



Full wwPDB X-ray Structure Validation Report i

Mar 16, 2022 – 02:14 PM EDT

PDB ID : 6C84
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 i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.27
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) : 2.27

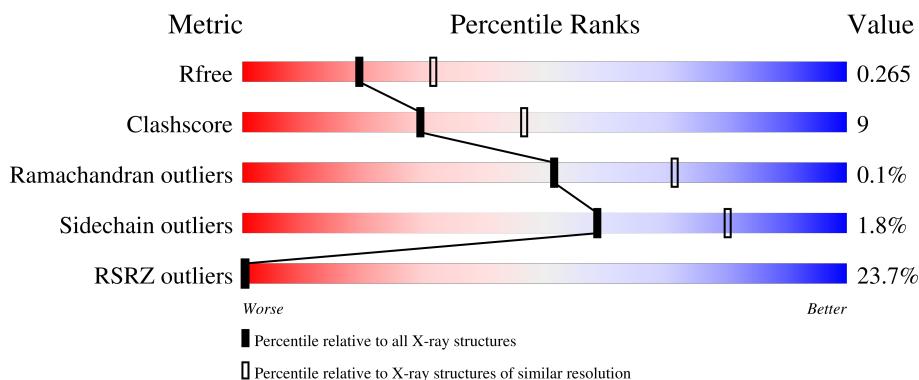
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

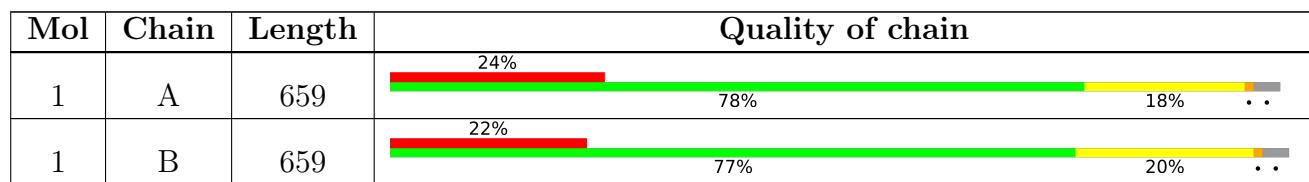
The reported resolution of this entry is 2.51 Å.

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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (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.



2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	640	4894	3062	808	1011	13	0	0	0
1	B	641	4903	3067	809	1014	13	0	0	0

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

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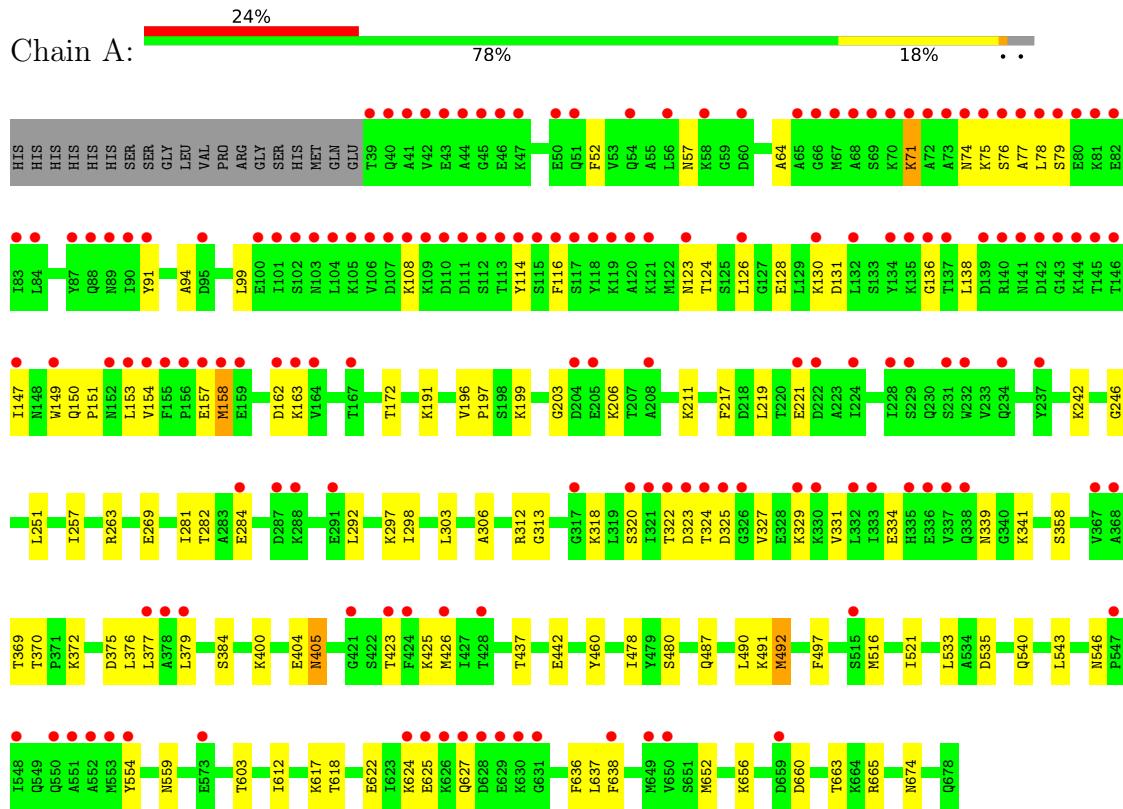
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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	SER	-	expression tag	UNP A0A133MY97
B	28	GLY	-	expression tag	UNP A0A133MY97
B	29	LEU	-	expression tag	UNP A0A133MY97
B	30	VAL	-	expression tag	UNP A0A133MY97
B	31	PRO	-	expression tag	UNP A0A133MY97
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

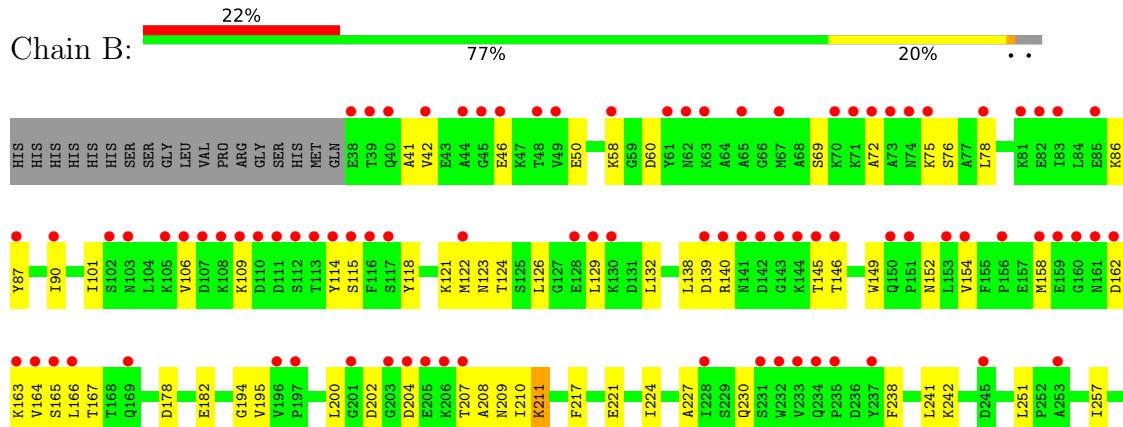
3 Residue-property plots

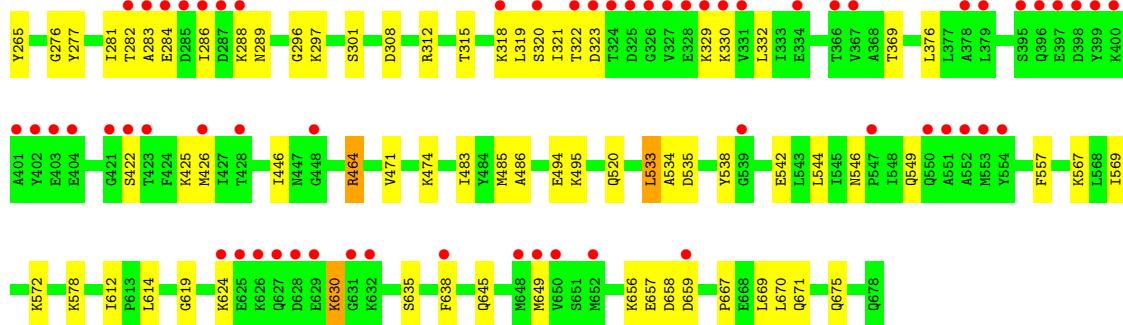
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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) 94.7 (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 0.224 , 0.265	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)	0.32 , 45.8	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	0.93	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 [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/4969	0.55	0/6719
1	B	0.34	0/4978	0.55	0/6731
All	All	0.33	0/9947	0.55	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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4894	0	4834	90	0
1	B	4903	0	4840	94	0
All	All	9797	0	9674	184	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 9.

All (184) 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

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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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:426:MET:HE2	1:B:557:PHE:CE2	2.41	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: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: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:358:SER:O	1:A:665:ARG:HD3	2.09	0.52
1:B:114:TYR:HB2	1:B:138:LEU:HB2	1.93	0.51
1:B:426:MET:HE1	1:B:638:PHE:CE2	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:211:LYS:HE2	1:A:221:GLU:CD	2.31	0.49
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: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:N	1:A:325:ASP:OD1	2.46	0.48
1:A:637:LEU:HB2	1:A:663:THR:HG22	1.95	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:157:GLU:HG3	1:A:329:LYS:HZ1	1.80	0.47
1:A:149:TRP:NE1	1:A:154:VAL:HG23	2.29	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: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:B:217:PHE:O	1:B:242:LYS:NZ	2.43	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ILE:HD11	1:B:330:LYS:H	1.81	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:B:649:MET:HE3	1:B:670:LEU:HG	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:B:649:MET:HE2	1:B:669:LEU:HD23	1.99	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:191:LYS:HZ3	1:A:246:GLY:C	2.19	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: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
1:B:494:GLU:HB2	1:B:533:LEU:HD13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:SER:HA	1:B:166:LEU:HA	1.75	0.42
1:A:492:MET:HE1	1:A:497:PHE:HD1	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: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: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: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:A:405:ASN:C	1:A:405:ASN:HD22	2.24	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%)	47 67
All	All	1277/1318 (97%)	1197 (94%)	79 (6%)	1 (0%)	51 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	658	ASP

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	530/547 (97%)	521 (98%)	9 (2%)	60 81
1	B	531/547 (97%)	521 (98%)	10 (2%)	57 79
All	All	1061/1094 (97%)	1042 (98%)	19 (2%)	59 80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LYS
1	A	108	LYS
1	A	158	MET
1	A	163	LYS
1	A	263	ARG
1	A	405	ASN
1	A	487	GLN
1	A	492	MET
1	A	624	LYS
1	B	121	LYS
1	B	211	LYS
1	B	319	LEU
1	B	464	ARG
1	B	495	LYS
1	B	533	LEU
1	B	578	LYS
1	B	630	LYS
1	B	645	GLN
1	B	659	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	169	GLN
1	A	258	GLN
1	A	405	ASN
1	A	482	ASN
1	A	496	ASN
1	A	517	ASN
1	A	520	GLN
1	A	559	ASN
1	A	674	ASN
1	B	482	ASN
1	B	487	GLN
1	B	549	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 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 i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	640/659 (97%)	1.22	156 (24%) 0 0	35, 60, 166, 204	0
1	B	641/659 (97%)	1.18	148 (23%) 0 0	34, 62, 162, 207	0
All	All	1281/1318 (97%)	1.20	304 (23%) 0 0	34, 61, 165, 207	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	LEU	14.3
1	B	232	TRP	11.9
1	B	631	GLY	11.7
1	A	109	LYS	10.1
1	A	140	ARG	10.1
1	A	76	SER	10.0
1	B	624	LYS	9.6
1	B	626	LYS	9.6
1	A	107	ASP	9.5
1	B	165	SER	9.4
1	B	628	ASP	9.1
1	A	105	LYS	8.7
1	A	332	LEU	8.5
1	B	143	GLY	8.3
1	A	143	GLY	8.0
1	B	627	GLN	7.8
1	B	107	ASP	7.8
1	A	163	LYS	7.7
1	B	108	LYS	7.5
1	A	102	SER	7.5
1	B	402	TYR	7.3
1	A	322	THR	7.3
1	B	330	LYS	7.3
1	A	72	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	161	ASN	7.1
1	A	65	ALA	7.0
1	B	117	SER	6.8
1	A	73	ALA	6.7
1	A	333	ILE	6.7
1	A	142	ASP	6.7
1	B	130	LYS	6.6
1	A	111	ASP	6.4
1	B	625	GLU	6.4
1	A	629	GLU	6.3
1	B	327	VAL	6.3
1	A	117	SER	6.3
1	B	201	GLY	6.2
1	B	62	ASN	6.1
1	B	139	ASP	6.1
1	B	142	ASP	6.1
1	B	325	ASP	6.0
1	A	116	PHE	6.0
1	A	108	LYS	5.9
1	A	115	SER	5.8
1	A	229	SER	5.8
1	B	71	LYS	5.8
1	A	75	LYS	5.7
1	A	70	LYS	5.7
1	A	104	LEU	5.7
1	A	121	LYS	5.7
1	B	113	THR	5.6
1	A	118	TYR	5.6
1	A	141	ASN	5.6
1	B	164	VAL	5.6
1	A	103	ASN	5.5
1	A	627	GLN	5.5
1	A	324	THR	5.5
1	A	58	LYS	5.4
1	A	106	VAL	5.4
1	A	628	ASP	5.4
1	A	155	PHE	5.4
1	A	83	ILE	5.4
1	B	331	VAL	5.3
1	A	74	ASN	5.3
1	B	156	PRO	5.3
1	B	396	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	5.2
1	A	167	THR	5.1
1	A	110	ASP	5.1
1	B	158	MET	5.1
1	A	630	LYS	5.0
1	A	113	THR	5.0
1	A	326	GLY	5.0
1	A	87	TYR	4.9
1	A	77	ALA	4.8
1	A	81	LYS	4.8
1	A	649	MET	4.8
1	A	42	VAL	4.7
1	B	109	LYS	4.7
1	A	325	ASP	4.7
1	B	159	GLU	4.7
1	B	75	LYS	4.7
1	B	110	ASP	4.7
1	A	626	LYS	4.7
1	B	551	ALA	4.7
1	A	147	ILE	4.7
1	B	231	SER	4.6
1	A	47	LYS	4.6
1	B	632	LYS	4.6
1	A	231	SER	4.5
1	A	162	ASP	4.5
1	B	111	ASP	4.5
1	A	45	GLY	4.5
1	B	397	GLU	4.4
1	B	395	SER	4.4
1	A	40	GLN	4.4
1	B	233	VAL	4.4
1	B	318	LYS	4.3
1	A	139	ASP	4.3
1	A	625	GLU	4.3
1	B	648	MET	4.3
1	A	551	ALA	4.3
1	B	166	LEU	4.2
1	A	68	ALA	4.2
1	B	326	GLY	4.2
1	B	328	GLU	4.2
1	A	144	LYS	4.2
1	A	39	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	287	ASP	4.2
1	A	90	ILE	4.2
1	A	145	THR	4.1
1	A	650	VAL	4.1
1	B	61	TYR	4.1
1	A	137	THR	4.1
1	B	74	ASN	4.1
1	B	329	LYS	4.0
1	A	101	ILE	4.0
1	A	95	ASP	4.0
1	A	43	GLU	3.9
1	B	145	THR	3.9
1	B	141	ASN	3.9
1	A	321	ILE	3.9
1	A	159	GLU	3.9
1	B	72	ALA	3.8
1	B	629	GLU	3.8
1	A	337	VAL	3.8
1	B	67	MET	3.8
1	A	100	GLU	3.8
1	B	288	LYS	3.7
1	A	71	LYS	3.7
1	A	82	GLU	3.7
1	B	234	GLN	3.7
1	A	336	GLU	3.6
1	B	401	ALA	3.6
1	B	403	GLU	3.6
1	A	66	GLY	3.6
1	A	89	ASN	3.6
1	A	69	SER	3.6
1	B	114	TYR	3.6
1	A	237	TYR	3.5
1	B	399	TYR	3.5
1	A	232	TRP	3.5
1	A	157	GLU	3.5
1	A	112	SER	3.5
1	A	88	GLN	3.5
1	B	550	GLN	3.5
1	B	196	VAL	3.4
1	B	87	TYR	3.4
1	B	115	SER	3.4
1	B	82	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	114	TYR	3.4
1	B	105	LYS	3.4
1	B	398	ASP	3.4
1	B	81	LYS	3.4
1	A	659	ASP	3.4
1	B	49	VAL	3.3
1	A	132	LEU	3.3
1	B	116	PHE	3.2
1	A	67	MET	3.2
1	B	206	LYS	3.2
1	B	48	THR	3.2
1	A	204	ASP	3.2
1	A	51	GLN	3.2
1	B	282	THR	3.2
1	B	379	LEU	3.2
1	A	130	LYS	3.2
1	B	140	ARG	3.2
1	B	46	GLU	3.2
1	A	554	TYR	3.1
1	B	40	GLN	3.1
1	B	400	LYS	3.1
1	B	42	VAL	3.1
1	A	329	LYS	3.1
1	B	153	LEU	3.1
1	A	317	GLY	3.1
1	A	367	VAL	3.1
1	B	154	VAL	3.1
1	A	234	GLN	3.1
1	A	50	GLU	3.1
1	A	323	ASP	3.1
1	B	283	ALA	3.1
1	B	323	ASP	3.0
1	B	65	ALA	3.0
1	B	404	GLU	3.0
1	A	60	ASP	3.0
1	B	204	ASP	3.0
1	A	154	VAL	3.0
1	A	149	TRP	3.0
1	B	112	SER	2.9
1	B	554	TYR	2.9
1	A	553	MET	2.9
1	A	46	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	550	GLN	2.9
1	A	515	SER	2.9
1	B	324	THR	2.9
1	B	70	LYS	2.9
1	B	103	ASN	2.9
1	B	162	ASP	2.9
1	A	41	ALA	2.9
1	A	338	GLN	2.9
1	B	106	VAL	2.8
1	A	44	ALA	2.8
1	B	197	PRO	2.8
1	B	237	TYR	2.8
1	A	54	GLN	2.8
1	B	58	LYS	2.8
1	B	144	LYS	2.8
1	B	235	PRO	2.8
1	B	129	LEU	2.7
1	B	205	GLU	2.7
1	B	207	THR	2.7
1	B	160	GLY	2.7
1	A	368	ALA	2.7
1	A	547	PRO	2.7
1	A	134	TYR	2.7
1	B	128	GLU	2.7
1	A	428	THR	2.7
1	A	146	THR	2.7
1	A	284	GLU	2.7
1	A	152	ASN	2.7
1	B	245	ASP	2.6
1	B	366	THR	2.6
1	A	153	LEU	2.6
1	A	287	ASP	2.6
1	B	547	PRO	2.6
1	B	163	LYS	2.6
1	B	150	GLN	2.6
1	A	335	HIS	2.6
1	B	44	ALA	2.6
1	A	423	THR	2.5
1	B	367	VAL	2.5
1	A	164	VAL	2.5
1	B	552	ALA	2.5
1	B	638	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	426	MET	2.5
1	B	85	GLU	2.5
1	B	553	MET	2.5
1	B	378	ALA	2.5
1	B	63	LYS	2.5
1	B	334	GLU	2.4
1	A	624	LYS	2.4
1	A	424	PHE	2.4
1	A	156	PRO	2.4
1	B	45	GLY	2.4
1	B	203	GLY	2.4
1	A	205	GLU	2.4
1	B	285	ASP	2.4
1	B	38	GLU	2.4
1	B	151	PRO	2.4
1	A	330	LYS	2.4
1	B	78	LEU	2.4
1	A	119	LYS	2.3
1	A	158	MET	2.3
1	B	322	THR	2.3
1	A	377	LEU	2.3
1	A	135	LYS	2.3
1	B	169	GLN	2.3
1	A	208	ALA	2.3
1	A	291	GLU	2.3
1	A	631	GLY	2.3
1	B	652	MET	2.3
1	A	548	ILE	2.3
1	A	378	ALA	2.3
1	B	428	THR	2.3
1	A	79	SER	2.3
1	B	286	ILE	2.3
1	B	659	ASP	2.2
1	A	228	ILE	2.2
1	A	573	GLU	2.2
1	B	284	GLU	2.2
1	A	80	GLU	2.2
1	B	39	THR	2.2
1	B	448	GLY	2.2
1	A	224	ILE	2.2
1	A	552	ALA	2.2
1	A	379	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	320	SER	2.2
1	A	421	GLY	2.2
1	A	221	GLU	2.2
1	B	146	THR	2.2
1	A	638	PHE	2.2
1	B	102	SER	2.2
1	B	422	SER	2.2
1	A	78	LEU	2.1
1	B	649	MET	2.1
1	B	90	ILE	2.1
1	A	56	LEU	2.1
1	B	122	MET	2.1
1	B	421	GLY	2.1
1	A	136	GLY	2.1
1	B	539	GLY	2.1
1	B	253	ALA	2.1
1	B	228	ILE	2.1
1	A	123	ASN	2.1
1	A	120	ALA	2.0
1	A	222	ASP	2.0
1	A	126	LEU	2.0
1	A	288	LYS	2.0
1	B	83	ILE	2.0
1	B	426	MET	2.0
1	B	423	THR	2.0
1	B	320	SER	2.0
1	B	650	VAL	2.0
1	A	91	TYR	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.