



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:12 AM UTC

PDB ID : 6C84 / pdb_00006c84
Title : Crystal structure of PBP5 from Enterococcus faecium
Authors : Shamoo, Y.; Davlieva, M.
Deposited on : 2018-01-24
Resolution : 2.51 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

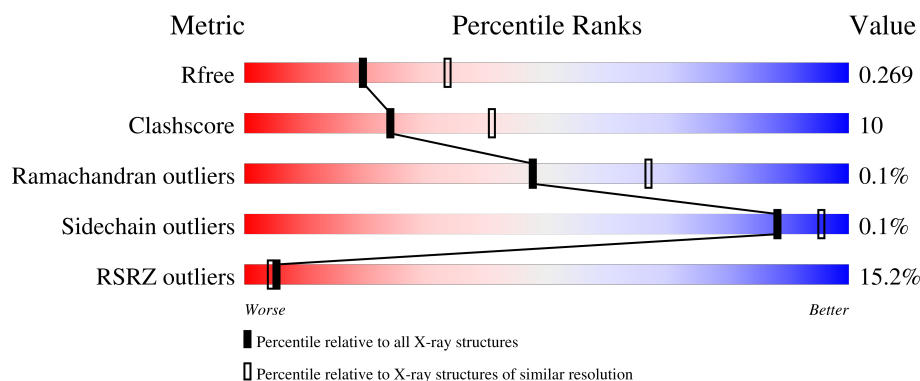
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	659	15% 78% 19% .
1	B	659	14% 77% 20% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9797 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 Penicillin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			4894	3062	808	1011	13			
1	B	641	Total	C	N	O	S	0	0	0
			4903	3067	809	1014	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	HIS	-	expression tag	UNP A0A133MY97
A	21	HIS	-	expression tag	UNP A0A133MY97
A	22	HIS	-	expression tag	UNP A0A133MY97
A	23	HIS	-	expression tag	UNP A0A133MY97
A	24	HIS	-	expression tag	UNP A0A133MY97
A	25	HIS	-	expression tag	UNP A0A133MY97
A	26	SER	-	expression tag	UNP A0A133MY97
A	27	SER	-	expression tag	UNP A0A133MY97
A	28	GLY	-	expression tag	UNP A0A133MY97
A	29	LEU	-	expression tag	UNP A0A133MY97
A	30	VAL	-	expression tag	UNP A0A133MY97
A	31	PRO	-	expression tag	UNP A0A133MY97
A	32	ARG	-	expression tag	UNP A0A133MY97
A	33	GLY	-	expression tag	UNP A0A133MY97
A	34	SER	-	expression tag	UNP A0A133MY97
A	35	HIS	-	expression tag	UNP A0A133MY97
A	36	MET	-	expression tag	UNP A0A133MY97
A	646	GLU	GLY	conflict	UNP A0A133MY97
B	20	HIS	-	expression tag	UNP A0A133MY97
B	21	HIS	-	expression tag	UNP A0A133MY97
B	22	HIS	-	expression tag	UNP A0A133MY97
B	23	HIS	-	expression tag	UNP A0A133MY97
B	24	HIS	-	expression tag	UNP A0A133MY97
B	25	HIS	-	expression tag	UNP A0A133MY97
B	26	SER	-	expression tag	UNP A0A133MY97

Continued on next page...

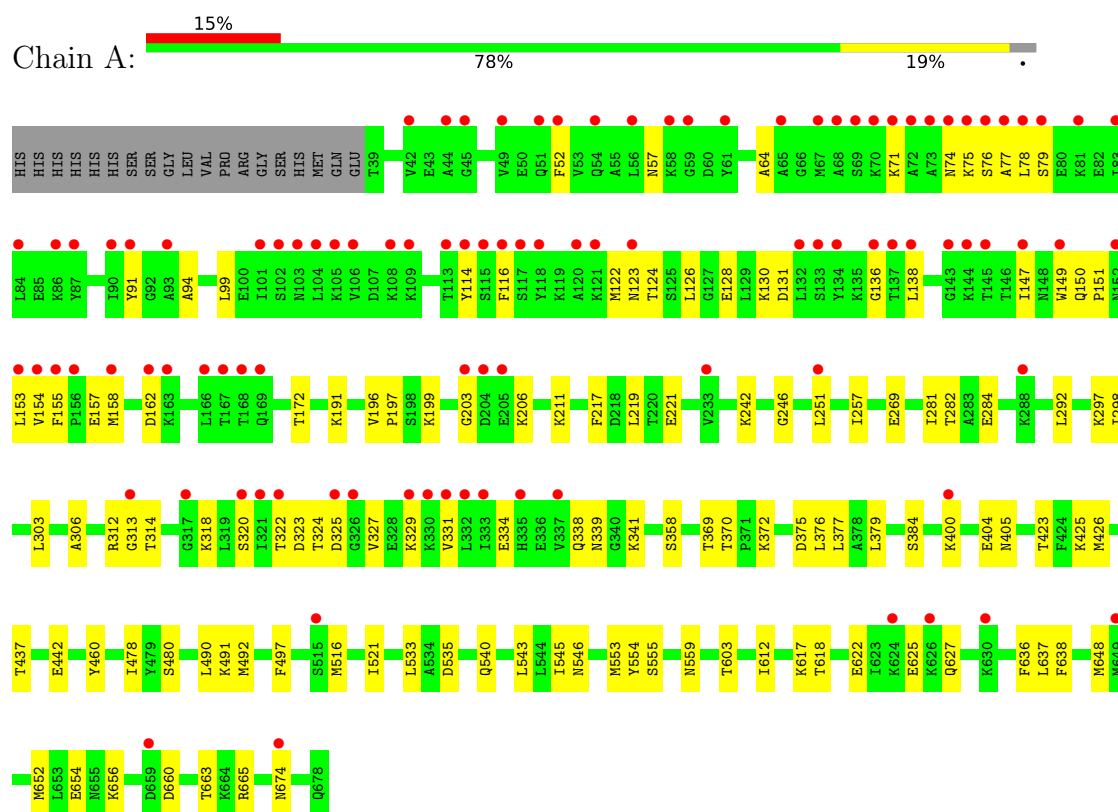
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	27	SER	-	expression tag	UNP A0A133MY97
B	28	GLY	-	expression tag	UNP A0A133MY97
B	29	LEU	-	expression tag	UNP A0A133MY97
B	30	VAL	-	expression tag	UNP A0A133MY97
B	31	PRO	-	expression tag	UNP A0A133MY97
B	32	ARG	-	expression tag	UNP A0A133MY97
B	33	GLY	-	expression tag	UNP A0A133MY97
B	34	SER	-	expression tag	UNP A0A133MY97
B	35	HIS	-	expression tag	UNP A0A133MY97
B	36	MET	-	expression tag	UNP A0A133MY97
B	646	GLU	GLY	conflict	UNP A0A133MY97

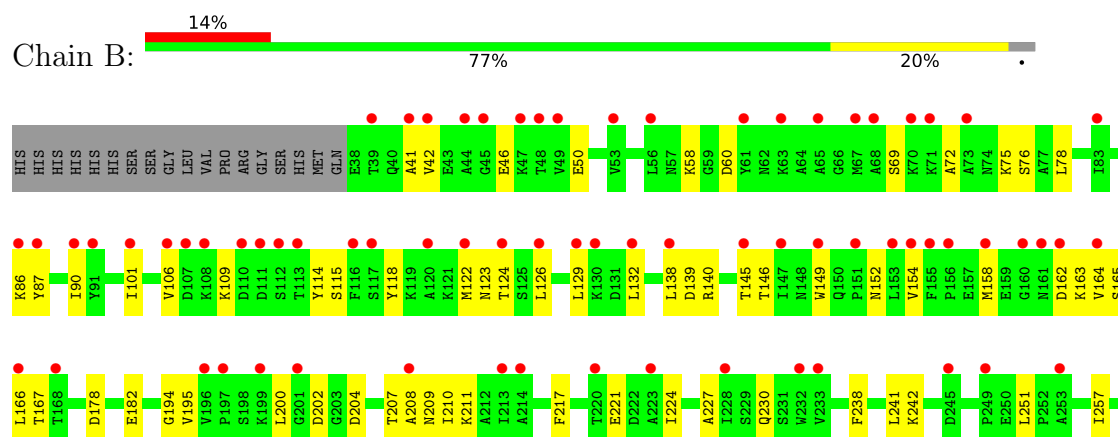
3 Residue-property plots [i](#)

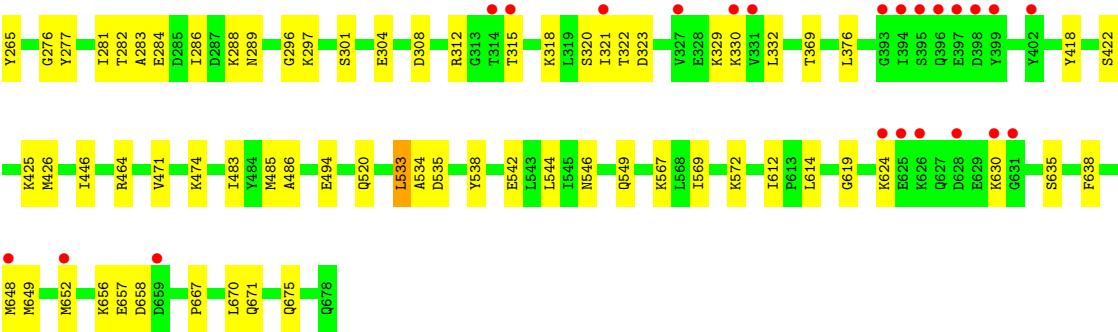
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Penicillin-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.98Å 73.07Å 131.44Å 90.00° 114.97° 90.00°	Depositor
Resolution (Å)	29.79 – 2.51 29.79 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.79-2.51) 94.6 (29.79-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.224 , 0.265 0.227 , 0.269	Depositor DCC
R_{free} test set	2003 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9797	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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	0.26	0/4969	0.49	0/6719
1	B	0.26	0/4978	0.49	0/6731
All	All	0.26	0/9947	0.49	0/13450

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4894	0	4834	96	0
1	B	4903	0	4840	98	0
All	All	9797	0	9674	194	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 10.

All (194) 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:41:ALA:HB1	1:B:140:ARG:HH11	0.97	1.10
1:A:191:LYS:NZ	1:A:246:GLY:O	1.91	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:HB1	1:B:140:ARG:NH1	1.77	1.00
1:A:191:LYS:CE	1:A:246:GLY:O	2.11	0.98
1:B:41:ALA:CB	1:B:140:ARG:HH11	1.76	0.96
1:A:191:LYS:HE2	1:A:246:GLY:O	1.74	0.84
1:A:425:LYS:NZ	1:A:480:SER:HA	1.97	0.80
1:B:162:ASP:HB2	1:B:322:THR:HG23	1.63	0.78
1:A:425:LYS:HZ1	1:A:480:SER:HA	1.51	0.76
1:A:151:PRO:HB2	1:A:158:MET:HB3	1.69	0.75
1:A:77:ALA:HB1	1:A:150:GLN:HG3	1.70	0.73
1:A:116:PHE:HB2	1:A:136:GLY:H	1.54	0.71
1:A:217:PHE:CB	1:A:219:LEU:HD13	2.22	0.70
1:B:251:LEU:HD21	1:B:257:ILE:HG12	1.74	0.70
1:B:140:ARG:NH2	1:B:145:THR:HB	2.08	0.69
1:B:124:THR:HG23	1:B:126:LEU:H	1.57	0.68
1:B:546:ASN:H	1:B:549:GLN:HE21	1.41	0.68
1:A:297:LYS:O	1:A:312:ARG:NH2	2.25	0.68
1:B:464:ARG:HD2	1:B:483:ILE:HD12	1.75	0.68
1:B:86:LYS:NZ	1:B:162:ASP:O	2.20	0.68
1:B:101:ILE:HD11	1:B:118:TYR:CD2	2.29	0.68
1:B:426:MET:HE1	1:B:638:PHE:CE2	2.28	0.68
1:B:41:ALA:CB	1:B:140:ARG:NH1	2.47	0.67
1:A:78:LEU:HD23	1:A:79:SER:H	1.59	0.67
1:B:200:LEU:O	1:B:209:ASN:ND2	2.28	0.66
1:A:217:PHE:HB3	1:A:219:LEU:HD13	1.78	0.66
1:A:149:TRP:HD1	1:A:153:LEU:HD23	1.61	0.64
1:B:675:GLN:NE2	1:B:675:GLN:O	2.31	0.64
1:A:251:LEU:HD21	1:A:257:ILE:HD11	1.79	0.64
1:A:555:SER:HA	1:A:648:MET:HE1	1.79	0.64
1:A:147:ILE:HD11	1:A:153:LEU:CD2	2.29	0.63
1:A:149:TRP:CD1	1:A:153:LEU:HB3	2.34	0.63
1:A:147:ILE:HD11	1:A:153:LEU:HD21	1.80	0.62
1:B:422:SER:HB2	1:B:619:GLY:HA2	1.81	0.62
1:B:520:GLN:NE2	1:B:542:GLU:O	2.33	0.61
1:A:124:THR:HG23	1:A:126:LEU:H	1.64	0.61
1:A:269:GLU:HG2	1:A:384:SER:HB3	1.83	0.60
1:B:194:GLY:HA2	1:B:241:LEU:HD23	1.83	0.60
1:A:149:TRP:HE1	1:A:154:VAL:HG23	1.66	0.60
1:B:207:THR:HA	1:B:210:ILE:HD12	1.83	0.60
1:B:86:LYS:HE3	1:B:90:ILE:HD12	1.83	0.60
1:B:72:ALA:HB3	1:B:75:LYS:HB2	1.84	0.59
1:A:114:TYR:HB2	1:A:138:LEU:HG	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:CA	1:B:140:ARG:NH1	2.66	0.58
1:B:321:ILE:HG23	1:B:332:LEU:HD21	1.84	0.58
1:B:546:ASN:H	1:B:549:GLN:NE2	2.01	0.58
1:A:281:ILE:HD12	1:A:292:LEU:HD23	1.84	0.58
1:A:442:GLU:OE1	1:A:491:LYS:NZ	2.36	0.58
1:B:109:LYS:HE3	1:B:115:SER:HB3	1.85	0.58
1:A:123:ASN:ND2	1:A:128:GLU:HA	2.19	0.58
1:A:217:PHE:HB2	1:A:219:LEU:HD13	1.86	0.56
1:B:58:LYS:HD3	1:B:60:ASP:OD1	2.05	0.56
1:A:372:LYS:HA	1:A:559:ASN:HD21	1.70	0.56
1:B:124:THR:HG23	1:B:126:LEU:N	2.21	0.56
1:A:217:PHE:HB3	1:A:219:LEU:CD1	2.36	0.56
1:B:122:MET:HB3	1:B:129:LEU:HD11	1.88	0.56
1:B:635:SER:HB2	1:B:656:LYS:HD3	1.88	0.56
1:B:152:ASN:HB3	1:B:158:MET:O	2.06	0.55
1:A:57:ASN:OD1	1:A:99:LEU:N	2.33	0.55
1:A:157:GLU:HG3	1:A:329:LYS:NZ	2.21	0.55
1:B:369:THR:HG22	1:B:376:LEU:HD23	1.90	0.54
1:A:535:ASP:HB3	1:A:540:GLN:HB2	1.89	0.54
1:A:211:LYS:HE2	1:A:221:GLU:CD	2.31	0.54
1:A:656:LYS:HE2	1:A:660:ASP:O	2.08	0.54
1:B:195:VAL:HB	1:B:200:LEU:HD21	1.89	0.54
1:B:46:GLU:O	1:B:50:GLU:HG3	2.08	0.54
1:A:217:PHE:O	1:A:219:LEU:HD12	2.07	0.53
1:B:164:VAL:HG11	1:B:320:SER:O	2.08	0.53
1:A:57:ASN:ND2	1:A:99:LEU:O	2.30	0.53
1:B:567:LYS:HB2	1:B:572:LYS:HE3	1.90	0.53
1:A:460:TYR:OH	1:A:535:ASP:OD1	2.24	0.53
1:A:545:ILE:HD13	1:A:553:MET:HE1	1.90	0.52
1:A:618:THR:HG22	1:A:663:THR:HG21	1.92	0.52
1:B:297:LYS:O	1:B:312:ARG:NH2	2.42	0.52
1:A:162:ASP:HA	1:A:324:THR:HG23	1.92	0.52
1:A:191:LYS:HZ3	1:A:246:GLY:C	2.15	0.52
1:A:358:SER:O	1:A:665:ARG:HD3	2.09	0.52
1:A:191:LYS:NZ	1:A:246:GLY:C	2.68	0.51
1:B:114:TYR:HB2	1:B:138:LEU:HB2	1.93	0.51
1:A:203:GLY:H	1:A:206:LYS:NZ	2.08	0.51
1:B:281:ILE:HD11	1:B:312:ARG:HH22	1.74	0.51
1:B:221:GLU:N	1:B:221:GLU:OE2	2.43	0.51
1:B:535:ASP:HA	1:B:538:TYR:CE1	2.46	0.51
1:B:569:ILE:H	1:B:572:LYS:HE2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LYS:NZ	1:A:480:SER:CA	2.72	0.51
1:B:87:TYR:HE1	1:B:154:VAL:HG11	1.76	0.51
1:A:149:TRP:CZ2	1:A:151:PRO:HA	2.46	0.50
1:A:521:ILE:HA	1:A:543:LEU:HD23	1.92	0.50
1:B:322:THR:OG1	1:B:323:ASP:N	2.44	0.50
1:A:172:THR:HG22	1:A:339:ASN:ND2	2.27	0.50
1:B:667:PRO:O	1:B:671:GLN:HG3	2.12	0.50
1:B:78:LEU:HD23	1:B:149:TRP:HZ3	1.77	0.49
1:A:52:PHE:HE1	1:A:64:ALA:HB1	1.78	0.49
1:B:418:TYR:CD1	1:B:652:MET:HE1	2.47	0.49
1:A:426:MET:HG3	1:A:617:LYS:HG2	1.94	0.49
1:A:400:LYS:O	1:A:404:GLU:N	2.36	0.48
1:A:219:LEU:HD11	1:A:242:LYS:HD2	1.95	0.48
1:B:329:LYS:HG3	1:B:330:LYS:HG2	1.94	0.48
1:A:325:ASP:OD1	1:A:325:ASP:N	2.46	0.47
1:A:637:LEU:HB2	1:A:663:THR:HG22	1.95	0.47
1:B:217:PHE:O	1:B:242:LYS:NZ	2.43	0.47
1:A:318:LYS:HG2	1:A:334:GLU:HB3	1.96	0.47
1:A:123:ASN:HD22	1:A:128:GLU:HA	1.78	0.47
1:A:369:THR:HG22	1:A:376:LEU:HD23	1.96	0.47
1:B:486:ALA:HB1	1:B:534:ALA:HB1	1.96	0.47
1:A:149:TRP:NE1	1:A:154:VAL:HG23	2.29	0.47
1:A:492:MET:HE2	1:A:497:PHE:HA	1.97	0.47
1:B:649:MET:HE3	1:B:670:LEU:HG	1.97	0.47
1:B:657:GLU:OE2	1:B:657:GLU:HA	2.15	0.47
1:A:625:GLU:O	1:A:627:GLN:N	2.45	0.46
1:B:210:ILE:HG23	1:B:224:ILE:HD12	1.98	0.46
1:B:425:LYS:HG2	1:B:485:MET:HG2	1.97	0.46
1:A:341:LYS:HA	1:A:341:LYS:HD3	1.62	0.46
1:A:490:LEU:HD23	1:A:533:LEU:HD23	1.97	0.46
1:B:101:ILE:HD12	1:B:101:ILE:HA	1.66	0.46
1:A:91:TYR:HA	1:A:94:ALA:HB3	1.96	0.46
1:A:78:LEU:HD23	1:A:79:SER:N	2.27	0.46
1:A:157:GLU:HG3	1:A:329:LYS:HZ1	1.81	0.46
1:B:129:LEU:HD13	1:B:132:LEU:HD22	1.98	0.46
1:A:75:LYS:HB2	1:A:150:GLN:OE1	2.16	0.46
1:B:86:LYS:NZ	1:B:163:LYS:HA	2.31	0.46
1:A:540:GLN:HE22	1:A:622:GLU:H	1.64	0.45
1:A:162:ASP:CB	1:A:323:ASP:HA	2.46	0.45
1:B:286:ILE:HD12	1:B:289:ASN:O	2.17	0.45
1:B:474:LYS:HB2	1:B:474:LYS:HE3	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:HB2	1:B:76:SER:H	1.81	0.45
1:B:208:ALA:HA	1:B:211:LYS:HD2	1.99	0.45
1:B:283:ALA:HA	1:B:286:ILE:HG22	1.99	0.45
1:A:636:PHE:CE1	1:A:652:MET:HG3	2.52	0.45
1:B:194:GLY:HA3	1:B:238:PHE:CE1	2.52	0.45
1:B:446:ILE:HD12	1:B:471:VAL:CG1	2.47	0.45
1:B:321:ILE:HD11	1:B:330:LYS:H	1.81	0.45
1:A:405:ASN:C	1:A:405:ASN:HD22	2.24	0.45
1:A:122:MET:HE1	1:A:155:PHE:HE1	1.82	0.45
1:B:194:GLY:HA3	1:B:238:PHE:HE1	1.82	0.44
1:B:42:VAL:HB	1:B:106:VAL:HG22	2.00	0.44
1:B:139:ASP:HB3	1:B:146:THR:HB	1.98	0.44
1:B:520:GLN:HG2	1:B:544:LEU:HB2	2.00	0.44
1:A:196:VAL:CG2	1:A:199:LYS:HD3	2.48	0.44
1:B:129:LEU:HD12	1:B:129:LEU:O	2.18	0.44
1:B:202:ASP:N	1:B:202:ASP:OD1	2.49	0.44
1:B:204:ASP:HA	1:B:207:THR:HG22	2.00	0.44
1:A:370:THR:HG23	1:A:377:LEU:HD21	2.00	0.44
1:B:123:ASN:ND2	1:B:286:ILE:HD11	2.33	0.44
1:B:308:ASP:O	1:B:312:ARG:HG2	2.18	0.44
1:B:624:LYS:HE2	1:B:630:LYS:HB2	1.98	0.44
1:B:569:ILE:HB	1:B:572:LYS:HG3	2.00	0.43
1:A:74:ASN:HA	1:A:75:LYS:HA	1.69	0.43
1:A:376:LEU:HD22	1:A:379:LEU:HD21	2.00	0.43
1:A:612:ILE:CG2	1:A:674:ASN:HD21	2.31	0.43
1:A:162:ASP:HB3	1:A:323:ASP:HA	2.00	0.43
1:A:162:ASP:HB2	1:A:322:THR:O	2.19	0.43
1:A:303:LEU:HA	1:A:306:ALA:HB3	1.99	0.43
1:A:516:MET:HG3	1:A:546:ASN:HD21	1.82	0.43
1:A:312:ARG:HG2	1:A:313:GLY:O	2.18	0.43
1:A:423:THR:HA	1:A:617:LYS:HG3	2.00	0.43
1:B:178:ASP:OD1	1:B:182:GLU:N	2.51	0.43
1:B:227:ALA:O	1:B:230:GLN:HG3	2.18	0.43
1:B:648:MET:HE3	1:B:648:MET:HB2	1.92	0.43
1:A:282:THR:HG23	1:A:284:GLU:H	1.84	0.43
1:A:130:LYS:HA	1:A:131:ASP:HA	1.62	0.43
1:A:370:THR:OG1	1:A:375:ASP:HB2	2.19	0.43
1:B:126:LEU:HA	1:B:315:THR:OG1	2.19	0.43
1:B:265:TYR:OH	1:B:277:TYR:HA	2.19	0.43
1:A:71:LYS:HB3	1:A:79:SER:HA	2.01	0.42
1:A:292:LEU:HD21	1:A:298:ILE:HD12	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:GLU:HB2	1:B:533:LEU:HD13	2.01	0.42
1:B:630:LYS:HD2	1:B:630:LYS:C	2.44	0.42
1:B:139:ASP:N	1:B:146:THR:O	2.52	0.42
1:B:318:LYS:HD3	1:B:320:SER:OG	2.20	0.42
1:A:437:THR:HB	1:A:492:MET:HB2	2.00	0.42
1:B:612:ILE:HG13	1:B:614:LEU:HG	2.00	0.42
1:A:320:SER:H	1:A:331:VAL:HG21	1.85	0.42
1:B:165:SER:HA	1:B:166:LEU:HA	1.75	0.42
1:A:314:THR:HG1	1:A:338:GLN:HB3	1.84	0.42
1:B:282:THR:HG22	1:B:284:GLU:H	1.85	0.42
1:B:284:GLU:OE2	1:B:288:LYS:HE3	2.20	0.42
1:B:86:LYS:HZ2	1:B:163:LYS:HA	1.85	0.41
1:B:446:ILE:HD12	1:B:471:VAL:HG11	2.02	0.41
1:A:322:THR:HA	1:A:327:VAL:O	2.21	0.41
1:B:123:ASN:CG	1:B:286:ILE:HD11	2.45	0.41
1:B:265:TYR:OH	1:B:304:GLU:OE2	2.37	0.41
1:B:41:ALA:HA	1:B:140:ARG:NH1	2.35	0.41
1:A:196:VAL:HA	1:A:197:PRO:HD3	1.89	0.41
1:A:76:SER:H	1:A:77:ALA:HA	1.86	0.41
1:B:281:ILE:HG13	1:B:296:GLY:O	2.20	0.41
1:A:478:ILE:O	1:A:603:THR:HG23	2.20	0.41
1:A:652:MET:HE2	1:A:654:GLU:HB2	2.03	0.41
1:B:283:ALA:HA	1:B:286:ILE:CG2	2.51	0.40
1:B:276:GLY:HA3	1:B:301:SER:O	2.22	0.40
1:B:569:ILE:HB	1:B:572:LYS:HE2	2.02	0.40
1:A:147:ILE:HD13	1:A:147:ILE:HG21	1.88	0.40
1:A:554:TYR:HB3	1:A:638:PHE:CE1	2.56	0.40
1:B:167:THR:HG23	1:B:167:THR: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	638/659 (97%)	590 (92%)	48 (8%)	0	100	100
1	B	639/659 (97%)	607 (95%)	31 (5%)	1 (0%)	43	62
All	All	1277/1318 (97%)	1197 (94%)	79 (6%)	1 (0%)	48	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	658	ASP

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	530/547 (97%)	530 (100%)	0	100	100
1	B	531/547 (97%)	530 (100%)	1 (0%)	87	95
All	All	1061/1094 (97%)	1060 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	533	LEU

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	123	ASN
1	A	169	GLN
1	A	180	ASN
1	A	405	ASN
1	A	452	GLN
1	A	470	GLN
1	A	487	GLN
1	A	496	ASN
1	A	517	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	520	GLN
1	A	559	ASN
1	A	605	HIS
1	A	627	GLN
1	A	674	ASN
1	B	230	GLN
1	B	392	ASN
1	B	482	ASN
1	B	487	GLN
1	B	496	ASN
1	B	549	GLN
1	B	627	GLN
1	B	645	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	640/659 (97%)	0.77	101 (15%) 5 4	35, 60, 166, 204	0
1	B	641/659 (97%)	0.74	94 (14%) 6 4	34, 62, 162, 207	0
All	All	1281/1318 (97%)	0.75	195 (15%) 5 4	34, 61, 165, 207	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	LEU	6.6
1	A	321	ILE	6.3
1	B	402	TYR	6.2
1	A	147	ILE	6.2
1	B	233	VAL	5.6
1	A	90	ILE	5.5
1	A	116	PHE	5.3
1	B	631	GLY	5.2
1	B	49	VAL	5.1
1	B	394	ILE	5.0
1	A	332	LEU	5.0
1	B	164	VAL	4.9
1	A	83	ILE	4.8
1	A	87	TYR	4.8
1	B	87	TYR	4.8
1	A	93	ALA	4.7
1	B	154	VAL	4.6
1	B	153	LEU	4.6
1	A	52	PHE	4.3
1	B	625	GLU	4.3
1	A	56	LEU	4.2
1	B	129	LEU	4.2
1	A	77	ALA	4.2
1	A	44	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	155	PHE	4.1
1	A	317	GLY	4.0
1	B	116	PHE	4.0
1	B	166	LEU	3.9
1	B	65	ALA	3.9
1	A	149	TRP	3.8
1	B	197	PRO	3.7
1	B	106	VAL	3.7
1	A	74	ASN	3.7
1	B	626	LYS	3.6
1	A	138	LEU	3.6
1	B	196	VAL	3.6
1	A	515	SER	3.6
1	A	78	LEU	3.5
1	A	145	THR	3.5
1	B	659	ASP	3.4
1	A	163	LYS	3.4
1	A	158	MET	3.4
1	A	331	VAL	3.4
1	B	201	GLY	3.4
1	A	67	MET	3.4
1	B	108	LYS	3.4
1	A	137	THR	3.4
1	A	73	ALA	3.3
1	A	104	LEU	3.3
1	A	143	GLY	3.3
1	B	42	VAL	3.2
1	A	105	LYS	3.2
1	B	71	LYS	3.2
1	B	147	ILE	3.2
1	B	117	SER	3.2
1	B	245	ASP	3.2
1	B	156	PRO	3.2
1	B	61	TYR	3.1
1	A	65	ALA	3.1
1	A	72	ALA	3.1
1	A	71	LYS	3.1
1	A	649	MET	3.1
1	B	83	ILE	3.1
1	A	106	VAL	3.1
1	A	79	SER	3.0
1	A	58	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	624	LYS	3.0
1	A	102	SER	3.0
1	B	330	LYS	3.0
1	B	624	LYS	3.0
1	B	315	THR	3.0
1	A	204	ASP	3.0
1	A	626	LYS	3.0
1	A	68	ALA	2.9
1	B	73	ALA	2.9
1	B	90	ILE	2.9
1	A	205	GLU	2.9
1	B	630	LYS	2.9
1	B	91	TYR	2.9
1	B	232	TRP	2.8
1	A	326	GLY	2.8
1	A	203	GLY	2.8
1	B	393	GLY	2.8
1	A	115	SER	2.8
1	A	330	LYS	2.8
1	A	630	LYS	2.8
1	A	320	SER	2.7
1	B	249	PRO	2.7
1	A	322	THR	2.7
1	A	132	LEU	2.7
1	A	167	THR	2.7
1	A	108	LYS	2.7
1	A	109	LYS	2.7
1	B	113	THR	2.7
1	A	69	SER	2.7
1	A	233	VAL	2.7
1	B	70	LYS	2.6
1	B	56	LEU	2.6
1	B	132	LEU	2.6
1	B	395	SER	2.6
1	B	214	ALA	2.6
1	A	659	ASP	2.6
1	B	331	VAL	2.6
1	A	117	SER	2.6
1	A	61	TYR	2.6
1	A	86	LYS	2.6
1	A	101	ILE	2.6
1	B	158	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	42	VAL	2.6
1	B	130	LYS	2.6
1	B	149	TRP	2.6
1	B	124	THR	2.6
1	A	114	TYR	2.6
1	B	107	ASP	2.5
1	A	91	TYR	2.5
1	A	136	GLY	2.5
1	A	75	LYS	2.5
1	B	68	ALA	2.5
1	B	120	ALA	2.5
1	B	398	ASP	2.5
1	A	153	LEU	2.5
1	B	223	ALA	2.5
1	B	220	THR	2.5
1	B	45	GLY	2.5
1	A	118	TYR	2.5
1	A	134	TYR	2.5
1	B	39	THR	2.5
1	B	112	SER	2.5
1	A	313	GLY	2.4
1	A	335	HIS	2.4
1	A	162	ASP	2.4
1	B	48	THR	2.4
1	A	76	SER	2.4
1	B	628	ASP	2.4
1	B	44	ALA	2.4
1	A	45	GLY	2.4
1	A	169	GLN	2.4
1	B	138	LEU	2.4
1	A	51	GLN	2.3
1	B	228	ILE	2.3
1	B	321	ILE	2.3
1	B	41	ALA	2.3
1	B	67	MET	2.3
1	A	70	LYS	2.3
1	A	154	VAL	2.3
1	A	337	VAL	2.3
1	A	120	ALA	2.3
1	A	49	VAL	2.3
1	B	145	THR	2.3
1	A	54	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	111	ASP	2.3
1	A	156	PRO	2.3
1	A	133	SER	2.2
1	A	144	LYS	2.2
1	B	168	THR	2.2
1	A	333	ILE	2.2
1	B	101	ILE	2.2
1	B	397	GLU	2.2
1	B	199	LYS	2.2
1	B	208	ALA	2.2
1	B	648	MET	2.2
1	B	160	GLY	2.2
1	A	121	LYS	2.2
1	B	155	PHE	2.2
1	A	123	ASN	2.1
1	B	161	ASN	2.1
1	B	253	ALA	2.1
1	B	126	LEU	2.1
1	B	213	ILE	2.1
1	B	396	GLN	2.1
1	A	674	ASN	2.1
1	A	166	LEU	2.1
1	B	314	THR	2.1
1	B	110	ASP	2.1
1	B	63	LYS	2.1
1	B	151	PRO	2.1
1	A	113	THR	2.1
1	B	399	TYR	2.1
1	A	81	LYS	2.1
1	A	329	LYS	2.1
1	B	47	LYS	2.1
1	B	122	MET	2.1
1	A	59	GLY	2.1
1	A	288	LYS	2.1
1	A	325	ASP	2.1
1	B	53	VAL	2.0
1	B	327	VAL	2.0
1	A	152	ASN	2.0
1	B	86	LYS	2.0
1	B	162	ASP	2.0
1	B	652	MET	2.0
1	A	251	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	2.0
1	A	400	LYS	2.0
1	A	168	THR	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.