



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:48 PM UTC

PDB ID : 6LYQ / pdb_00006lyq
Title : Structure of the BAM complex
Authors : Xiao, L.; Huang, Y.
Deposited on : 2020-02-15
Resolution : 3.19 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

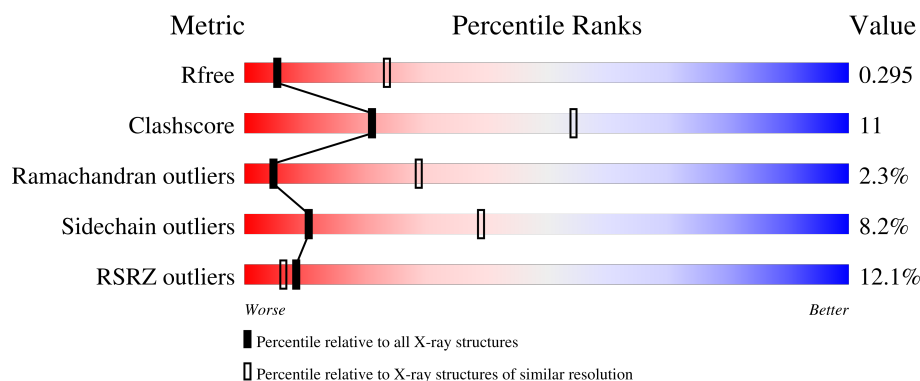
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	
2	B	400	
3	C	344	
4	D	245	
5	E	119	

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Mol	Chain	Length	Quality of chain
6	O	16	12% 56% 25% 19%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11463 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	787	Total	C	N	O	S	0	0	0
			6078	3825	1024	1213	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
			2610	1640	444	520	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 Phospholipase A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	13	Total	C	N	O	S	0	0	0
			98	63	17	17	1			

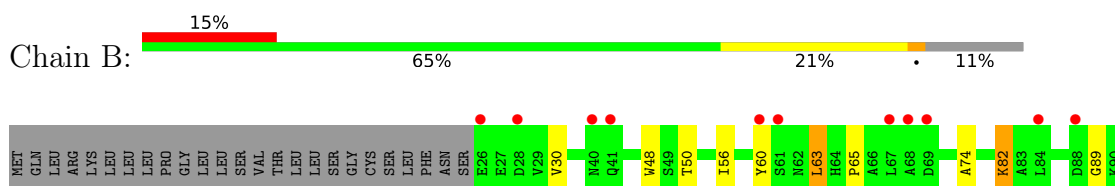
3 Residue-property plots [i](#)

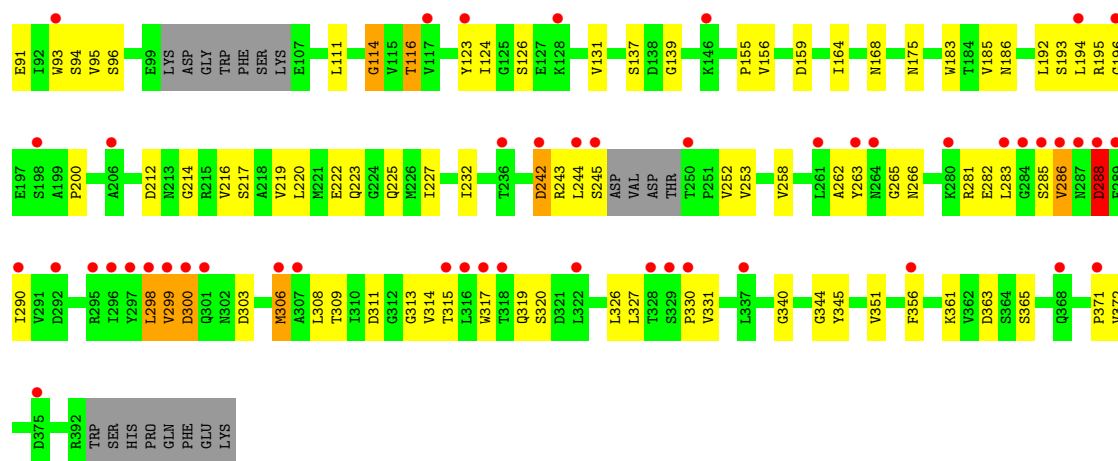
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

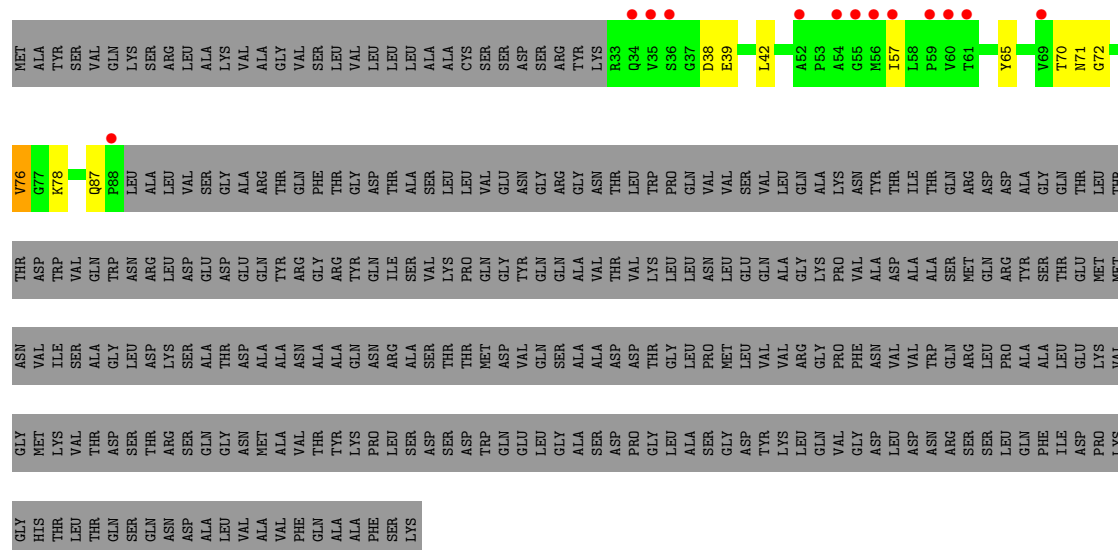


- Molecule 2: Outer membrane protein assembly factor BamB

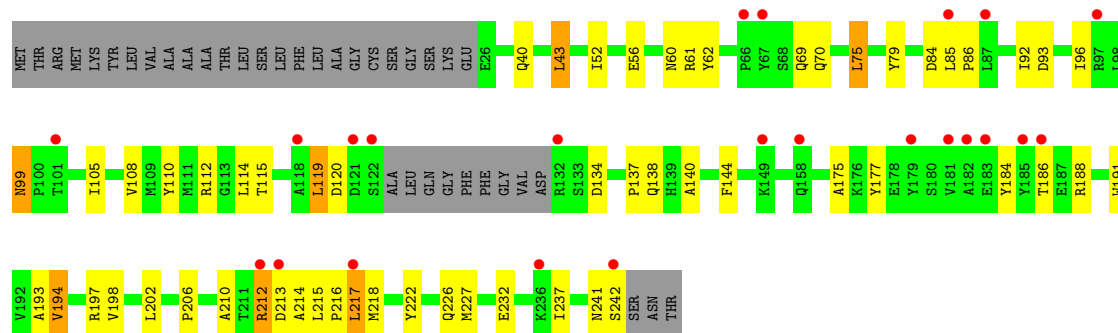




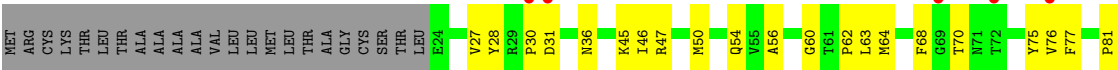
• Molecule 3: Outer membrane protein assembly factor BamC



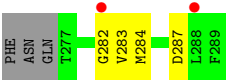
• Molecule 4: Outer membrane protein assembly factor BamD



• Molecule 5: Outer membrane protein assembly factor BamE



● Molecule 6: Peptide from Phospholipase A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.27Å 117.27Å 429.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 3.19 49.41 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.41-3.19) 98.7 (49.41-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.18Å)	Xtriage
Refinement program	PHENIX 3.1	Depositor
R, R_{free}	0.265 , 0.293 0.262 , 0.295	Depositor DCC
R_{free} test set	2548 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	113.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11463	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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	1.01	1/6216 (0.0%)	1.37	3/8453 (0.0%)
2	B	1.06	0/2654	1.35	3/3627 (0.1%)
3	C	1.06	0/387	1.37	0/533
4	D	0.98	0/1678	1.57	0/2285
5	E	1.03	0/671	1.36	0/919
6	O	1.18	0/98	1.84	2/131 (1.5%)
All	All	1.02	1/11704 (0.0%)	1.40	8/15948 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	VAL	N-CA	5.48	1.50	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASN	N-CA-C	-11.05	95.85	112.54
6	O	282	GLY	N-CA-C	-10.36	88.63	113.18
1	A	206	TRP	CB-CA-C	-9.74	91.04	110.42
6	O	283	VAL	N-CA-C	-6.72	95.37	109.34
1	A	126	ASP	CA-CB-CG	5.54	118.14	112.60
2	B	288	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	286	VAL	N-CA-C	-5.15	107.69	112.43
2	B	159	ASP	N-CA-C	-5.03	99.59	108.08

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	550	TYR	Peptide
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	6078	0	5676	128	0
2	B	2610	0	2528	61	0
3	C	378	0	362	6	0
4	D	1642	0	1559	54	0
5	E	657	0	615	14	0
6	O	98	0	102	1	0
All	All	11463	0	10842	246	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 11.

All (246) 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:208:VAL:CG1	1:A:779:PRO:HD3	1.97	0.94
1:A:208:VAL:HG13	1:A:779:PRO:HD3	1.45	0.94
4:D:217:LEU:HD12	4:D:217:LEU:H	1.30	0.93
4:D:214:ALA:O	4:D:217:LEU:CD1	2.21	0.88
4:D:214:ALA:HA	4:D:217:LEU:HD11	1.56	0.86
1:A:213:LYS:CB	1:A:215:GLN:OE1	2.24	0.86
1:A:678:GLN:HG2	1:A:693:GLN:HE22	1.39	0.85
1:A:208:VAL:HG11	1:A:779:PRO:CD	2.07	0.84
1:A:208:VAL:CG1	1:A:779:PRO:CD	2.60	0.79
1:A:722:THR:HG22	1:A:735:THR:HG23	1.63	0.79
2:B:63:LEU:HA	2:B:114:GLY:HA2	1.67	0.76
2:B:266:ASN:HD22	2:B:282:GLU:HA	1.49	0.76
1:A:329:ASN:ND2	1:A:332:ASP:OD1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:ARG:HG3	4:D:62:TYR:CZ	2.22	0.73
1:A:247:LEU:HD23	2:B:192:LEU:HD11	1.70	0.72
1:A:692:THR:HA	1:A:696:ALA:HB2	1.72	0.72
1:A:363:ALA:O	1:A:367:ARG:HB3	1.90	0.71
2:B:82:LYS:HZ1	2:B:95:VAL:H	1.39	0.71
1:A:765:ASN:HB3	1:A:794:TYR:CD2	2.26	0.70
4:D:214:ALA:O	4:D:217:LEU:HD12	1.91	0.69
1:A:192:GLU:O	1:A:195:SER:HB3	1.94	0.67
1:A:647:PRO:HB3	1:A:649:TYR:CZ	2.29	0.67
2:B:214:GLY:HA3	2:B:243:ARG:CB	2.24	0.67
1:A:735:THR:HG22	1:A:774:LEU:CD2	2.25	0.66
2:B:308:LEU:CD2	2:B:315:THR:HA	2.26	0.66
4:D:61:ARG:HG3	4:D:62:TYR:CE2	2.30	0.65
4:D:212:ARG:HG3	4:D:213:ASP:H	1.61	0.65
1:A:126:ASP:O	1:A:129:THR:OG1	2.09	0.65
4:D:212:ARG:HG3	4:D:213:ASP:N	2.12	0.65
2:B:214:GLY:CA	2:B:243:ARG:CB	2.75	0.64
4:D:75:LEU:HD22	4:D:79:TYR:CE2	2.32	0.63
1:A:54:VAL:HG23	1:A:58:ASP:HB2	1.81	0.63
1:A:205:TRP:HA	1:A:208:VAL:HG23	1.81	0.62
4:D:214:ALA:O	4:D:217:LEU:HD13	1.97	0.62
4:D:217:LEU:HD12	4:D:217:LEU:N	2.11	0.62
1:A:745:TRP:CE3	1:A:763:PRO:HB3	2.35	0.62
4:D:214:ALA:C	4:D:217:LEU:CD1	2.72	0.61
4:D:191:TRP:HA	4:D:194:VAL:CG2	2.30	0.61
4:D:214:ALA:CA	4:D:217:LEU:HD11	2.29	0.61
4:D:40:GLN:HA	4:D:43:LEU:HD22	1.83	0.59
2:B:298:LEU:CD2	2:B:306:MET:HG2	2.33	0.58
5:E:47:ARG:O	5:E:50:MET:HG3	2.03	0.58
4:D:92:ILE:HG23	4:D:108:VAL:HG12	1.85	0.58
5:E:62:PRO:HB3	5:E:75:TYR:CE1	2.38	0.58
4:D:214:ALA:HA	4:D:217:LEU:CD1	2.30	0.58
1:A:205:TRP:HA	1:A:208:VAL:CB	2.35	0.57
1:A:223:LEU:CD2	1:A:243:THR:HG21	2.35	0.57
2:B:308:LEU:HD22	2:B:315:THR:HA	1.86	0.56
1:A:102:ASN:ND2	1:A:107:ASP:OD1	2.38	0.56
2:B:50:THR:OG1	2:B:89:GLY:O	2.21	0.56
1:A:244:GLN:HE22	2:B:168:ASN:HB3	1.69	0.56
1:A:538:ASN:O	1:A:538:ASN:ND2	2.38	0.56
1:A:722:THR:CG2	1:A:735:THR:HG23	2.35	0.56
5:E:88:GLN:HB3	5:E:110:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:LEU:HD13	2:B:124:ILE:HG21	1.87	0.56
1:A:137:LEU:O	1:A:140:PHE:HB3	2.06	0.55
1:A:367:ARG:HD2	1:A:477:TYR:CG	2.41	0.55
1:A:714:ALA:O	1:A:741:MET:HG2	2.07	0.55
1:A:177:ILE:HD11	1:A:180:ILE:CG1	2.36	0.55
1:A:208:VAL:HG11	1:A:779:PRO:HD2	1.89	0.55
1:A:401:ASP:OD2	1:A:403:GLN:NE2	2.36	0.55
1:A:177:ILE:HG22	1:A:214:TYR:O	2.06	0.54
1:A:352:ILE:HG13	1:A:373:GLU:HB2	1.89	0.54
4:D:92:ILE:HG21	4:D:112:ARG:HB2	1.90	0.54
1:A:479:THR:HB	1:A:483:VAL:HB	1.90	0.54
4:D:93:ASP:OD1	4:D:112:ARG:NH1	2.40	0.54
4:D:191:TRP:O	4:D:194:VAL:HG23	2.08	0.54
1:A:182:ILE:HG12	1:A:258:VAL:HG22	1.89	0.53
1:A:177:ILE:HD11	1:A:180:ILE:HG13	1.90	0.53
2:B:156:VAL:HG21	2:B:200:PRO:O	2.08	0.52
2:B:266:ASN:ND2	2:B:282:GLU:HA	2.23	0.52
3:C:39:GLU:OE2	3:C:78:LYS:N	2.41	0.52
1:A:247:LEU:CD2	2:B:192:LEU:HD11	2.38	0.52
1:A:719:ILE:HD13	1:A:734:ARG:CZ	2.39	0.52
2:B:131:VAL:HG21	2:B:164:ILE:HG12	1.91	0.52
1:A:472:SER:HB2	1:A:488:ARG:CZ	2.40	0.52
1:A:722:THR:HG22	1:A:735:THR:H	1.75	0.52
2:B:303:ASP:O	2:B:327:LEU:HD12	2.10	0.52
1:A:425:SER:HB2	6:O:284:MET:HA	1.92	0.52
1:A:745:TRP:CD2	1:A:763:PRO:HB3	2.45	0.52
4:D:52:ILE:O	4:D:56:GLU:N	2.40	0.52
4:D:75:LEU:HD22	4:D:79:TYR:CZ	2.45	0.52
4:D:226:GLN:HG3	5:E:110:LEU:HD23	1.92	0.51
5:E:50:MET:HE2	5:E:54:GLN:HB3	1.90	0.51
1:A:647:PRO:HB3	1:A:649:TYR:CE1	2.45	0.51
1:A:205:TRP:C	1:A:207:ASN:H	2.19	0.51
1:A:324:SER:HB3	1:A:337:LEU:HD11	1.93	0.51
1:A:585:TYR:O	1:A:587:PRO:HD3	2.12	0.50
1:A:676:PRO:CB	1:A:696:ALA:HB1	2.41	0.50
1:A:678:GLN:CG	1:A:693:GLN:HE22	2.18	0.50
1:A:435:GLU:CD	1:A:657:SER:H	2.19	0.50
3:C:70:THR:O	3:C:72:GLY:N	2.45	0.50
1:A:244:GLN:NE2	2:B:168:ASN:HB3	2.27	0.50
1:A:158:LEU:HD11	1:A:164:ASP:CG	2.37	0.49
1:A:205:TRP:HA	1:A:208:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ASP:OD1	4:D:188:ARG:NH2	2.38	0.49
1:A:348:TYR:CE1	5:E:36:ASN:HA	2.47	0.49
1:A:508:SER:HA	1:A:533:HIS:O	2.11	0.49
1:A:678:GLN:HG2	1:A:693:GLN:NE2	2.19	0.49
2:B:212:ASP:OD1	2:B:245:SER:HA	2.12	0.49
1:A:244:GLN:NE2	1:A:259:ASN:OD1	2.44	0.49
1:A:558:THR:HG23	1:A:675:PHE:CD2	2.47	0.49
1:A:663:PHE:CZ	1:A:767:ARG:HB3	2.46	0.49
2:B:116:THR:HG21	2:B:155:PRO:O	2.13	0.49
4:D:193:ALA:O	4:D:197:ARG:HB2	2.13	0.49
2:B:183:TRP:CE3	2:B:185:VAL:HG23	2.48	0.49
1:A:432:TYR:O	1:A:806:ILE:HG12	2.12	0.48
2:B:214:GLY:O	2:B:232:ILE:HG22	2.13	0.48
2:B:281:ARG:NH2	2:B:315:THR:OG1	2.46	0.48
4:D:198:VAL:HG11	4:D:218:MET:HB2	1.95	0.48
4:D:85:LEU:HB2	4:D:86:PRO:HD3	1.95	0.48
4:D:175:ALA:HB1	4:D:210:ALA:HB3	1.94	0.48
1:A:676:PRO:HB2	1:A:696:ALA:HB1	1.96	0.48
2:B:82:LYS:HE3	2:B:94:SER:HA	1.95	0.48
1:A:634:ARG:HB3	1:A:713:VAL:HG22	1.95	0.48
1:A:147:TYR:C	1:A:149:ALA:H	2.22	0.48
1:A:554:GLU:C	1:A:556:PRO:HD3	2.38	0.48
2:B:327:LEU:HA	2:B:340:GLY:O	2.14	0.48
4:D:110:TYR:CE2	4:D:114:LEU:HD11	2.48	0.48
5:E:88:GLN:HB3	5:E:110:LEU:HD11	1.96	0.48
1:A:311:LEU:O	1:A:314:ARG:HB3	2.14	0.47
1:A:582:ASP:OD1	1:A:589:ASP:N	2.44	0.47
1:A:726:SER:HB3	1:A:729:TYR:CE1	2.49	0.47
2:B:243:ARG:O	2:B:263:TYR:N	2.45	0.47
4:D:115:THR:O	4:D:119:LEU:HD12	2.14	0.47
1:A:233:ARG:NH2	1:A:624:ASP:OD1	2.35	0.47
2:B:299:VAL:HG23	2:B:330:PRO:HD3	1.97	0.47
2:B:288:ASP:OD1	2:B:288:ASP:N	2.46	0.47
1:A:585:TYR:CE2	1:A:586:PHE:CE1	3.02	0.47
1:A:587:PRO:HB2	1:A:618:TYR:CE2	2.48	0.47
2:B:232:ILE:HG23	2:B:262:ALA:HB2	1.97	0.47
2:B:220:LEU:HD12	2:B:223:GLN:NE2	2.30	0.47
3:C:42:LEU:HD21	3:C:76:VAL:CG1	2.45	0.47
5:E:60:GLY:O	5:E:75:TYR:OH	2.33	0.47
1:A:361:LYS:HG2	4:D:134:ASP:OD2	2.16	0.46
2:B:223:GLN:HE21	2:B:225:GLN:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:TYR:CE2	1:A:493:ASP:OD1	2.68	0.46
4:D:96:ILE:HG12	4:D:105:ILE:HD11	1.96	0.46
2:B:363:ASP:OD1	2:B:365:SER:HB3	2.15	0.46
5:E:56:ALA:O	5:E:60:GLY:N	2.45	0.46
2:B:48:TRP:CE3	2:B:89:GLY:HA3	2.51	0.46
1:A:210:GLY:N	1:A:777:MET:O	2.47	0.46
5:E:64:MET:HE1	5:E:76:VAL:HG21	1.97	0.46
1:A:150:SER:OG	1:A:151:VAL:N	2.48	0.46
3:C:65:TYR:HA	4:D:144:PHE:CE2	2.50	0.45
4:D:61:ARG:HG3	4:D:62:TYR:CE1	2.51	0.45
2:B:223:GLN:HG3	2:B:225:GLN:CB	2.46	0.45
4:D:92:ILE:HG23	4:D:108:VAL:CG1	2.46	0.45
4:D:61:ARG:CG	4:D:62:TYR:CZ	2.97	0.45
2:B:253:VAL:HG22	2:B:258:VAL:HG22	1.97	0.45
1:A:207:ASN:ND2	1:A:207:ASN:O	2.49	0.45
1:A:735:THR:HG22	1:A:774:LEU:HD23	1.98	0.45
1:A:663:PHE:CE1	1:A:790:PRO:HB3	2.52	0.45
1:A:615:THR:HB	1:A:633:THR:OG1	2.17	0.45
1:A:352:ILE:O	1:A:366:ARG:NH1	2.44	0.45
2:B:308:LEU:HD23	2:B:315:THR:HA	1.97	0.45
1:A:205:TRP:HA	1:A:208:VAL:CA	2.47	0.44
1:A:219:LEU:O	1:A:219:LEU:HD12	2.16	0.44
2:B:156:VAL:HG11	2:B:200:PRO:O	2.17	0.44
2:B:82:LYS:CE	2:B:94:SER:HA	2.47	0.44
1:A:610:LYS:HE3	1:A:650:GLU:O	2.17	0.44
1:A:776:TRP:CZ2	1:A:783:LEU:HD23	2.53	0.44
1:A:595:LEU:HD12	1:A:613:LEU:HD13	2.00	0.44
4:D:237:ILE:O	4:D:241:ASN:ND2	2.49	0.44
4:D:191:TRP:HA	4:D:194:VAL:HG22	2.00	0.44
2:B:194:LEU:HB2	2:B:245:SER:HB3	2.00	0.44
1:A:26:VAL:HG12	1:A:52:ASP:O	2.18	0.44
2:B:309:THR:OG1	2:B:314:VAL:HG22	2.18	0.44
4:D:214:ALA:CA	4:D:217:LEU:CD1	2.94	0.44
2:B:220:LEU:HD23	2:B:220:LEU:HA	1.84	0.43
1:A:48:VAL:HG13	1:A:62:THR:OG1	2.18	0.43
1:A:367:ARG:HA	4:D:184:TYR:OH	2.19	0.43
2:B:283:LEU:HD12	2:B:283:LEU:N	2.33	0.43
5:E:36:ASN:O	5:E:77:PHE:HA	2.18	0.43
4:D:215:LEU:N	4:D:216:PRO:HD2	2.33	0.43
1:A:105:VAL:HG13	1:A:109:MET:HE3	1.99	0.43
1:A:162:ARG:CD	4:D:60:ASN:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ASN:OD1	1:A:688:TYR:OH	2.36	0.43
2:B:65:PRO:HB3	2:B:74:ALA:HB2	2.00	0.43
2:B:220:LEU:HG	2:B:227:ILE:HD11	1.99	0.43
4:D:137:PRO:HD3	4:D:177:TYR:CE2	2.54	0.43
4:D:222:TYR:CD1	4:D:227:MET:HE2	2.54	0.43
5:E:27:VAL:HG12	5:E:28:TYR:N	2.34	0.43
2:B:344:GLY:HA3	2:B:363:ASP:O	2.19	0.43
4:D:75:LEU:O	4:D:79:TYR:CD2	2.72	0.43
2:B:93:TRP:CE3	2:B:139:GLY:HA3	2.54	0.43
2:B:193:SER:HB2	2:B:245:SER:HB2	2.00	0.43
1:A:76:ARG:NH2	1:A:87:GLN:OE1	2.47	0.43
1:A:368:GLU:OE1	1:A:388:ARG:HD3	2.19	0.43
1:A:373:GLU:HG2	4:D:193:ALA:HB1	2.00	0.42
1:A:751:SER:OG	1:A:759:ASP:OD1	2.35	0.42
1:A:765:ASN:CB	1:A:794:TYR:CD2	2.98	0.42
4:D:202:LEU:O	4:D:206:PRO:HB3	2.19	0.42
1:A:162:ARG:HD2	4:D:60:ASN:O	2.18	0.42
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.91	0.42
2:B:317:TRP:NE1	2:B:351:VAL:O	2.50	0.42
1:A:218:LYS:O	1:A:218:LYS:CG	2.68	0.42
4:D:120:ASP:OD1	4:D:140:ALA:HB2	2.19	0.42
2:B:242:ASP:OD1	2:B:242:ASP:N	2.53	0.42
5:E:64:MET:HE1	5:E:76:VAL:CG2	2.49	0.42
1:A:722:THR:HG21	1:A:733:VAL:HG13	2.02	0.42
2:B:286:VAL:HG12	2:B:286:VAL:O	2.19	0.42
1:A:147:TYR:CD2	1:A:247:LEU:HD11	2.55	0.42
1:A:478:PHE:HB3	1:A:483:VAL:O	2.20	0.42
2:B:91:GLU:OE2	2:B:94:SER:HB2	2.20	0.42
2:B:319:GLN:NE2	2:B:356:PHE:CE2	2.88	0.42
1:A:219:LEU:HG	1:A:223:LEU:HD11	2.02	0.41
2:B:283:LEU:HD21	2:B:306:MET:HE2	2.02	0.41
1:A:99:PHE:O	1:A:100:SER:HB3	2.19	0.41
1:A:460:GLY:HA2	1:A:469:ALA:HA	2.03	0.41
1:A:585:TYR:C	1:A:587:PRO:HD3	2.45	0.41
1:A:679:ALA:C	1:A:681:ASN:H	2.27	0.41
2:B:345:TYR:CE1	2:B:361:LYS:HG2	2.55	0.41
4:D:99:ASN:O	4:D:105:ILE:HD13	2.20	0.41
1:A:547:ARG:HH22	1:A:746:ASP:CG	2.27	0.41
2:B:298:LEU:O	2:B:298:LEU:HD23	2.21	0.41
1:A:203:VAL:HA	1:A:204:PRO:HD3	1.87	0.41
1:A:373:GLU:HG2	4:D:193:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ARG:HD2	2:B:313:GLY:O	2.20	0.41
2:B:298:LEU:HD21	2:B:306:MET:SD	2.61	0.41
4:D:79:TYR:O	4:D:84:ASP:N	2.51	0.41
1:A:138:GLU:O	1:A:141:TYR:N	2.53	0.41
1:A:246:SER:HB3	2:B:194:LEU:O	2.21	0.41
1:A:283:GLU:O	1:A:286:GLN:NE2	2.54	0.41
1:A:559:SER:O	1:A:677:HIS:HA	2.21	0.41
1:A:541:PRO:HA	1:A:546:TRP:HE1	1.86	0.41
2:B:116:THR:HG22	2:B:123:TYR:HB2	2.03	0.41
2:B:185:VAL:HG11	2:B:219:VAL:HG11	2.02	0.41
1:A:207:ASN:O	1:A:207:ASN:CG	2.62	0.41
1:A:230:TYR:CE1	1:A:262:GLU:HG2	2.56	0.41
1:A:341:VAL:HG12	1:A:342:ASP:N	2.36	0.41
1:A:356:GLY:O	1:A:358:ASP:N	2.54	0.41
1:A:628:VAL:HB	1:A:719:ILE:HD12	2.02	0.41
3:C:57:ILE:O	5:E:68:PHE:HA	2.21	0.41
1:A:205:TRP:HA	1:A:208:VAL:HB	2.03	0.40
1:A:366:ARG:HG2	4:D:184:TYR:CD2	2.56	0.40
4:D:61:ARG:CG	4:D:62:TYR:CE2	3.03	0.40
1:A:217:GLN:O	1:A:218:LYS:C	2.64	0.40
1:A:367:ARG:HD2	1:A:477:TYR:CD1	2.57	0.40
2:B:285:SER:HB2	2:B:300:ASP:HA	2.04	0.40
3:C:38:ASP:OD1	3:C:39:GLU:N	2.54	0.40
1:A:223:LEU:HD22	1:A:243:THR:HG21	2.03	0.40
1:A:274:SER:O	1:A:340:ASN:HA	2.20	0.40
1:A:477:TYR:CD2	1:A:482:GLY:HA2	2.56	0.40
1:A:586:PHE:O	1:A:587:PRO:C	2.64	0.40
1:A:595:LEU:HD23	1:A:595:LEU:O	2.21	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	785/810 (97%)	697 (89%)	73 (9%)	15 (2%)	6	33
2	B	350/400 (88%)	305 (87%)	34 (10%)	11 (3%)	3	22
3	C	54/344 (16%)	45 (83%)	7 (13%)	2 (4%)	2	18
4	D	204/245 (83%)	183 (90%)	20 (10%)	1 (0%)	24	59
5	E	86/119 (72%)	69 (80%)	12 (14%)	5 (6%)	1	10
6	O	11/16 (69%)	7 (64%)	4 (36%)	0	100	100
All	All	1490/1934 (77%)	1306 (88%)	150 (10%)	34 (2%)	5	29

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	VAL
1	A	357	ASN
1	A	684	PRO
1	A	697	LYS
2	B	137	SER
2	B	326	LEU
3	C	71	ASN
1	A	210	GLY
2	B	60	TYR
2	B	196	GLY
2	B	265	GLY
2	B	311	ASP
5	E	45	LYS
2	B	63	LEU
2	B	186	ASN
4	D	138	GLN
5	E	81	PRO
1	A	148	SER
1	A	149	ALA
1	A	150	SER
1	A	218	LYS
5	E	83	HIS
2	B	371	PRO
3	C	87	GLN
5	E	31	ASP
1	A	24	PHE
1	A	401	ASP
1	A	542	GLN
1	A	683	ASP
5	E	30	PRO

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Mol	Chain	Res	Type
2	B	372	VAL
1	A	208	VAL
1	A	784	VAL
2	B	114	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	639/688 (93%)	584 (91%)	55 (9%)	10	36
2	B	274/329 (83%)	252 (92%)	22 (8%)	11	40
3	C	36/276 (13%)	35 (97%)	1 (3%)	38	68
4	D	166/204 (81%)	154 (93%)	12 (7%)	13	44
5	E	71/101 (70%)	64 (90%)	7 (10%)	7	31
6	O	11/14 (79%)	10 (91%)	1 (9%)	9	34
All	All	1197/1612 (74%)	1099 (92%)	98 (8%)	10	39

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	59	ILE
1	A	61	ASN
1	A	93	THR
1	A	120	ARG
1	A	126	ASP
1	A	135	LYS
1	A	138	GLU
1	A	143	SER
1	A	146	LYS
1	A	155	VAL
1	A	163	VAL
1	A	177	ILE
1	A	202	GLU

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Mol	Chain	Res	Type
1	A	203	VAL
1	A	208	VAL
1	A	209	VAL
1	A	219	LEU
1	A	243	THR
1	A	268	LEU
1	A	273	VAL
1	A	325	MET
1	A	335	VAL
1	A	366	ARG
1	A	367	ARG
1	A	372	MET
1	A	373	GLU
1	A	388	ARG
1	A	389	LEU
1	A	422	ASN
1	A	430	ILE
1	A	459	ASN
1	A	466	GLN
1	A	472	SER
1	A	479	THR
1	A	512	ASP
1	A	519	ILE
1	A	520	ASN
1	A	540	GLN
1	A	542	GLN
1	A	559	SER
1	A	571	THR
1	A	606	ASN
1	A	611	VAL
1	A	612	THR
1	A	621	ILE
1	A	660	VAL
1	A	690	CYS
1	A	706	VAL
1	A	713	VAL
1	A	743	THR
1	A	765	ASN
1	A	786	SER
1	A	803	GLN
1	A	806	ILE
2	B	30	VAL

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Mol	Chain	Res	Type
2	B	56	ILE
2	B	82	LYS
2	B	96	SER
2	B	116	THR
2	B	126	SER
2	B	175	ASN
2	B	195	ARG
2	B	216	VAL
2	B	217	SER
2	B	222	GLU
2	B	242	ASP
2	B	244	LEU
2	B	252	VAL
2	B	288	ASP
2	B	290	ILE
2	B	298	LEU
2	B	299	VAL
2	B	300	ASP
2	B	306	MET
2	B	320	SER
2	B	331	VAL
3	C	76	VAL
4	D	43	LEU
4	D	69	GLN
4	D	70	GLN
4	D	75	LEU
4	D	99	ASN
4	D	119	LEU
4	D	186	THR
4	D	194	VAL
4	D	212	ARG
4	D	217	LEU
4	D	232	GLU
4	D	242	SER
5	E	46	ILE
5	E	63	LEU
5	E	70	THR
5	E	86	VAL
5	E	90	THR
5	E	94	THR
5	E	102	THR
6	O	287	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	244	GLN
1	A	259	ASN
1	A	323	GLN
1	A	340	ASN
1	A	520	ASN
1	A	540	GLN
1	A	555	HIS
1	A	573	ASN
1	A	748	ASN
2	B	165	HIS
2	B	175	ASN
2	B	223	GLN
2	B	324	HIS
2	B	359	GLN
3	C	34	GLN
4	D	30	ASN
4	D	41	GLN
4	D	60	ASN
4	D	99	ASN
5	E	52	GLN
6	O	286	ASN

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	787/810 (97%)	0.47	79 (10%) 12 8	91, 125, 156, 201	0
2	B	356/400 (89%)	0.84	60 (16%) 4 3	96, 126, 156, 204	0
3	C	56/344 (16%)	0.81	13 (23%) 2 2	113, 136, 165, 193	0
4	D	208/245 (84%)	0.53	23 (11%) 10 7	100, 125, 168, 199	0
5	E	88/119 (73%)	0.36	6 (6%) 23 15	100, 132, 166, 194	0
6	O	13/16 (81%)	0.93	2 (15%) 5 4	142, 161, 181, 182	0
All	All	1508/1934 (77%)	0.58	183 (12%) 8 6	91, 126, 161, 204	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	285	SER	6.9
1	A	488	ARG	6.9
2	B	299	VAL	6.7
1	A	537	SER	6.6
2	B	297	TYR	6.5
2	B	244	LEU	6.5
2	B	301	GLN	6.4
2	B	316	LEU	6.4
2	B	287	ASN	6.4
2	B	298	LEU	6.2
1	A	41	ALA	6.1
2	B	68	ALA	6.1
2	B	306	MET	5.9
2	B	61	SER	5.6
2	B	263	TYR	5.5
2	B	300	ASP	5.5
2	B	286	VAL	5.4
1	A	495	GLN	5.4
2	B	368	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	5.2
5	E	30	PRO	5.2
2	B	329	SER	5.1
1	A	725	ILE	5.0
1	A	502	SER	5.0
4	D	87	LEU	4.9
2	B	330	PRO	4.8
1	A	70	GLY	4.8
4	D	118	ALA	4.7
6	O	288	LEU	4.7
2	B	289	PHE	4.7
2	B	284	GLY	4.6
4	D	97	ARG	4.5
2	B	288	ASP	4.5
1	A	73	GLU	4.4
1	A	801	GLN	4.4
1	A	74	ASP	4.4
1	A	401	ASP	4.3
2	B	198	SER	4.3
1	A	400	THR	4.3
1	A	503	ASP	4.2
2	B	69	ASP	4.2
1	A	72	PHE	4.1
4	D	179	TYR	4.1
2	B	242	ASP	4.0
1	A	414	VAL	4.0
2	B	292	ASP	4.0
1	A	619	VAL	3.9
2	B	295	ARG	3.9
1	A	383	ASP	3.9
1	A	71	ASN	3.8
1	A	42	ALA	3.7
1	A	504	TYR	3.7
2	B	307	ALA	3.7
1	A	399	ASP	3.7
5	E	69	GLY	3.7
4	D	242	SER	3.6
1	A	415	VAL	3.6
1	A	585	TYR	3.6
1	A	497	ASP	3.6
3	C	54	ALA	3.6
1	A	785	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	55	GLY	3.6
4	D	185	TYR	3.5
4	D	122	SER	3.5
1	A	34	LEU	3.4
1	A	445	GLN	3.4
2	B	375	ASP	3.3
4	D	236	LYS	3.3
1	A	91	ARG	3.3
1	A	539	MET	3.3
1	A	808	LYS	3.3
1	A	687	ASP	3.2
4	D	121	ASP	3.2
1	A	128	THR	3.2
1	A	505	THR	3.2
1	A	90	GLU	3.2
2	B	283	LEU	3.2
1	A	269	SER	3.2
1	A	726	SER	3.2
2	B	41	GLN	3.1
2	B	328	THR	3.1
3	C	36	SER	3.1
1	A	799	ALA	3.1
2	B	245	SER	3.1
3	C	57	ILE	3.1
4	D	186	THR	3.1
1	A	300	LYS	3.0
3	C	88	PRO	2.9
2	B	60	TYR	2.9
1	A	40	GLY	2.9
1	A	729	TYR	2.9
2	B	356	PHE	2.9
1	A	589	ASP	2.9
1	A	621	ILE	2.9
1	A	409	PRO	2.9
2	B	123	TYR	2.9
1	A	237	ARG	2.9
1	A	236	ALA	2.9
4	D	149	LYS	2.9
1	A	385	GLY	2.9
1	A	75	VAL	2.8
1	A	564	SER	2.8
1	A	786	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	35	VAL	2.8
4	D	212	ARG	2.7
2	B	40	ASN	2.7
4	D	181	VAL	2.7
2	B	315	THR	2.7
4	D	67	TYR	2.7
6	O	282	GLY	2.7
4	D	217	LEU	2.7
5	E	76	VAL	2.7
2	B	290	ILE	2.6
1	A	380	ASP	2.6
4	D	183	GLU	2.6
2	B	322	LEU	2.6
1	A	370	ARG	2.6
2	B	28	ASP	2.6
1	A	326	PRO	2.6
2	B	128	LYS	2.6
2	B	317	TRP	2.6
2	B	296	ILE	2.5
2	B	196	GLY	2.5
2	B	117	VAL	2.5
1	A	703	ASP	2.5
1	A	727	ASP	2.5
3	C	56	MET	2.5
4	D	182	ALA	2.5
1	A	805	ASN	2.5
2	B	250	THR	2.5
2	B	194	LEU	2.5
2	B	371	PRO	2.5
3	C	59	PRO	2.5
4	D	101	THR	2.4
2	B	26	GLU	2.4
4	D	132	ARG	2.4
2	B	236	THR	2.4
1	A	416	TYR	2.4
1	A	331	ALA	2.4
2	B	93	TRP	2.4
1	A	498	ASP	2.4
2	B	84	LEU	2.4
2	B	318	THR	2.3
3	C	61	THR	2.3
2	B	264	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	213	ASP	2.3
4	D	66	PRO	2.3
1	A	408	SER	2.3
3	C	34	GLN	2.3
2	B	67	LEU	2.3
1	A	382	VAL	2.3
3	C	69	VAL	2.3
1	A	307	ASP	2.3
1	A	43	LEU	2.2
1	A	789	GLN	2.2
2	B	146	LYS	2.2
1	A	472	SER	2.2
3	C	60	VAL	2.2
1	A	766	ILE	2.2
5	E	31	ASP	2.2
3	C	52	ALA	2.2
4	D	85	LEU	2.2
1	A	507	LYS	2.2
1	A	218	LYS	2.1
2	B	280	LYS	2.1
1	A	657	SER	2.1
1	A	211	ASP	2.1
1	A	546	TRP	2.1
1	A	704	ASP	2.1
2	B	88	ASP	2.1
1	A	386	LYS	2.1
1	A	728	LYS	2.1
1	A	290	ILE	2.1
1	A	304	MET	2.1
2	B	206	ALA	2.1
5	E	85	GLY	2.1
2	B	337	LEU	2.0
5	E	72	THR	2.0
4	D	158	GLN	2.0
1	A	556	PRO	2.0
1	A	745	TRP	2.0
1	A	402	THR	2.0
2	B	261	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.