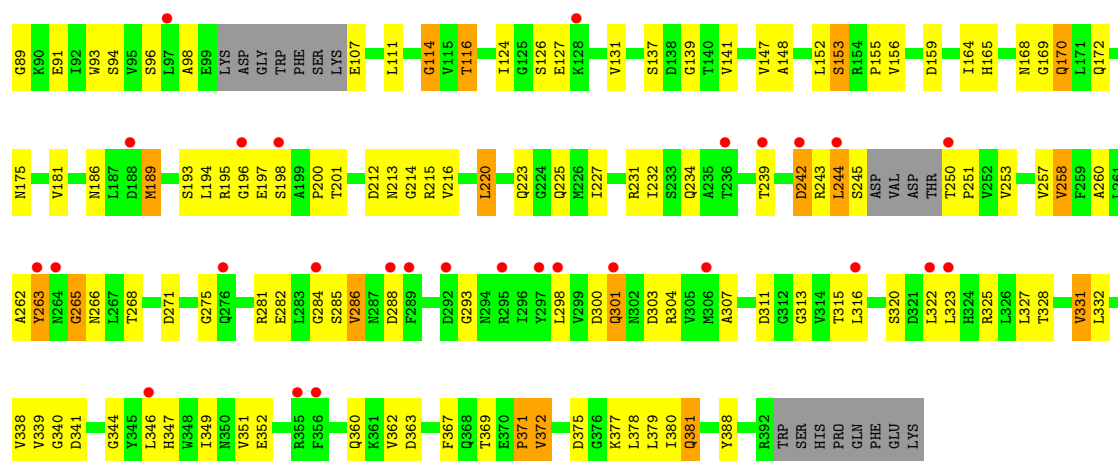
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	88	Total	C	N	O	S	0	0	0
			657	415	108	132	2			

There are 6 discrepancies between the modelled and reference sequences:

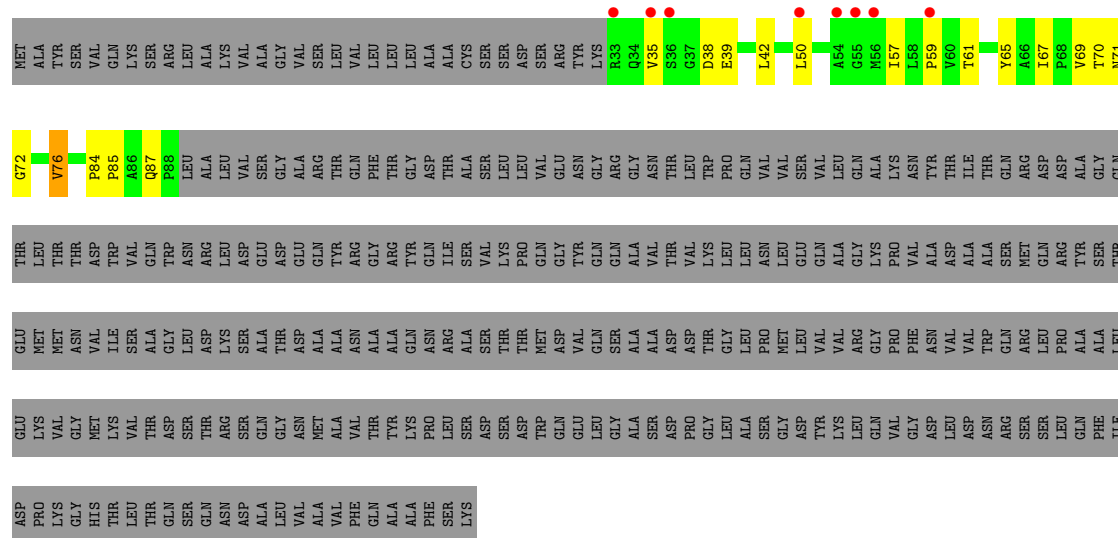
Chain	Residue	Modelled	Actual	Comment	Reference
E	114	HIS	-	expression tag	UNP P0A937
E	115	HIS	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937

- Molecule 6 is a protein called Peptide from Outer membrane protein A.

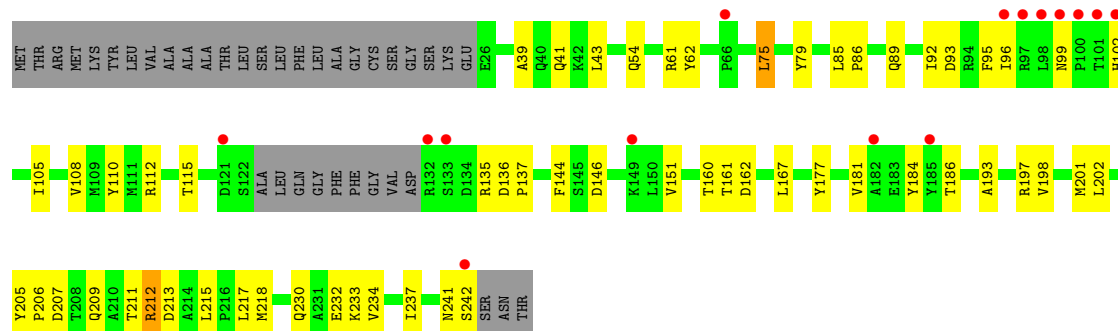
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	P	9	Total	C	N	O	S	0	0	0
			59	36	10	12	1			



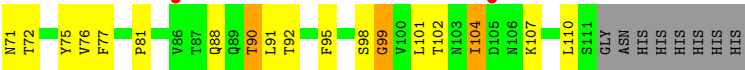
• Molecule 3: Outer membrane protein assembly factor BamC



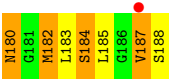
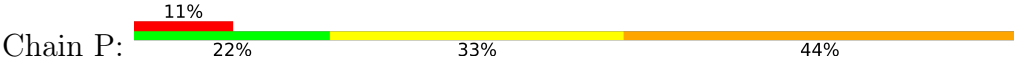
• Molecule 4: Outer membrane protein assembly factor BamD



• Molecule 5: Outer membrane protein assembly factor BamE



● Molecule 6: Peptide from Outer membrane protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.88Å 116.88Å 430.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 3.28 49.37 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.37-3.28) 99.4 (49.37-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.246 , 0.280 0.250 , 0.283	Depositor DCC
R_{free} test set	2302 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	103.1	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11439	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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	0.98	0/6212	1.32	1/8446 (0.0%)
2	B	1.01	0/2674	1.32	2/3652 (0.1%)
3	C	1.05	0/387	1.32	0/533
4	D	0.97	0/1678	1.56	0/2285
5	E	1.00	0/671	1.32	1/919 (0.1%)
6	P	1.05	0/58	1.81	1/76 (1.3%)
All	All	0.99	0/11680	1.36	5/15911 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	P	184	SER	N-CA-CB	-9.58	94.86	110.77
2	B	159	ASP	N-CA-C	-6.58	98.30	108.31
5	E	60	GLY	CA-C-O	-5.14	117.61	122.39
2	B	286	VAL	N-CA-C	-5.11	108.29	113.20
1	A	126	ASP	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	722	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6074	0	5674	126	0
2	B	2629	0	2556	72	0
3	C	378	0	362	11	0
4	D	1642	0	1559	40	0
5	E	657	0	615	25	0
6	P	59	0	61	4	0
All	All	11439	0	10827	259	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 12.

All (259) 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:205:TRP:HA	1:A:208:VAL:HG23	1.33	1.07
2:B:223:GLN:HE21	2:B:225:GLN:HB3	1.24	1.02
6:P:183:LEU:HG	6:P:184:SER:N	1.92	0.83
1:A:681:ASN:OD1	1:A:688:TYR:OH	1.95	0.82
1:A:205:TRP:HA	1:A:208:VAL:CG2	2.11	0.80
4:D:93:ASP:OD1	4:D:112:ARG:NH1	2.15	0.78
1:A:676:PRO:HB2	1:A:696:ALA:HB1	1.69	0.73
1:A:692:THR:HA	1:A:696:ALA:HB2	1.71	0.73
6:P:180:ASN:N	6:P:180:ASN:HD22	1.87	0.72
2:B:63:LEU:HA	2:B:114:GLY:HA2	1.72	0.72
2:B:266:ASN:HD22	2:B:282:GLU:HA	1.55	0.71
4:D:209:GLN:OE1	4:D:212:ARG:NH1	2.24	0.71
1:A:329:ASN:ND2	1:A:332:ASP:OD1	2.22	0.70
1:A:290:ILE:HD11	1:A:304:MET:HE1	1.75	0.69
1:A:54:VAL:HG23	1:A:58:ASP:HB2	1.75	0.69
1:A:659:THR:OG1	1:A:660:VAL:N	2.21	0.69
1:A:663:PHE:CE1	1:A:790:PRO:HB3	2.29	0.68
5:E:27:VAL:HG12	5:E:28:TYR:H	1.60	0.67
1:A:423:THR:OG1	1:A:446:GLN:OE1	2.13	0.66
1:A:213:LYS:CB	1:A:215:GLN:OE1	2.44	0.66
2:B:197:GLU:OE2	2:B:245:SER:OG	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:ASP:OD1	2:B:242:ASP:N	2.29	0.65
2:B:263:TYR:O	2:B:284:GLY:HA3	1.98	0.64
1:A:315:TYR:C	5:E:37:TYR:HE2	2.06	0.64
1:A:136:GLY:O	1:A:139:ASP:OD1	2.15	0.64
4:D:92:ILE:HG23	4:D:108:VAL:HG12	1.80	0.64
2:B:266:ASN:ND2	2:B:282:GLU:HA	2.13	0.63
4:D:61:ARG:HG3	4:D:62:TYR:CZ	2.34	0.63
2:B:82:LYS:NZ	2:B:94:SER:HA	2.15	0.62
2:B:168:ASN:HA	2:B:189:MET:HE1	1.81	0.62
1:A:205:TRP:CA	1:A:208:VAL:HG23	2.21	0.62
4:D:110:TYR:OH	4:D:162:ASP:OD2	2.17	0.61
3:C:70:THR:O	3:C:72:GLY:N	2.34	0.61
2:B:156:VAL:HG21	2:B:200:PRO:O	2.00	0.61
1:A:247:LEU:HD12	1:A:251:LYS:HA	1.82	0.61
1:A:595:LEU:HD12	1:A:613:LEU:HD13	1.82	0.61
2:B:193:SER:HB2	2:B:245:SER:HB2	1.84	0.60
3:C:59:PRO:HG3	5:E:67:PRO:HB2	1.82	0.60
2:B:131:VAL:HG21	2:B:164:ILE:HG12	1.84	0.59
1:A:316:GLY:HA3	5:E:37:TYR:HD2	1.67	0.59
2:B:363:ASP:HB2	2:B:388:TYR:CE2	2.37	0.59
2:B:111:LEU:HD13	2:B:124:ILE:HG21	1.84	0.59
1:A:368:GLU:OE1	1:A:388:ARG:NH1	2.35	0.58
3:C:38:ASP:OD1	3:C:39:GLU:N	2.35	0.58
2:B:285:SER:HB2	2:B:300:ASP:HA	1.85	0.57
2:B:253:VAL:HG22	2:B:258:VAL:HG22	1.86	0.57
1:A:585:TYR:O	1:A:587:PRO:HD3	2.05	0.57
2:B:220:LEU:HD12	2:B:223:GLN:HE22	1.70	0.57
1:A:472:SER:HB2	1:A:488:ARG:CZ	2.35	0.56
2:B:284:GLY:O	2:B:301:GLN:HG3	2.06	0.56
1:A:520:ASN:OD1	1:A:521:GLU:N	2.38	0.56
4:D:75:LEU:HD22	4:D:79:TYR:CE2	2.41	0.56
1:A:243:THR:HB	1:A:258:VAL:HG12	1.88	0.56
1:A:567:THR:HG21	1:A:606:ASN:OD1	2.06	0.56
1:A:77:VAL:HG22	1:A:86:VAL:HG13	1.88	0.56
1:A:722:THR:HG21	1:A:733:VAL:HG13	1.88	0.55
1:A:182:ILE:HG12	1:A:258:VAL:HG22	1.88	0.55
1:A:244:GLN:HE22	2:B:168:ASN:HB3	1.71	0.55
2:B:116:THR:HG21	2:B:155:PRO:O	2.07	0.55
4:D:209:GLN:O	4:D:212:ARG:NH1	2.39	0.55
1:A:669:GLY:HA3	1:A:744:VAL:HB	1.88	0.55
2:B:67:LEU:HD21	2:B:375:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ALA:O	1:A:668:ILE:HB	2.07	0.54
1:A:538:ASN:O	1:A:538:ASN:ND2	2.32	0.54
1:A:477:TYR:CD1	1:A:482:GLY:HA2	2.42	0.54
1:A:37:VAL:HG22	1:A:71:ASN:HD22	1.73	0.53
1:A:722:THR:HG21	1:A:733:VAL:O	2.08	0.53
1:A:105:VAL:HG13	1:A:109:MET:HE3	1.91	0.53
1:A:244:GLN:NE2	2:B:168:ASN:HB3	2.24	0.53
2:B:82:LYS:HZ1	2:B:94:SER:HA	1.72	0.53
2:B:298:LEU:C	2:B:298:LEU:HD23	2.34	0.53
5:E:70:THR:HG22	5:E:72:THR:OG1	2.09	0.53
5:E:50:MET:HE2	5:E:54:GLN:HB3	1.91	0.52
1:A:711:MET:HG2	1:A:712:ALA:N	2.23	0.52
1:A:192:GLU:O	1:A:195:SER:HB3	2.10	0.52
2:B:344:GLY:HA3	2:B:363:ASP:O	2.11	0.51
2:B:281:ARG:HD2	2:B:313:GLY:O	2.11	0.51
5:E:70:THR:O	5:E:72:THR:N	2.43	0.51
1:A:348:TYR:HB3	5:E:63:LEU:HD21	1.92	0.51
1:A:177:ILE:HD11	1:A:180:ILE:HG13	1.93	0.51
1:A:435:GLU:HG2	1:A:656:GLY:HA3	1.93	0.51
2:B:201:THR:HG22	2:B:251:PRO:HG2	1.93	0.51
1:A:373:GLU:HG2	4:D:193:ALA:CB	2.41	0.50
1:A:717:GLU:HG2	1:A:736:SER:HB2	1.92	0.50
3:C:76:VAL:HG13	4:D:162:ASP:HA	1.93	0.50
1:A:745:TRP:CD2	1:A:763:PRO:HB3	2.47	0.50
2:B:243:ARG:O	2:B:263:TYR:N	2.23	0.50
4:D:209:GLN:O	4:D:212:ARG:HG3	2.11	0.50
1:A:268:LEU:HD13	1:A:290:ILE:HG21	1.94	0.50
2:B:232:ILE:CG2	2:B:262:ALA:HB2	2.42	0.50
2:B:360:GLN:CD	2:B:362:VAL:HG22	2.37	0.50
1:A:177:ILE:HD11	1:A:180:ILE:CG1	2.42	0.49
1:A:316:GLY:HA3	5:E:37:TYR:CD2	2.45	0.49
2:B:153:SER:HB3	2:B:165:HIS:O	2.12	0.49
1:A:519:ILE:HG22	1:A:520:ASN:HB3	1.94	0.49
1:A:713:VAL:HA	1:A:742:GLY:HA2	1.95	0.49
5:E:37:TYR:CD1	5:E:77:PHE:CE1	3.00	0.49
1:A:63:ILE:HG13	1:A:77:VAL:HG23	1.94	0.49
4:D:61:ARG:HG3	4:D:62:TYR:CE2	2.47	0.49
6:P:183:LEU:O	6:P:184:SER:HB2	2.12	0.49
1:A:160:ARG:NH2	4:D:61:ARG:HD3	2.28	0.49
1:A:200:ARG:NH1	1:A:728:LYS:O	2.45	0.48
1:A:634:ARG:HB3	1:A:713:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:PRO:HB3	1:A:649:TYR:CE1	2.48	0.48
3:C:72:GLY:HA3	4:D:161:THR:HB	1.94	0.48
1:A:380:ASP:O	1:A:383:ASP:N	2.47	0.48
2:B:307:ALA:O	2:B:316:LEU:HB2	2.14	0.48
4:D:95:PHE:CE2	4:D:108:VAL:HG21	2.49	0.48
5:E:37:TYR:CE1	5:E:77:PHE:CE1	3.01	0.48
1:A:373:GLU:HG2	4:D:193:ALA:HB1	1.95	0.48
1:A:613:LEU:HD23	1:A:635:TRP:CD1	2.49	0.48
1:A:247:LEU:HD12	1:A:251:LYS:HG3	1.96	0.48
3:C:65:TYR:HA	4:D:144:PHE:CE1	2.49	0.48
4:D:177:TYR:O	4:D:181:VAL:HG23	2.13	0.48
1:A:290:ILE:CD1	1:A:304:MET:HE1	2.44	0.48
1:A:217:GLN:O	1:A:218:LYS:C	2.56	0.47
1:A:546:TRP:HH2	1:A:556:PRO:HB2	1.79	0.47
5:E:60:GLY:O	5:E:75:TYR:OH	2.31	0.47
1:A:465:TYR:CD1	1:A:466:GLN:HG3	2.49	0.47
2:B:232:ILE:HD11	2:B:268:THR:HG1	1.80	0.47
4:D:85:LEU:HB2	4:D:86:PRO:HD3	1.96	0.47
1:A:66:LEU:O	1:A:69:THR:OG1	2.26	0.47
1:A:541:PRO:HA	1:A:546:TRP:HE1	1.80	0.47
2:B:147:VAL:HB	2:B:172:GLN:OE1	2.14	0.47
2:B:331:VAL:HG12	2:B:338:VAL:HB	1.97	0.47
1:A:763:PRO:C	1:A:765:ASN:H	2.23	0.47
2:B:303:ASP:O	2:B:327:LEU:HD12	2.15	0.47
1:A:366:ARG:NE	4:D:181:VAL:HG13	2.30	0.47
2:B:251:PRO:HB3	2:B:260:ALA:HB2	1.95	0.47
4:D:202:LEU:O	4:D:206:PRO:HB3	2.15	0.47
5:E:61:THR:HG22	5:E:62:PRO:HD2	1.97	0.47
5:E:88:GLN:H	5:E:110:LEU:HD11	1.80	0.46
5:E:98:SER:OG	5:E:99:GLY:N	2.46	0.46
2:B:93:TRP:CE3	2:B:139:GLY:HA3	2.50	0.46
2:B:72:VAL:HG22	2:B:379:LEU:HD11	1.97	0.46
2:B:346:LEU:HD21	2:B:380:ILE:HD13	1.97	0.46
1:A:205:TRP:HA	1:A:208:VAL:CB	2.45	0.46
2:B:223:GLN:NE2	2:B:225:GLN:HB3	2.08	0.46
1:A:508:SER:HA	1:A:533:HIS:O	2.16	0.46
1:A:181:ASN:ND2	2:B:127:GLU:O	2.47	0.46
1:A:662:GLY:CA	1:A:788:ALA:HB3	2.46	0.46
1:A:714:ALA:O	1:A:741:MET:HG2	2.15	0.46
2:B:48:TRP:CE3	2:B:89:GLY:HA3	2.51	0.46
2:B:214:GLY:O	2:B:232:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ASN:HA	1:A:794:TYR:HE2	1.81	0.45
2:B:65:PRO:HB3	2:B:74:ALA:HB2	1.99	0.45
5:E:46:ILE:HG22	5:E:55:VAL:HG22	1.98	0.45
1:A:276:ASN:N	1:A:276:ASN:OD1	2.47	0.45
1:A:633:THR:HA	1:A:714:ALA:HA	1.98	0.45
2:B:91:GLU:OE2	2:B:94:SER:HB2	2.17	0.45
4:D:230:GLN:O	4:D:233:LYS:HB2	2.16	0.45
1:A:733:VAL:HG23	1:A:776:TRP:HE3	1.82	0.45
1:A:129:THR:O	1:A:133:ILE:HG13	2.17	0.45
1:A:538:ASN:ND2	1:A:561:GLN:HE21	2.15	0.45
2:B:46:THR:O	2:B:47:ALA:C	2.60	0.45
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.86	0.45
2:B:351:VAL:HG23	2:B:352:GLU:HG2	1.99	0.45
1:A:552:MET:HE1	1:A:605:ASP:O	2.17	0.44
1:A:678:GLN:HG2	1:A:693:GLN:HE22	1.82	0.44
3:C:65:TYR:HA	4:D:144:PHE:CZ	2.53	0.44
1:A:324:SER:HB3	1:A:337:LEU:HD11	1.98	0.44
4:D:135:ARG:O	4:D:136:ASP:C	2.59	0.44
5:E:63:LEU:HD13	5:E:63:LEU:HA	1.81	0.44
1:A:684:PRO:HB2	1:A:685:ASP:H	1.70	0.44
2:B:148:ALA:N	2:B:172:GLN:OE1	2.48	0.44
3:C:39:GLU:HB3	3:C:42:LEU:HD12	1.99	0.44
1:A:367:ARG:HA	4:D:184:TYR:OH	2.17	0.44
2:B:65:PRO:HD3	2:B:381:GLN:HB2	2.00	0.44
1:A:554:GLU:C	1:A:556:PRO:HD3	2.42	0.44
2:B:271:ASP:O	2:B:275:GLY:N	2.46	0.44
2:B:338:VAL:HG11	2:B:378:LEU:HD21	2.00	0.44
2:B:281:ARG:NH2	2:B:315:THR:OG1	2.51	0.44
1:A:354:PHE:CE1	1:A:369:MET:HE3	2.53	0.44
2:B:286:VAL:HG12	2:B:286:VAL:O	2.18	0.43
1:A:129:THR:HA	1:A:132:ASP:HB2	2.00	0.43
1:A:258:VAL:HG23	1:A:258:VAL:O	2.18	0.43
4:D:201:MET:HE2	4:D:211:THR:HA	1.99	0.43
4:D:202:LEU:HD21	4:D:215:LEU:HD21	1.99	0.43
1:A:546:TRP:CH2	1:A:556:PRO:HB2	2.54	0.43
2:B:234:GLN:H	2:B:265:GLY:HA2	1.83	0.43
2:B:232:ILE:HD11	2:B:268:THR:OG1	2.18	0.43
2:B:193:SER:HB2	2:B:245:SER:CB	2.49	0.43
1:A:158:LEU:O	1:A:160:ARG:N	2.52	0.43
1:A:312:LEU:HD11	1:A:341:VAL:CG1	2.49	0.43
1:A:678:GLN:NE2	1:A:693:GLN:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:MET:HE3	1:A:711:MET:HB3	1.79	0.43
2:B:215:ARG:HH11	2:B:231:ARG:HB2	1.84	0.43
2:B:322:LEU:HD21	2:B:347:HIS:NE2	2.32	0.43
2:B:341:ASP:O	2:B:367:PHE:HB2	2.19	0.43
1:A:97:ILE:HA	1:A:165:LEU:O	2.19	0.42
2:B:152:LEU:HD12	2:B:197:GLU:HG2	2.00	0.42
4:D:96:ILE:HG12	4:D:105:ILE:HD11	2.00	0.42
1:A:722:THR:HB	1:A:735:THR:CG2	2.49	0.42
5:E:34:GLN:NE2	5:E:34:GLN:HA	2.34	0.42
5:E:56:ALA:O	5:E:60:GLY:N	2.52	0.42
1:A:673:VAL:HG23	1:A:760:TRP:HZ3	1.84	0.42
5:E:88:GLN:HB3	5:E:110:LEU:HD21	2.00	0.42
1:A:223:LEU:CD2	1:A:243:THR:HG21	2.49	0.42
1:A:360:SER:OG	1:A:420:GLU:OE2	2.29	0.42
1:A:647:PRO:HB3	1:A:649:TYR:CZ	2.54	0.42
1:A:209:VAL:HB	1:A:211:ASP:HB2	2.02	0.42
1:A:541:PRO:HB2	1:A:675:PHE:HB2	2.00	0.42
2:B:169:GLY:O	2:B:170:GLN:C	2.62	0.42
2:B:322:LEU:HD22	2:B:325:ARG:HD3	2.02	0.42
3:C:57:ILE:O	5:E:68:PHE:HA	2.20	0.42
1:A:281:SER:O	1:A:285:GLU:HB2	2.20	0.42
1:A:294:GLU:OE2	1:A:300:LYS:NZ	2.36	0.42
1:A:352:ILE:HD11	1:A:371:GLN:HG3	2.01	0.42
4:D:137:PRO:HD3	4:D:177:TYR:CE2	2.55	0.42
4:D:151:VAL:HG12	4:D:160:THR:HG23	2.02	0.42
4:D:201:MET:CE	4:D:211:THR:HA	2.49	0.42
1:A:244:GLN:NE2	1:A:259:ASN:OD1	2.52	0.42
1:A:280:HIS:ND1	1:A:283:GLU:OE1	2.53	0.42
1:A:477:TYR:CE1	1:A:482:GLY:HA2	2.55	0.42
2:B:86:ALA:HB1	2:B:377:LYS:HD2	2.01	0.42
4:D:89:GLN:HG3	4:D:115:THR:HG21	2.02	0.42
1:A:209:VAL:HG11	1:A:732:SER:OG	2.20	0.42
1:A:432:TYR:HD1	1:A:438:VAL:HG22	1.84	0.42
1:A:609:TYR:HD2	1:A:641:LEU:HD21	1.84	0.42
1:A:725:ILE:HD11	1:A:729:TYR:CE2	2.55	0.42
5:E:76:VAL:HG22	5:E:90:THR:HG23	2.02	0.42
1:A:541:PRO:HA	1:A:546:TRP:NE1	2.34	0.41
2:B:220:LEU:CD2	2:B:227:ILE:HD11	2.50	0.41
4:D:99:ASN:HB3	4:D:102:HIS:HB2	2.02	0.41
5:E:52:GLN:HG2	5:E:95:PHE:CE2	2.55	0.41
2:B:371:PRO:O	2:B:372:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:VAL:HG11	1:A:668:ILE:HD12	2.01	0.41
2:B:332:LEU:HD23	2:B:332:LEU:HA	1.84	0.41
1:A:24:PHE:HE1	1:A:81:GLY:O	2.02	0.41
1:A:431:GLY:HA3	1:A:808:LYS:HA	2.03	0.41
1:A:710:ALA:HB1	1:A:745:TRP:CZ2	2.56	0.41
1:A:219:LEU:O	1:A:219:LEU:HD12	2.20	0.41
1:A:765:ASN:HA	1:A:794:TYR:CE2	2.55	0.41
2:B:328:THR:HG23	2:B:340:GLY:O	2.21	0.41
4:D:193:ALA:O	4:D:197:ARG:HB2	2.21	0.41
5:E:101:LEU:HD11	5:E:104:ILE:HG22	2.03	0.41
1:A:496:ALA:HB3	1:A:504:TYR:H	1.86	0.41
4:D:39:ALA:HB2	4:D:54:GLN:HB3	2.02	0.41
1:A:745:TRP:CE3	1:A:763:PRO:HB3	2.56	0.41
3:C:67:ILE:HG12	4:D:167:LEU:HB3	2.01	0.41
4:D:198:VAL:HG11	4:D:218:MET:HB2	2.03	0.41
1:A:630:LEU:HB3	1:A:717:GLU:HB3	2.03	0.41
1:A:784:VAL:O	1:A:804:PHE:HA	2.20	0.41
2:B:300:ASP:OD1	2:B:304:ARG:HG2	2.20	0.41
2:B:339:VAL:HG22	2:B:347:HIS:HB2	2.02	0.41
6:P:182:MET:HB3	6:P:183:LEU:H	1.67	0.41
1:A:543:VAL:HG21	1:A:754:TYR:CE2	2.56	0.41
2:B:98:ALA:HB1	2:B:107:GLU:O	2.20	0.41
3:C:84:PRO:HA	3:C:85:PRO:HD3	1.96	0.41
4:D:207:ASP:OD1	4:D:207:ASP:N	2.53	0.41
4:D:212:ARG:NH2	4:D:213:ASP:CA	2.84	0.41
1:A:717:GLU:HA	1:A:738:PHE:HA	2.02	0.40
4:D:41:GLN:C	4:D:43:LEU:H	2.29	0.40
4:D:237:ILE:O	4:D:241:ASN:ND2	2.53	0.40
1:A:350:ARG:NH1	1:A:413:ASP:OD2	2.55	0.40
2:B:250:THR:HB	2:B:288:ASP:HB3	2.04	0.40
1:A:182:ILE:HG12	1:A:258:VAL:CG2	2.50	0.40
1:A:223:LEU:HD22	1:A:243:THR:HG21	2.03	0.40
5:E:75:TYR:HB2	5:E:91:LEU: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	782/810 (96%)	680 (87%)	86 (11%)	16 (2%)	6	27
2	B	350/400 (88%)	300 (86%)	35 (10%)	15 (4%)	2	13
3	C	54/344 (16%)	45 (83%)	7 (13%)	2 (4%)	2	16
4	D	204/245 (83%)	189 (93%)	15 (7%)	0	100	100
5	E	86/119 (72%)	66 (77%)	13 (15%)	7 (8%)	1	5
6	P	7/9 (78%)	2 (29%)	4 (57%)	1 (14%)	0	1
All	All	1483/1927 (77%)	1282 (86%)	160 (11%)	41 (3%)	4	21

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	TYR
1	A	697	LYS
2	B	137	SER
2	B	244	LEU
2	B	263	TYR
2	B	265	GLY
2	B	311	ASP
2	B	371	PRO
3	C	71	ASN
5	E	71	ASN
1	A	684	PRO
2	B	63	LEU
2	B	114	GLY
2	B	186	ASN
2	B	194	LEU
2	B	196	GLY
3	C	87	GLN
5	E	81	PRO
1	A	24	PHE
1	A	149	ALA

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	436	SER
5	E	31	ASP
1	A	150	SER
1	A	213	LYS
1	A	218	LYS
1	A	585	TYR
1	A	683	ASP
1	A	808	LYS
2	B	170	GLN
5	E	45	LYS
1	A	342	ASP
1	A	435	GLU
2	B	239	THR
2	B	293	GLY
5	E	99	GLY
1	A	159	PRO
5	E	27	VAL
6	P	187	VAL
5	E	30	PRO
2	B	53	GLY

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	638/688 (93%)	558 (88%)	80 (12%)	4	19
2	B	278/329 (84%)	246 (88%)	32 (12%)	5	22
3	C	36/276 (13%)	31 (86%)	5 (14%)	3	16
4	D	166/204 (81%)	157 (95%)	9 (5%)	20	48
5	E	71/101 (70%)	59 (83%)	12 (17%)	2	10
6	P	7/7 (100%)	2 (29%)	5 (71%)	0	0
All	All	1196/1605 (74%)	1053 (88%)	143 (12%)	5	21

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	28	ASP
1	A	44	LEU
1	A	54	VAL
1	A	59	ILE
1	A	76	ARG
1	A	86	VAL
1	A	93	THR
1	A	98	THR
1	A	100	SER
1	A	126	ASP
1	A	138	GLU
1	A	146	LYS
1	A	150	SER
1	A	163	VAL
1	A	174	SER
1	A	177	ILE
1	A	203	VAL
1	A	209	VAL
1	A	219	LEU
1	A	223	LEU
1	A	243	THR
1	A	244	GLN
1	A	247	LEU
1	A	251	LYS
1	A	268	LEU
1	A	273	VAL
1	A	276	ASN
1	A	290	ILE
1	A	295	LEU
1	A	323	GLN
1	A	325	MET
1	A	335	VAL
1	A	358	ASP
1	A	359	THR
1	A	361	LYS
1	A	373	GLU
1	A	380	ASP
1	A	388	ARG
1	A	389	LEU
1	A	398	VAL
1	A	400	THR

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Mol	Chain	Res	Type
1	A	402	THR
1	A	408	SER
1	A	412	VAL
1	A	430	ILE
1	A	458	ILE
1	A	463	ASN
1	A	471	LEU
1	A	479	THR
1	A	480	VAL
1	A	513	VAL
1	A	519	ILE
1	A	520	ASN
1	A	538	ASN
1	A	558	THR
1	A	563	ASN
1	A	564	SER
1	A	571	THR
1	A	596	THR
1	A	600	THR
1	A	612	THR
1	A	614	ASP
1	A	621	ILE
1	A	626	LYS
1	A	629	VAL
1	A	633	THR
1	A	647	PRO
1	A	659	THR
1	A	660	VAL
1	A	690	CYS
1	A	692	THR
1	A	711	MET
1	A	713	VAL
1	A	722	THR
1	A	735	THR
1	A	784	VAL
1	A	786	SER
1	A	803	GLN
1	A	806	ILE
2	B	29	VAL
2	B	30	VAL
2	B	52	VAL
2	B	56	ILE

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Mol	Chain	Res	Type
2	B	82	LYS
2	B	84	LEU
2	B	96	SER
2	B	116	THR
2	B	126	SER
2	B	141	VAL
2	B	153	SER
2	B	175	ASN
2	B	181	VAL
2	B	189	MET
2	B	195	ARG
2	B	198	SER
2	B	212	ASP
2	B	213	ASN
2	B	216	VAL
2	B	220	LEU
2	B	242	ASP
2	B	244	LEU
2	B	257	VAL
2	B	258	VAL
2	B	301	GLN
2	B	320	SER
2	B	323	LEU
2	B	331	VAL
2	B	349	ILE
2	B	369	THR
2	B	372	VAL
2	B	381	GLN
3	C	35	VAL
3	C	50	LEU
3	C	61	THR
3	C	69	VAL
3	C	76	VAL
4	D	75	LEU
4	D	146	ASP
4	D	186	THR
4	D	205	TYR
4	D	212	ARG
4	D	217	LEU
4	D	232	GLU
4	D	234	VAL
4	D	242	SER

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Mol	Chain	Res	Type
5	E	39	THR
5	E	42	ASP
5	E	46	ILE
5	E	51	THR
5	E	61	THR
5	E	63	LEU
5	E	67	PRO
5	E	90	THR
5	E	92	THR
5	E	102	THR
5	E	104	ILE
5	E	107	LYS
6	P	180	ASN
6	P	182	MET
6	P	185	LEU
6	P	187	VAL
6	P	188	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	217	GLN
1	A	244	GLN
1	A	265	GLN
1	A	340	ASN
1	A	422	ASN
1	A	427	ASN
1	A	466	GLN
1	A	561	GLN
2	B	223	GLN
2	B	264	ASN
2	B	381	GLN
4	D	41	GLN
4	D	47	ASN
4	D	82	ASN
4	D	99	ASN
4	D	220	ASN
4	D	224	GLN
4	D	228	ASN
5	E	79	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 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	786/810 (97%)	0.45	67 (8%) 16 13	74, 102, 134, 170	0
2	B	356/400 (89%)	0.44	33 (9%) 14 11	75, 103, 132, 160	0
3	C	56/344 (16%)	0.78	8 (14%) 6 5	87, 111, 151, 165	0
4	D	208/245 (84%)	0.22	15 (7%) 21 16	79, 101, 136, 156	0
5	E	88/119 (73%)	0.26	4 (4%) 38 25	84, 107, 143, 184	0
6	P	9/9 (100%)	0.85	1 (11%) 10 9	133, 153, 160, 163	0
All	All	1503/1927 (77%)	0.42	128 (8%) 16 13	74, 103, 138, 184	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	ARG	7.2
1	A	73	GLU	6.3
2	B	244	LEU	5.5
1	A	809	THR	5.4
1	A	269	SER	5.1
1	A	495	GLN	5.0
3	C	55	GLY	4.9
1	A	41	ALA	4.7
1	A	70	GLY	4.6
1	A	800	GLU	4.5
1	A	808	LYS	4.5
1	A	789	GLN	4.4
1	A	795	ASP	4.4
2	B	236	THR	4.2
1	A	472	SER	3.9
3	C	54	ALA	3.9
1	A	71	ASN	3.8
1	A	686	TYR	3.8
2	B	301	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	3.7
1	A	799	ALA	3.7
1	A	401	ASP	3.7
1	A	117	SER	3.7
1	A	500	ASP	3.6
1	A	91	ARG	3.6
1	A	116	ALA	3.6
1	A	683	ASP	3.5
1	A	457	GLY	3.4
1	A	127	ARG	3.4
4	D	96	ILE	3.4
4	D	98	LEU	3.3
4	D	97	ARG	3.3
2	B	298	LEU	3.3
1	A	445	GLN	3.2
2	B	322	LEU	3.2
1	A	128	THR	3.2
1	A	166	LYS	3.1
2	B	264	ASN	3.1
2	B	295	ARG	3.1
2	B	297	TYR	3.1
2	B	196	GLY	3.1
1	A	48	VAL	3.0
3	C	35	VAL	3.0
1	A	202	GLU	3.0
1	A	74	ASP	3.0
3	C	33	ARG	3.0
1	A	90	GLU	3.0
2	B	289	PHE	3.0
4	D	242	SER	2.9
1	A	687	ASP	2.9
4	D	100	PRO	2.9
4	D	182	ALA	2.9
1	A	801	GLN	2.8
1	A	499	ALA	2.8
1	A	72	PHE	2.8
2	B	316	LEU	2.8
2	B	61	SER	2.8
1	A	498	ASP	2.8
4	D	102	HIS	2.8
2	B	263	TYR	2.7
3	C	36	SER	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	57	TYR	2.7
2	B	250	THR	2.7
2	B	82	LYS	2.6
1	A	470	GLU	2.6
1	A	729	TYR	2.6
2	B	242	ASP	2.6
3	C	56	MET	2.6
1	A	61	ASN	2.5
2	B	292	ASP	2.5
1	A	50	THR	2.5
4	D	66	PRO	2.5
3	C	50	LEU	2.5
2	B	188	ASP	2.5
4	D	121	ASP	2.5
1	A	787	TYR	2.5
4	D	132	ARG	2.5
2	B	28	ASP	2.5
2	B	43	THR	2.5
1	A	126	ASP	2.4
1	A	237	ARG	2.4
2	B	288	ASP	2.4
4	D	133	SER	2.4
2	B	239	THR	2.4
1	A	332	ASP	2.4
2	B	30	VAL	2.4
2	B	356	PHE	2.4
1	A	124	SER	2.4
1	A	270	GLY	2.3
1	A	430	ILE	2.3
4	D	185	TYR	2.3
1	A	431	GLY	2.3
4	D	101	THR	2.3
1	A	211	ASP	2.3
1	A	481	ASP	2.3
1	A	33	GLY	2.3
1	A	558	THR	2.3
1	A	471	LEU	2.3
1	A	218	LYS	2.3
2	B	355	ARG	2.3
1	A	246	SER	2.3
2	B	198	SER	2.2
4	D	99	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	725	ILE	2.2
1	A	497	ASP	2.2
2	B	346	LEU	2.2
1	A	220	ALA	2.2
5	E	105	ASP	2.2
1	A	400	THR	2.2
2	B	128	LYS	2.2
2	B	284	GLY	2.2
1	A	338	ARG	2.2
1	A	798	LYS	2.1
2	B	323	LEU	2.1
1	A	439	SER	2.1
4	D	149	LYS	2.1
1	A	118	GLY	2.1
6	P	187	VAL	2.1
2	B	97	LEU	2.1
5	E	69	GLY	2.1
1	A	47	PRO	2.1
3	C	59	PRO	2.1
1	A	726	SER	2.0
2	B	276	GLN	2.0
1	A	409	PRO	2.0
2	B	306	MET	2.0
1	A	585	TYR	2.0
5	E	86	VAL	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.