Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 08:34 AM EST

PDB ID	:	1VQQ
Title	:	Structure of Penicillin binding protein 2a from methicillin resistant Staphylococcus aureus strain 27r at 1.80 A resolution.
Authors	:	Lim, D.; Strynadka, N.C.J.
Deposited on	:	2004-12-17
Resolution	:	1.80 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:

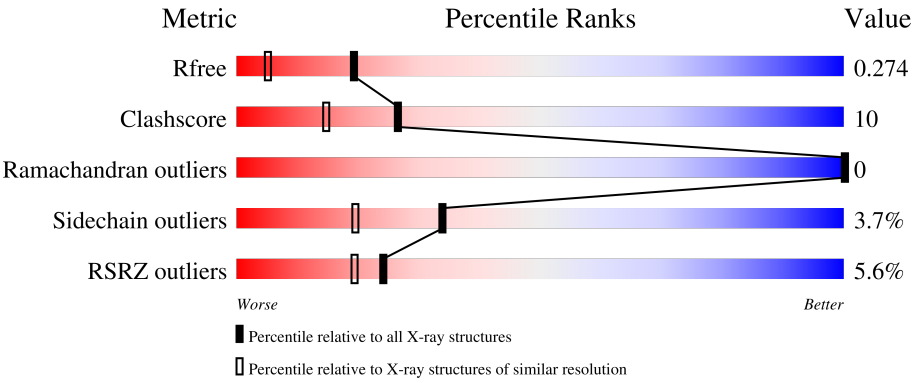
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	646	4% 76% 20%
1	B	646	7% 80% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10644 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 mecA, low-affinity.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total 5102	C 3218	N 860	O 1009	S 15	0	0	0
1	B	625	Total 5023	C 3171	N 843	O 994	S 15	0	0	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Cd 2	0	0
2	B	5	Total 5	Cd 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	3	Total 3	Cl 3	0	0

- Molecule 4 is water.

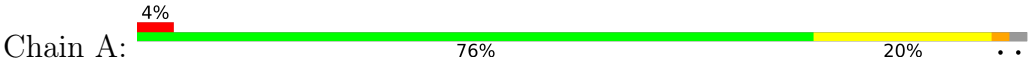
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total 246	O 246	0	0
4	B	262	Total 262	O 262	0	0

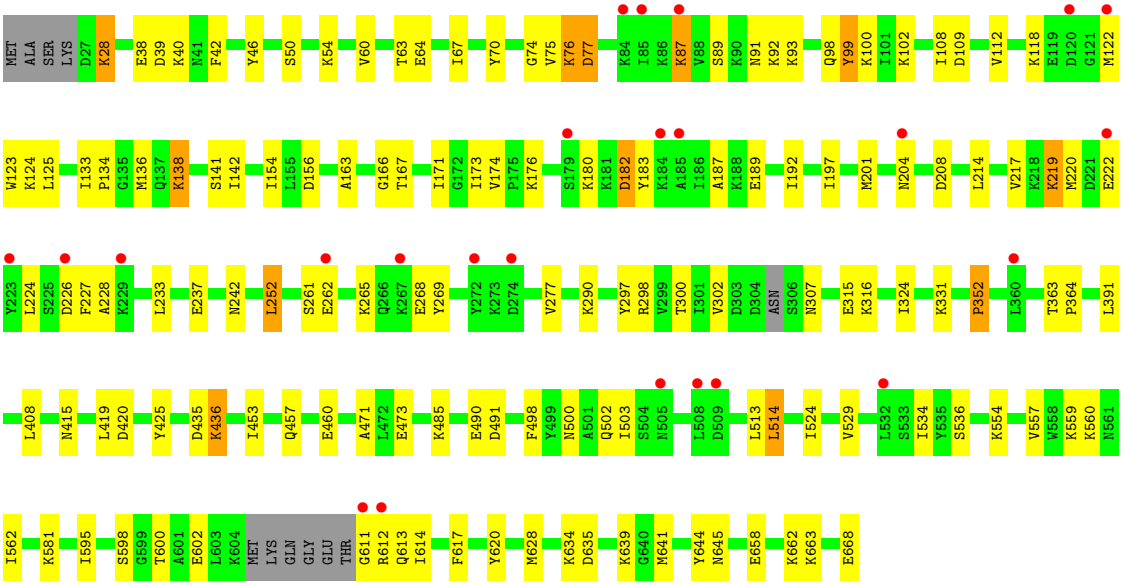
3 Residue-property plots (i)

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 mecA, low-affinity

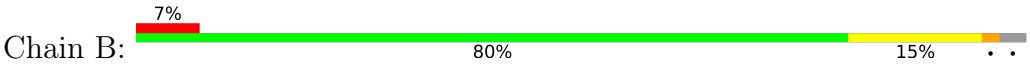
Chain A:

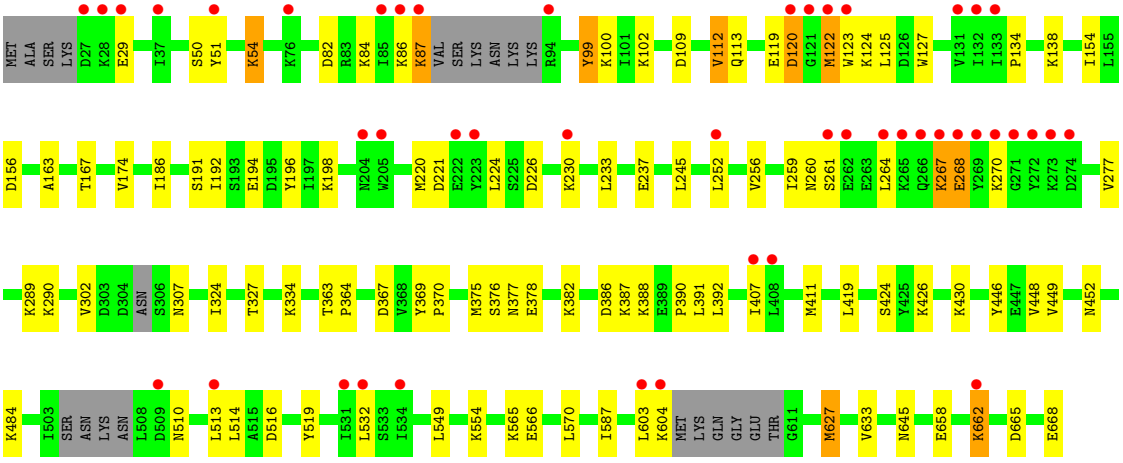




• Molecule 1: penicillin-binding protein mecA, low-affinity

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.87Å 100.61Å 186.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.92 – 1.80 24.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.92-1.80) 97.4 (24.92-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.274 0.237 , 0.274	Depositor DCC
R_{free} test set	6974 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.804	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10644	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CL

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	0.47	0/5186	0.70	2/6971 (0.0%)
1	B	0.46	0/5105	0.69	1/6862 (0.0%)
All	All	0.47	0/10291	0.69	3/13833 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	174	VAL	N-CA-C	-5.42	96.35	111.00
1	B	174	VAL	N-CA-C	-5.06	97.35	111.00

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	5102	0	5099	122	0
1	B	5023	0	5008	88	0
2	A	2	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	246	0	0	5	0
4	B	262	0	0	6	0
All	All	10644	0	10107	209	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 (209) 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:87:LYS:H	1:A:87:LYS:HE3	1.14	1.08
1:B:267:LYS:HD3	1:B:267:LYS:H	1.21	1.06
1:A:611:GLY:HA3	1:A:635:ASP:OD1	1.56	1.04
1:A:436:LYS:H	1:A:436:LYS:HD3	1.23	1.03
1:B:267:LYS:HD3	1:B:267:LYS:N	1.89	0.86
1:A:87:LYS:H	1:A:87:LYS:CE	1.92	0.82
1:B:87:LYS:N	1:B:87:LYS:HD3	1.93	0.82
1:A:138:LYS:HD2	1:A:138:LYS:H	1.43	0.81
1:A:122:MET:HG3	1:A:124:LYS:NZ	1.95	0.81
1:B:226:ASP:O	1:B:230:LYS:HG2	1.82	0.79
1:A:28:LYS:N	1:A:28:LYS:HD2	1.97	0.79
1:A:87:LYS:HE3	1:A:87:LYS:N	1.96	0.78
1:B:510:ASN:HB3	1:B:513:LEU:HD12	1.65	0.77
1:A:436:LYS:H	1:A:436:LYS:CD	1.96	0.77
1:A:70:TYR:HB3	1:A:75:VAL:CG2	2.15	0.76
1:A:138:LYS:H	1:A:138:LYS:CD	1.99	0.74
1:B:387:LYS:HA	1:B:387:LYS:HE2	1.69	0.73
1:A:70:TYR:HB3	1:A:75:VAL:HG21	1.69	0.73
1:A:557:VAL:HG11	1:A:560:LYS:HG2	1.71	0.73
1:A:112:VAL:CG1	1:A:134:PRO:HB3	2.19	0.72
1:A:485:LYS:HE3	4:A:1170:HOH:O	1.90	0.72
1:A:613:GLN:HG2	1:A:641:MET:SD	2.30	0.71
1:B:256:VAL:HG22	4:B:1059:HOH:O	1.90	0.71
1:B:426:LYS:HG2	1:B:452:ASN:OD1	1.91	0.70
1:B:267:LYS:HA	1:B:270:LYS:HE3	1.73	0.70
1:B:122:MET:HG3	1:B:124:LYS:HE2	1.73	0.70
1:A:536:SER:HA	1:A:628:MET:HE3	1.73	0.70
1:A:77:ASP:HB2	1:A:102:LYS:HD2	1.74	0.68
1:B:138:LYS:HE2	1:B:138:LYS:H	1.58	0.68
1:B:220:MET:HE1	1:B:224:LEU:HD23	1.75	0.68
1:B:378:GLU:HG3	1:B:382:LYS:NZ	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:CG1	1:B:134:PRO:HB3	2.25	0.67
1:B:603:LEU:HD23	1:B:604:LYS:N	2.11	0.66
1:A:268:GLU:HG3	1:A:269:TYR:CD1	2.31	0.65
1:A:133:ILE:HB	1:A:136:MET:CE	2.27	0.65
1:A:176:LYS:HG3	1:A:208:ASP:O	1.98	0.64
1:B:167:THR:HG23	1:B:237:GLU:HG3	1.80	0.64
1:A:171:ILE:HD11	1:A:217:VAL:HG13	1.79	0.64
1:B:112:VAL:HG13	1:B:134:PRO:HB3	1.80	0.64
1:A:436:LYS:HD3	1:A:436:LYS:N	2.06	0.63
1:A:614:ILE:HD11	1:A:634:LYS:HG3	1.79	0.63
1:A:171:ILE:HD11	1:A:217:VAL:CG1	2.29	0.63
1:A:176:LYS:HD2	1:B:113:GLN:NE2	2.15	0.62
1:B:627:MET:O	1:B:627:MET:HG3	1.98	0.62
1:A:420:ASP:OD1	4:A:1011:HOH:O	2.16	0.62
1:B:100:LYS:HG2	1:B:109:ASP:OD2	2.00	0.62
1:A:138:LYS:HD2	1:A:138:LYS:N	2.12	0.61
1:A:598:SER:HB3	1:A:617:PHE:CD1	2.36	0.61
1:A:602:GLU:OE1	1:A:613:GLN:NE2	2.29	0.61
1:B:29:GLU:OE1	1:B:123:TRP:HD1	1.84	0.61
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.83	0.61
1:B:99:TYR:HD1	1:B:112:VAL:HG11	1.66	0.60
1:A:46:TYR:O	1:A:54:LYS:HD3	2.01	0.60
1:B:186:ILE:HD13	1:B:233:LEU:HD21	1.84	0.60
1:B:226:ASP:HB3	1:B:230:LYS:HE3	1.83	0.60
1:A:133:ILE:HB	1:A:136:MET:HE2	1.84	0.60
1:B:220:MET:CE	1:B:224:LEU:HD23	2.32	0.60
1:A:261:SER:O	1:A:265:LYS:HE3	2.02	0.59
1:A:658:GLU:HB2	1:A:662:LYS:HG2	1.85	0.59
1:B:50:SER:O	1:B:54:LYS:HD2	2.02	0.59
1:B:261:SER:HA	1:B:264:LEU:HD12	1.84	0.59
1:A:503:ILE:O	1:A:524:ILE:HG12	2.04	0.58
1:B:277:VAL:HG23	4:B:1057:HOH:O	2.04	0.58
1:A:136:MET:HE2	1:A:142:ILE:HD11	1.85	0.58
1:A:290:LYS:HG3	4:A:1144:HOH:O	2.03	0.58
1:B:260:ASN:O	1:B:264:LEU:HG	2.05	0.57
1:B:449:VAL:HG23	1:B:449:VAL:O	2.04	0.57
1:A:89:SER:OG	1:A:92:LYS:HB3	2.05	0.56
1:A:612:ARG:HH11	1:A:612:ARG:HG3	1.69	0.56
1:A:70:TYR:HB3	1:A:75:VAL:HG22	1.87	0.56
1:A:425:TYR:OH	1:A:473:GLU:HG3	2.06	0.56
1:B:86:LYS:HG2	1:B:87:LYS:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:GLU:HG3	1:B:382:LYS:HZ3	1.70	0.56
1:B:125:LEU:HD13	1:B:127:TRP:N	2.21	0.56
1:A:28:LYS:N	1:A:28:LYS:CD	2.69	0.56
1:A:112:VAL:HG11	1:A:134:PRO:HB3	1.86	0.55
1:B:554:LYS:HG2	4:B:1196:HOH:O	2.06	0.55
1:A:219:LYS:HD2	1:A:219:LYS:H	1.71	0.55
1:A:277:VAL:HG23	4:A:1055:HOH:O	2.06	0.55
1:A:136:MET:CE	1:A:142:ILE:HD11	2.38	0.54
1:A:290:LYS:HB2	1:A:324:ILE:HD11	1.89	0.54
1:A:460:GLU:OE1	1:A:581:LYS:HE3	2.07	0.54
1:B:82:ASP:O	1:B:82:ASP:OD1	2.26	0.54
1:B:221:ASP:OD2	1:B:224:LEU:HB2	2.08	0.53
1:A:658:GLU:HG3	1:A:662:LYS:HD3	1.90	0.53
1:A:302:VAL:CG1	1:A:307:ASN:HA	2.39	0.53
1:A:122:MET:HG3	1:A:124:LYS:HZ1	1.71	0.53
1:B:484:LYS:NZ	1:B:484:LYS:HB2	2.22	0.53
1:A:614:ILE:CD1	1:A:634:LYS:HA	2.39	0.52
1:A:639:LYS:HD3	1:A:644:TYR:CE1	2.44	0.52
1:B:82:ASP:O	1:B:84:LYS:HG3	2.09	0.52
1:A:298:ARG:HD3	1:A:315:GLU:OE1	2.10	0.52
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.45	0.52
1:A:614:ILE:CD1	1:A:634:LYS:HG3	2.39	0.52
1:A:217:VAL:HG21	1:A:224:LEU:HD13	1.92	0.51
1:B:87:LYS:HD3	1:B:87:LYS:H	1.72	0.51
1:B:86:LYS:CG	1:B:87:LYS:N	2.73	0.51
1:B:424:SER:OG	1:B:452:ASN:HB3	2.10	0.51
1:A:64:GLU:O	1:A:67:ILE:HB	2.10	0.51
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.41	0.50
1:B:386:ASP:HB3	1:B:390:PRO:HD3	1.92	0.50
1:B:516:ASP:HA	1:B:519:TYR:CE2	2.46	0.50
1:A:70:TYR:CB	1:A:75:VAL:HG21	2.40	0.50
1:A:180:LYS:HA	1:A:183:TYR:CE1	2.47	0.50
1:A:268:GLU:HG3	1:A:269:TYR:CE1	2.47	0.50
1:A:598:SER:HB3	1:A:617:PHE:CE1	2.47	0.50
1:B:565:LYS:HE2	4:B:1262:HOH:O	2.11	0.50
1:B:125:LEU:CD1	1:B:127:TRP:HA	2.42	0.49
1:B:658:GLU:HG3	1:B:662:LYS:HE2	1.94	0.49
1:A:60:VAL:HG13	1:A:64:GLU:OE1	2.12	0.49
1:B:587:ILE:O	1:B:587:ILE:HG12	2.12	0.49
1:B:390:PRO:HD2	4:B:1085:HOH:O	2.10	0.49
1:A:189:GLU:HG2	1:A:227:PHE:CZ	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:HB	1:A:136:MET:HE3	1.94	0.49
1:A:220:MET:SD	1:A:224:LEU:HD23	2.52	0.49
1:A:262:GLU:H	1:A:262:GLU:CD	2.13	0.49
1:B:192:ILE:HD12	1:B:196:TYR:HD2	1.78	0.49
1:B:378:GLU:HG3	1:B:382:LYS:HZ1	1.78	0.49
1:A:98:GLN:NE2	1:A:109:ASP:OD2	2.42	0.49
1:A:180:LYS:HA	1:A:183:TYR:CD1	2.48	0.48
1:A:536:SER:HA	1:A:628:MET:CE	2.41	0.48
1:B:86:LYS:CG	1:B:87:LYS:H	2.27	0.48
1:B:289:LYS:NZ	1:B:289:LYS:HB2	2.28	0.48
1:B:194:GLU:O	1:B:198:LYS:HG3	2.14	0.48
1:A:261:SER:HB2	1:A:262:GLU:OE1	2.14	0.48
1:A:277:VAL:HG23	1:A:277:VAL:O	2.14	0.48
1:A:352:PRO:HA	1:A:536:SER:HB2	1.95	0.48
1:B:369:TYR:HB2	1:B:370:PRO:HD3	1.96	0.48
1:B:191:SER:HB3	1:B:376:SER:HB3	1.96	0.47
1:B:604:LYS:HE3	1:B:604:LYS:HA	1.96	0.47
1:B:665:ASP:HB3	1:B:668:GLU:HB2	1.97	0.47
1:B:668:GLU:OXT	1:B:668:GLU:HG2	2.15	0.47
1:A:222:GLU:O	1:A:226:ASP:HB2	2.14	0.47
1:A:331:LYS:NZ	1:A:668:GLU:OXT	2.47	0.47
1:B:364:PRO:HG2	1:B:388:LYS:HD3	1.96	0.47
1:B:370:PRO:HB2	1:B:375:MET:HE2	1.97	0.47
1:A:166:GLY:HA3	1:A:242:ASN:HB2	1.97	0.46
1:A:471:ALA:HB1	1:A:514:LEU:HD22	1.97	0.46
1:B:138:LYS:H	1:B:138:LYS:CE	2.26	0.46
1:A:182:ASP:N	1:A:182:ASP:OD1	2.49	0.46
1:B:119:GLU:O	1:B:120:ASP:C	2.53	0.46
1:B:220:MET:HA	1:B:220:MET:HE2	1.97	0.46
1:A:173:ILE:CD1	1:A:214:LEU:HD11	2.45	0.46
1:B:290:LYS:HB2	1:B:324:ILE:HD11	1.98	0.46
1:A:187:ALA:HB1	1:A:192:ILE:O	2.16	0.46
1:A:197:ILE:O	1:A:201:MET:HG2	2.16	0.46
1:A:93:LYS:HE3	1:A:123:TRP:CZ2	2.51	0.45
1:B:387:LYS:HA	1:B:387:LYS:CE	2.41	0.45
1:A:167:THR:CG2	1:A:237:GLU:HG3	2.47	0.45
1:B:510:ASN:CB	1:B:513:LEU:HD12	2.40	0.45
1:B:407:ILE:O	1:B:411:MET:HG3	2.15	0.45
1:B:302:VAL:CG1	1:B:307:ASN:HA	2.47	0.45
1:A:262:GLU:OE1	1:A:262:GLU:N	2.40	0.45
1:A:614:ILE:HD12	1:A:634:LYS:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLU:HG2	4:B:1188:HOH:O	2.16	0.45
1:A:297:TYR:CE1	1:A:316:LYS:HD3	2.51	0.45
1:B:363:THR:HA	1:B:364:PRO:C	2.37	0.45
1:A:100:LYS:HA	1:A:108:ILE:O	2.17	0.45
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.52	0.44
1:B:54:LYS:HB3	1:B:54:LYS:HE2	1.73	0.44
1:A:39:ASP:O	1:A:40:LYS:HB2	2.17	0.44
1:B:245:LEU:HD13	1:B:334:LYS:HG3	1.99	0.44
1:A:557:VAL:HG11	1:A:560:LYS:CG	2.45	0.44
1:B:267:LYS:H	1:B:267:LYS:CD	2.08	0.44
1:B:125:LEU:HD11	1:B:127:TRP:HA	2.00	0.44
1:B:658:GLU:CD	1:B:662:LYS:HG2	2.38	0.44
1:A:112:VAL:CG1	1:A:134:PRO:CB	2.94	0.43
1:A:490:GLU:OE1	1:A:559:LYS:NZ	2.39	0.43
1:B:267:LYS:HG2	1:B:268:GLU:HG2	1.99	0.43
1:A:138:LYS:H	1:A:138:LYS:CE	2.30	0.43
1:A:154:ILE:HB	1:A:163:ALA:HB3	2.00	0.43
1:A:559:LYS:HB3	1:A:562:ILE:HD11	2.00	0.43
1:A:363:THR:HA	1:A:364:PRO:C	2.38	0.43
1:A:415:ASN:HD21	1:A:485:LYS:HE2	1.84	0.43
1:A:498:PHE:CE2	1:A:529:VAL:HG21	2.53	0.43
1:A:658:GLU:CG	1:A:662:LYS:HD3	2.49	0.43
1:A:99:TYR:HD1	1:A:112:VAL:HG11	1.84	0.43
1:A:298:ARG:HG2	1:A:300:THR:HG23	2.01	0.43
1:A:70:TYR:CG	1:A:75:VAL:HG21	2.54	0.43
1:A:93:LYS:HG3	1:A:123:TRP:CH2	2.54	0.42
1:B:167:THR:CG2	1:B:237:GLU:HG3	2.47	0.42
1:A:112:VAL:HG12	1:A:134:PRO:CB	2.49	0.42
1:A:453:ILE:HG23	1:A:457:GLN:CG	2.49	0.42
1:A:645:ASN:HD22	1:A:645:ASN:H	1.67	0.42
1:B:51:TYR:O	1:B:54:LYS:HG2	2.20	0.42
1:B:430:LYS:HG3	1:B:448:VAL:CG2	2.49	0.42
1:A:74:GLY:O	1:A:76:LYS:HD3	2.19	0.42
1:A:50:SER:O	1:A:54:LYS:HG3	2.20	0.42
1:B:82:ASP:OD1	1:B:84:LYS:HD2	2.20	0.42
1:A:415:ASN:ND2	1:A:485:LYS:HE2	2.35	0.41
1:B:154:ILE:HB	1:B:163:ALA:HB3	2.02	0.41
1:A:138:LYS:HB3	1:A:138:LYS:HE3	1.86	0.41
1:A:435:ASP:HB2	1:A:436:LYS:HD3	2.02	0.41
1:A:112:VAL:HG12	1:A:134:PRO:HB3	2.01	0.41
1:A:502:GLN:O	1:A:502:GLN:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:OE2	1:A:222:GLU:HA	2.20	0.41
1:A:265:LYS:N	1:A:265:LYS:HD3	2.36	0.41
1:B:259:ILE:HG12	1:B:260:ASN:N	2.35	0.41
1:B:633:VAL:CG2	1:B:645:ASN:HD21	2.34	0.41
1:B:367:ASP:OD1	1:B:369:TYR:CD1	2.74	0.41
1:A:42:PHE:HB3	1:A:63:THR:HA	2.03	0.41
1:A:228:ALA:HA	1:A:233:LEU:HB2	2.02	0.41
1:B:424:SER:HG	1:B:452:ASN:HB3	1.84	0.41
1:B:327:THR:OG1	1:B:549:LEU:HA	2.22	0.40
1:A:663:LYS:HE2	4:A:1216:HOH:O	2.20	0.40
1:A:600:THR:HG21	1:A:641:MET:HB3	2.03	0.40
1:B:186:ILE:CD1	1:B:233:LEU:HD21	2.50	0.40
1:A:91:ASN:ND2	1:A:118:LYS:HB3	2.36	0.40
1:A:491:ASP:OD1	1:A:500:ASN:ND2	2.54	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	629/646 (97%)	612 (97%)	17 (3%)	0	100	100
1	B	615/646 (95%)	595 (97%)	20 (3%)	0	100	100
All	All	1244/1292 (96%)	1207 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	567/576 (98%)	546 (96%)	21 (4%)	34	19
1	B	557/576 (97%)	536 (96%)	21 (4%)	33	18
All	All	1124/1152 (98%)	1082 (96%)	42 (4%)	34	19

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	38	GLU
1	A	76	LYS
1	A	77	ASP
1	A	87	LYS
1	A	99	TYR
1	A	125	LEU
1	A	138	LYS
1	A	141	SER
1	A	156	ASP
1	A	182	ASP
1	A	204	ASN
1	A	219	LYS
1	A	252	LEU
1	A	352	PRO
1	A	391	LEU
1	A	419	LEU
1	A	436	LYS
1	A	513	LEU
1	A	514	LEU
1	A	554	LYS
1	B	54	LYS
1	B	87	LYS
1	B	99	TYR
1	B	102	LYS
1	B	112	VAL
1	B	120	ASP
1	B	122	MET
1	B	156	ASP
1	B	252	LEU
1	B	267	LYS
1	B	268	GLU
1	B	377	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	391	LEU
1	B	392	LEU
1	B	419	LEU
1	B	446	TYR
1	B	514	LEU
1	B	532	LEU
1	B	570	LEU
1	B	627	MET
1	B	662	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	81	GLN
1	A	91	ASN
1	A	113	GLN
1	A	115	ASN
1	A	203	GLN
1	A	207	GLN
1	A	266	GLN
1	A	415	ASN
1	A	645	ASN
1	B	32	ASN
1	B	81	GLN
1	B	111	ASN
1	B	377	ASN
1	B	433	GLN
1	B	632	ASN
1	B	645	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	635/646 (98%)	0.24	24 (3%)	40	35	17, 31, 51, 62	0
1	B	625/646 (96%)	0.29	46 (7%)	14	11	19, 31, 53, 62	0
All	All	1260/1292 (97%)	0.26	70 (5%)	24	19	17, 31, 52, 62	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	TYR	7.4
1	B	223	TYR	6.4
1	A	120	ASP	5.3
1	A	611	GLY	5.1
1	B	120	ASP	4.7
1	B	261	SER	4.3
1	B	204	ASN	4.2
1	A	222	GLU	4.1
1	B	267	LYS	3.9
1	B	603	LEU	3.9
1	B	28	LYS	3.8
1	B	51	TYR	3.7
1	A	204	ASN	3.5
1	A	226	ASP	3.4
1	B	122	MET	3.2
1	B	264	LEU	3.1
1	B	86	LYS	3.1
1	B	272	TYR	3.1
1	A	509	ASP	3.0
1	B	274	ASP	3.0
1	B	76	LYS	3.0
1	B	85	ILE	2.9
1	A	229	LYS	2.9
1	A	267	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	508	LEU	2.9
1	B	266	GLN	2.9
1	B	133	ILE	2.9
1	B	604	LYS	2.8
1	A	87	LYS	2.8
1	B	265	LYS	2.8
1	B	270	LYS	2.8
1	B	121	GLY	2.8
1	B	123	TRP	2.8
1	A	179	SER	2.7
1	B	271	GLY	2.7
1	B	273	LYS	2.7
1	A	360	LEU	2.6
1	B	262	GLU	2.6
1	A	184	LYS	2.6
1	B	87	LYS	2.5
1	B	222	GLU	2.5
1	A	185	ALA	2.5
1	A	612	ARG	2.5
1	A	274	ASP	2.5
1	B	252	LEU	2.4
1	B	532	LEU	2.4
1	B	205	TRP	2.4
1	B	94	ARG	2.4
1	B	269	TYR	2.3
1	B	29	GLU	2.3
1	A	272	TYR	2.3
1	B	268	GLU	2.3
1	A	505	ASN	2.3
1	A	84	LYS	2.3
1	B	662	LYS	2.2
1	B	131	VAL	2.2
1	B	531	ILE	2.2
1	B	513	LEU	2.2
1	A	122	MET	2.2
1	B	27	ASP	2.2
1	A	262	GLU	2.1
1	B	230	LYS	2.1
1	B	37	ILE	2.1
1	B	132	ILE	2.1
1	B	408	LEU	2.1
1	A	532	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	85	ILE	2.0
1	B	407	ILE	2.0
1	B	534	ILE	2.0
1	B	509	ASP	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CD	B	1006	1/1	0.93	0.08	57,57,57,57	0
3	CL	B	1010	1/1	0.97	0.06	29,29,29,29	0
3	CL	B	1008	1/1	0.98	0.06	27,27,27,27	0
3	CL	A	1009	1/1	0.98	0.10	27,27,27,27	0
3	CL	B	1011	1/1	0.98	0.09	27,27,27,27	0
2	CD	A	1004	1/1	0.99	0.05	50,50,50,50	0
2	CD	B	1007	1/1	0.99	0.04	31,31,31,31	0
2	CD	B	1003	1/1	0.99	0.09	27,27,27,27	0
2	CD	B	1001	1/1	1.00	0.08	25,25,25,25	0
2	CD	B	1002	1/1	1.00	0.08	24,24,24,24	0
2	CD	A	1005	1/1	1.00	0.07	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.