



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 29, 2020 – 12:08 PM JST

PDB ID : 6LYR
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

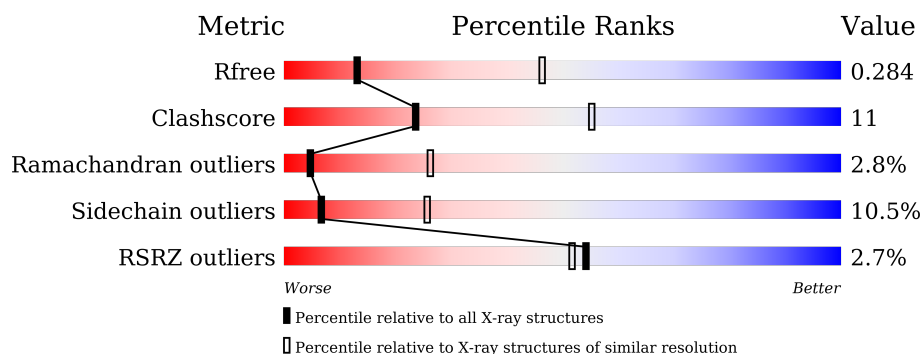
1 Overall quality at a glance

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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	 3% 70% 23% . .
2	B	400	 3% 58% 28% . 11%
3	C	344	 12% . 84%
4	D	245	 64% 20% . 15%
5	E	119	 2% 39% 26% 8% 26%
6	P	9	 33% 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

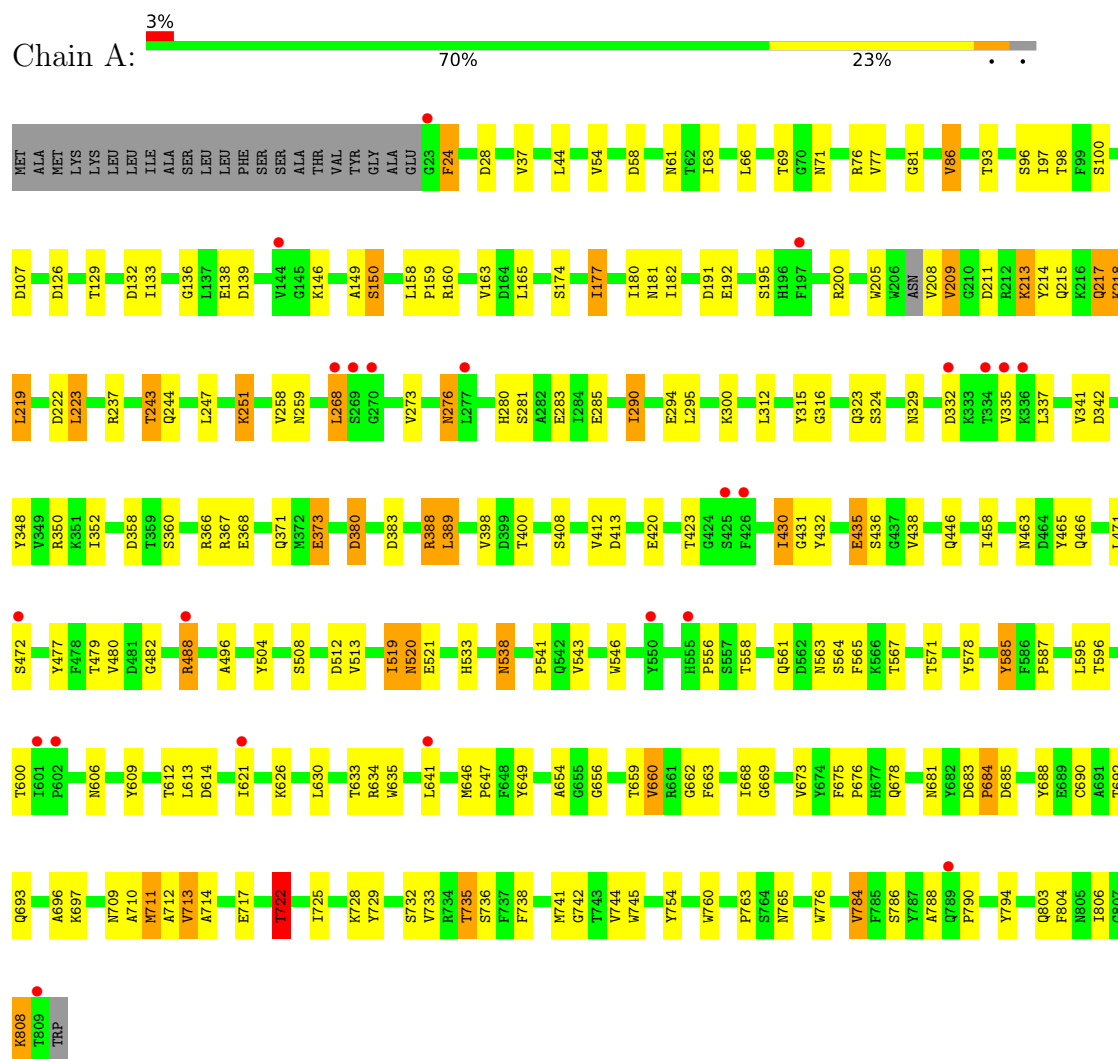
- Molecule 6 is a protein called Peptide from Outer membrane protein A.

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

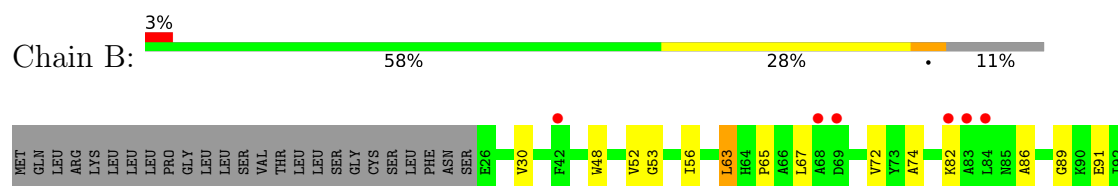
3 Residue-property plots [i](#)

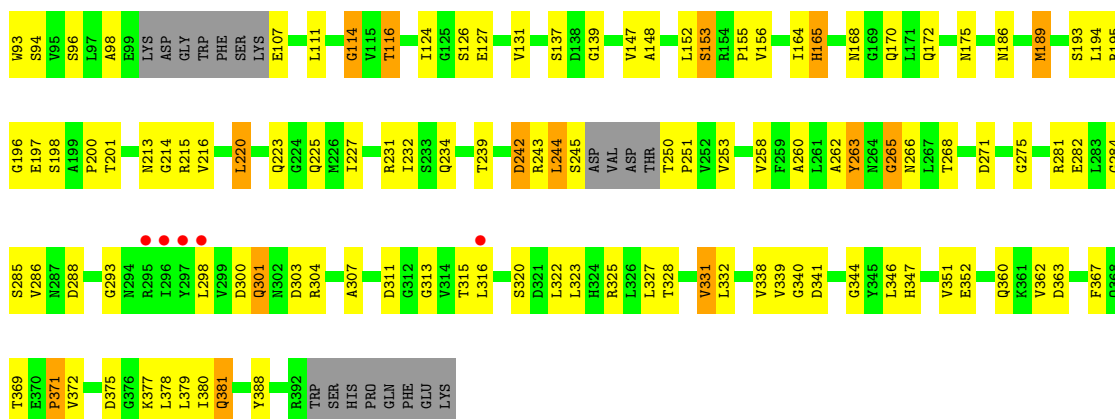
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

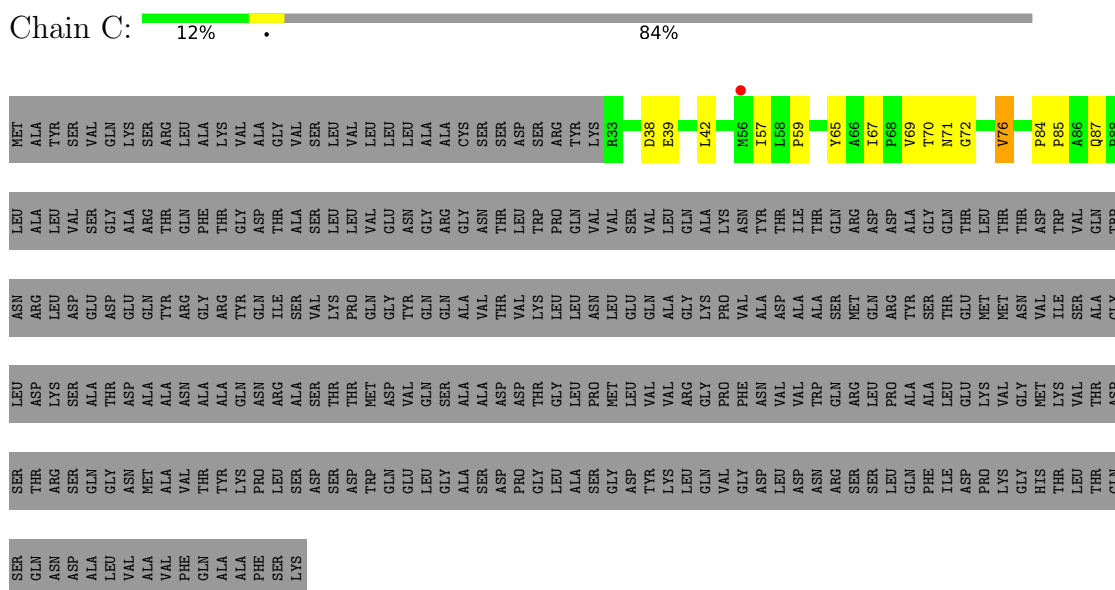


- Molecule 2: Outer membrane protein assembly factor BamB

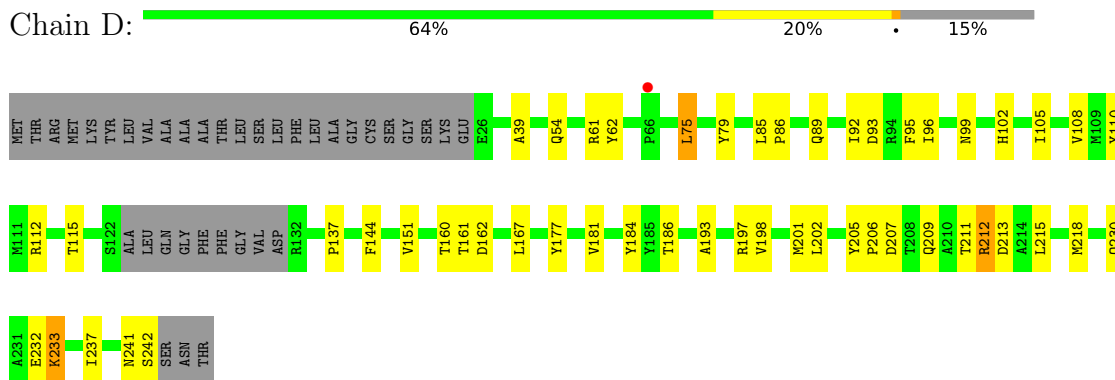




- Molecule 3: Outer membrane protein assembly factor BamC

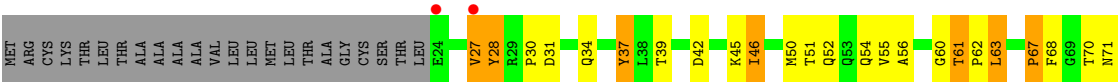


- Molecule 4: Outer membrane protein assembly factor BamD

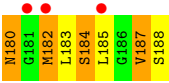
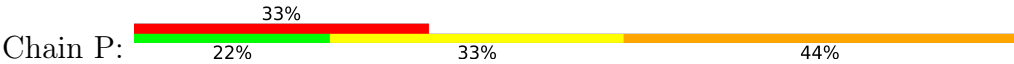


- Molecule 5: Outer membrane protein assembly factor BamE





● Molecule 6: Peptide from 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 49.32 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.37-3.28) 99.4 (49.32-3.28)	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 , 0.284	Depositor DCC
R_{free} test set	2302 reflections (4.93%)	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 , 55.8	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	0.64	0/6212	0.78	0/8446
2	B	0.66	0/2674	0.80	0/3652
3	C	0.67	0/387	0.76	0/533
4	D	0.64	0/1678	0.74	0/2285
5	E	0.65	0/671	0.81	0/919
6	P	0.70	0/58	1.57	1/76 (1.3%)
All	All	0.65	0/11680	0.79	1/15911 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	184	SER	N-CA-CB	-10.43	94.86	110.50

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	123	0
2	B	2629	0	2556	69	0
3	C	378	0	362	11	0
4	D	1642	0	1559	38	0
5	E	657	0	615	24	0
6	P	59	0	61	4	0
All	All	11439	0	10827	250	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 (250) 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:659:THR:OG1	1:A:660:VAL:N	2.21	0.73
1:A:692:THR:HA	1:A:696:ALA:HB2	1.71	0.73
6:P:180:ASN:HD22	6:P:180:ASN:N	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:54:VAL:HG23	1:A:58:ASP:HB2	1.75	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
2:B:242:ASP:N	2:B:242:ASP:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:TYR:O	2:B:284:GLY:HA3	1.98	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
1:A:205:TRP:CA	1:A:208:VAL:HG23	2.21	0.62
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
1:A:315:TYR:C	5:E:37:TYR:HE2	2.06	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
4:D:110:TYR:OH	4:D:162:ASP:OD2	2.17	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:244:GLN:HE22	2:B:168:ASN:HB3	1.71	0.55
1:A:182:ILE:HG12	1:A:258:VAL:HG22	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:GLN:NE2	2:B:168:ASN:HB3	2.24	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
4:D:201:MET:HE2	4:D:211:THR:HA	1.90	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:633:THR:HG1	1:A:635:TRP:HE1	1.59	0.51
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:373:GLU:HG2	4:D:193:ALA:CB	2.41	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:C	2:B:298:LEU:HD23	2.34	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:613:LEU:HD23	1:A:635:TRP:CD1	2.49	0.48
1:A:373:GLU:HG2	4:D:193:ALA:HB1	1.95	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:546:TRP:HH2	1:A:556:PRO:HB2	1.79	0.47
1:A:465:TYR:CD1	1:A:466:GLN:HG3	2.49	0.47
4:D:85:LEU:HB2	4:D:86:PRO:HD3	1.96	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:541:PRO:HA	1:A:546:TRP:HE1	1.80	0.47
1:A:66:LEU:O	1:A:69:THR:OG1	2.26	0.47
2:B:303:ASP:O	2:B:327:LEU:HD12	2.15	0.47
2:B:251:PRO:HB3	2:B:260:ALA:HB2	1.95	0.47
1:A:366:ARG:NE	4:D:181:VAL:HG13	2.30	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:232:ILE:HD11	2:B:268:THR:HG1	1.81	0.46
2:B:346:LEU:HD21	2:B:380:ILE:HD13	1.97	0.46
2:B:72:VAL:HG22	2:B:379:LEU:HD11	1.97	0.46
1:A:646:MET:HE2	1:A:709:ASN:HB3	1.98	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: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
1:A:181:ASN:ND2	2:B:127:GLU:O	2.47	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
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:OD1	1:A:276:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:230:GLN:O	4:D:233:LYS:HB2	2.16	0.45
2:B:360:GLN:CD	2:B:362:VAL:HG22	2.37	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
1:A:389:LEU:HA	1:A:389:LEU:HD23	1.86	0.45
2:B:351:VAL:HG23	2:B:352:GLU:HG2	1.99	0.45
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
5:E:63:LEU:HA	5:E:63:LEU:HD13	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
2:B:65:PRO:HD3	2:B:381:GLN:HB2	2.00	0.44
1:A:367:ARG:HA	4:D:184:TYR:OH	2.17	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:217:GLN:O	1:A:218:LYS:C	2.56	0.43
2:B:286:VAL:O	2:B:286:VAL:HG12	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: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
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
5:E:34:GLN:NE2	5:E:34:GLN:HA	2.34	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:711:MET:HE3	1:A:711:MET:HB3	1.76	0.42
1:A:722:THR:HB	1:A:735:THR:CG2	2.49	0.42
5:E:56:ALA:O	5:E:60:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:352:ILE:HD11	1:A:371:GLN:HG3	2.01	0.42
4:D:151:VAL:HG12	4:D:160:THR:HG23	2.02	0.42
4:D:137:PRO:HD3	4:D:177:TYR:CE2	2.55	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: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
1:A:209:VAL:HG11	1:A:732:SER:OG	2.20	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
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:710:ALA:HB1	1:A:745:TRP:CZ2	2.56	0.41
1:A:431:GLY:HA3	1:A:808:LYS:HA	2.03	0.41
1:A:219:LEU:HD12	1:A:219:LEU:O	2.20	0.41
1:A:763:PRO:C	1:A:765:ASN:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:784:VAL:O	1:A:804:PHE:HA	2.20	0.41
2:B:339:VAL:HG22	2:B:347:HIS:HB2	2.02	0.41
1:A:430:ILE:HG13	1:A:430:ILE:O	2.21	0.41
1:A:630:LEU:HB3	1:A:717:GLU:HB3	2.03	0.41
2:B:168:ASN:HA	2:B:189:MET:CE	2.51	0.41
2:B:300:ASP:OD1	2:B:304:ARG:HG2	2.20	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:N	4:D:207:ASP:OD1	2.53	0.41
4:D:212:ARG:NH2	4:D:213:ASP:CA	2.84	0.41
1:A:294:GLU:OE2	1:A:300:LYS:NZ	2.36	0.40
1:A:717:GLU:HA	1:A:738:PHE:HA	2.02	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%)	7 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	350/400 (88%)	300 (86%)	35 (10%)	15 (4%)	2	17
3	C	54/344 (16%)	45 (83%)	7 (13%)	2 (4%)	3	20
4	D	204/245 (83%)	189 (93%)	15 (7%)	0	100	100
5	E	86/119 (72%)	66 (77%)	13 (15%)	7 (8%)	1	6
6	P	7/9 (78%)	2 (29%)	4 (57%)	1 (14%)	0	1
All	All	1483/1927 (77%)	1282 (86%)	160 (11%)	41 (3%)	5	26

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
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

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Mol	Chain	Res	Type
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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	638/688 (93%)	563 (88%)	75 (12%)	5	21
2	B	278/329 (84%)	255 (92%)	23 (8%)	11	35
3	C	36/276 (13%)	34 (94%)	2 (6%)	21	51
4	D	166/204 (81%)	159 (96%)	7 (4%)	30	60
5	E	71/101 (70%)	57 (80%)	14 (20%)	1	5
6	P	7/7 (100%)	2 (29%)	5 (71%)	0	0
All	All	1196/1605 (74%)	1070 (90%)	126 (10%)	7	26

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	44	LEU
1	A	61	ASN
1	A	76	ARG
1	A	86	VAL
1	A	93	THR
1	A	96	SER

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Mol	Chain	Res	Type
1	A	98	THR
1	A	100	SER
1	A	107	ASP
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	191	ASP
1	A	209	VAL
1	A	219	LEU
1	A	222	ASP
1	A	223	LEU
1	A	237	ARG
1	A	243	THR
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	335	VAL
1	A	358	ASP
1	A	373	GLU
1	A	380	ASP
1	A	388	ARG
1	A	389	LEU
1	A	398	VAL
1	A	400	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	488	ARG
1	A	512	ASP

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Mol	Chain	Res	Type
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	565	PHE
1	A	571	THR
1	A	578	TYR
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	660	VAL
1	A	690	CYS
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	30	VAL
2	B	52	VAL
2	B	56	ILE
2	B	96	SER
2	B	116	THR
2	B	126	SER
2	B	153	SER
2	B	165	HIS
2	B	175	ASN
2	B	189	MET
2	B	195	ARG
2	B	198	SER
2	B	213	ASN
2	B	216	VAL
2	B	220	LEU
2	B	242	ASP

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Mol	Chain	Res	Type
2	B	244	LEU
2	B	301	GLN
2	B	320	SER
2	B	323	LEU
2	B	331	VAL
2	B	369	THR
2	B	381	GLN
3	C	69	VAL
3	C	76	VAL
4	D	75	LEU
4	D	186	THR
4	D	205	TYR
4	D	212	ARG
4	D	232	GLU
4	D	233	LYS
4	D	242	SER
5	E	28	TYR
5	E	37	TYR
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	259	ASN
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	466	GLN
1	A	561	GLN
2	B	223	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 monosaccharides 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%)	0.09	23 (2%) 51 50	74, 102, 134, 170	0
2	B	356/400 (89%)	0.16	11 (3%) 49 48	75, 103, 132, 160	0
3	C	56/344 (16%)	0.13	1 (1%) 68 66	87, 111, 151, 165	0
4	D	208/245 (84%)	-0.14	1 (0%) 91 91	79, 101, 136, 156	0
5	E	88/119 (73%)	0.02	2 (2%) 60 58	84, 107, 143, 184	0
6	P	9/9 (100%)	1.91	3 (33%) 0 0	133, 153, 160, 163	0
All	All	1503/1927 (77%)	0.09	41 (2%) 54 52	74, 103, 138, 184	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	SER	4.9
1	A	809	THR	4.4
1	A	488	ARG	3.7
6	P	185	LEU	3.6
2	B	295	ARG	3.4
2	B	316	LEU	3.3
2	B	84	LEU	3.3
2	B	297	TYR	3.2
5	E	24	GLU	3.2
1	A	268	LEU	3.0
1	A	332	ASP	2.9
1	A	555	HIS	2.8
1	A	335	VAL	2.8
1	A	550	TYR	2.7
1	A	270	GLY	2.7
1	A	641	LEU	2.6
1	A	144	VAL	2.5
1	A	789	GLN	2.5
2	B	296	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
6	P	182	MET	2.4
1	A	23	GLY	2.3
2	B	83	ALA	2.3
1	A	621	ILE	2.3
6	P	181	GLY	2.3
1	A	602	PRO	2.2
3	C	56	MET	2.2
2	B	82	LYS	2.2
2	B	298	LEU	2.2
1	A	425	SER	2.2
2	B	42	PHE	2.2
2	B	68	ALA	2.2
5	E	27	VAL	2.2
1	A	197	PHE	2.1
1	A	426	PHE	2.1
4	D	66	PRO	2.1
1	A	277	LEU	2.1
1	A	336	LYS	2.0
1	A	334	THR	2.0
1	A	601	ILE	2.0
2	B	69	ASP	2.0
1	A	472	SER	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 monosaccharides 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.