



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

PDB ID : 1MWS
Title : Structure of nitrocefin acyl-Penicillin binding protein 2a from methicillin resistant *Staphylococcus aureus* strain 27r at 2.00 Å resolution.
Authors : Lim, D.C.; Strynadka, N.C.J.
Deposited on : 2002-10-01
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

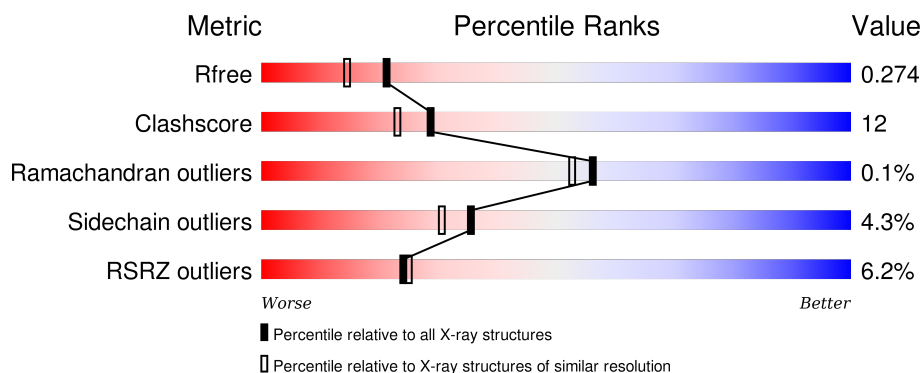
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	646	<div> <div>5%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	B	646	<div> <div>7%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10592 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 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5130	3235	861	1017	17			
1	B	629	Total	C	N	O	S	0	0	0
			5056	3192	850	999	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cd	0	0
			3	3		
2	A	5	Total	Cd	0	0
			5	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		

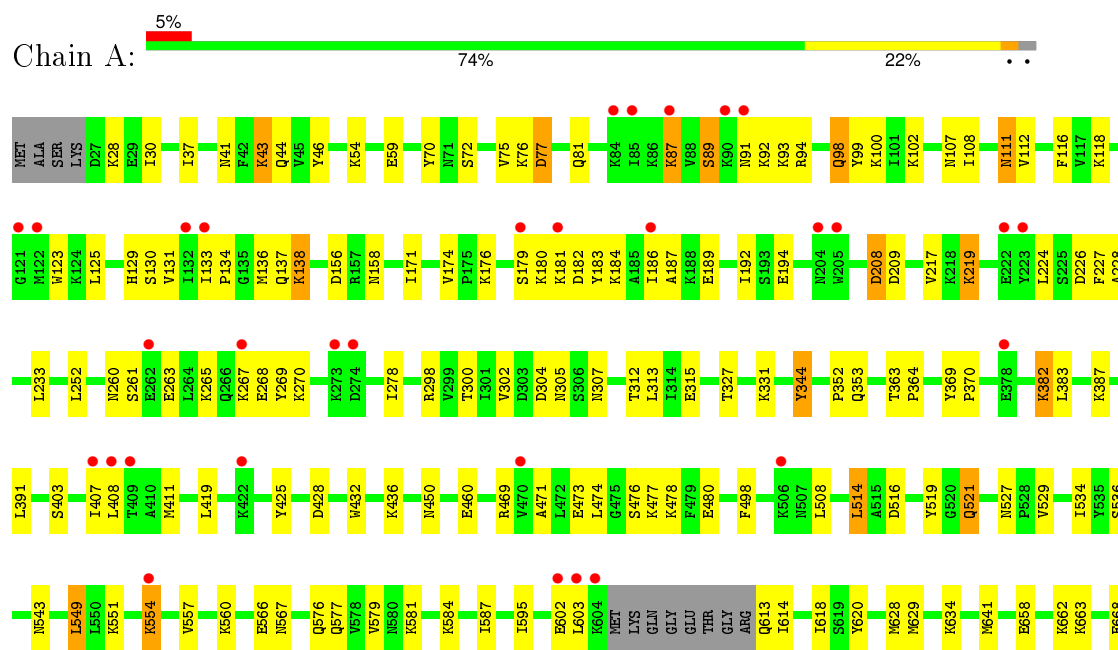
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	0
			205	205		
4	B	189	Total	O	0	0
			189	189		

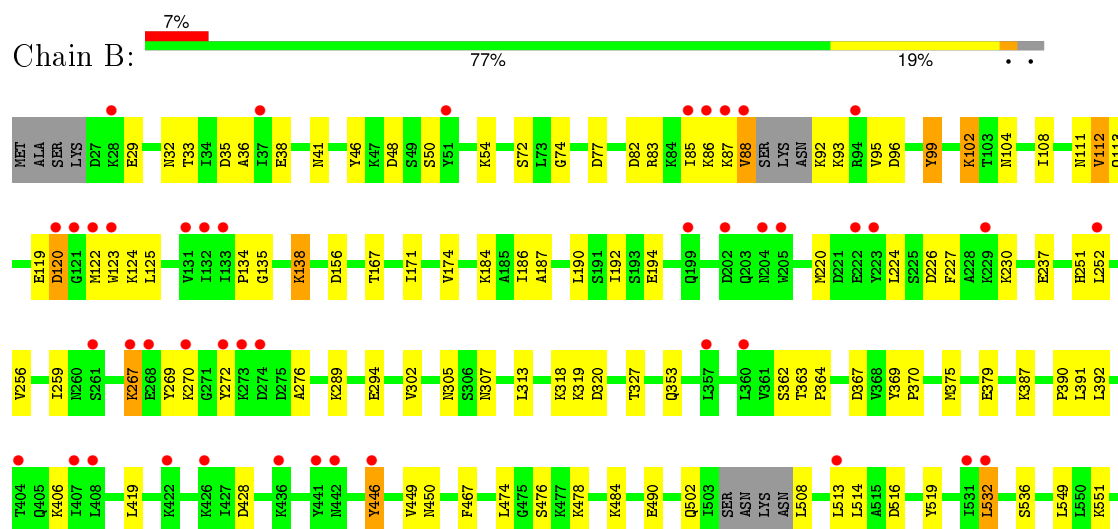
3 Residue-property plots

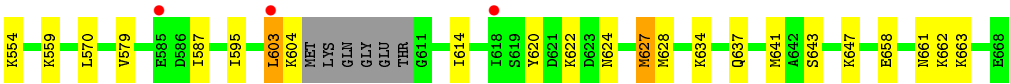
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 2a



• Molecule 1: penicillin-binding protein 2a





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.58Å 100.75Å 187.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 2.00 24.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (24.96-2.00) 96.6 (24.96-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.274 0.236 , 0.274	Depositor DCC
R_{free} test set	5059 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 100014 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10592	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NC1, CL, CD

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	0.46	0/5173	0.70	1/6955 (0.0%)
1	B	0.48	0/5132	0.70	1/6897 (0.0%)
All	All	0.47	0/10305	0.70	2/13852 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	VAL	N-CA-C	-5.50	96.14	111.00
1	A	174	VAL	N-CA-C	-5.09	97.27	111.00

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	5130	0	5105	137	0
1	B	5056	0	5049	106	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	205	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	189	0	0	3	0
All	All	10592	0	10154	234	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 12.

All (234) 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:138:LYS:H	1:B:138:LYS:HD2	1.13	1.07
1:A:138:LYS:H	1:A:138:LYS:HD2	1.38	0.87
1:B:226:ASP:O	1:B:230:LYS:HG2	1.75	0.85
1:B:387:LYS:HE2	1:B:387:LYS:HA	1.57	0.84
1:A:138:LYS:CD	1:A:138:LYS:H	1.89	0.84
1:B:184:LYS:HG2	1:B:194:GLU:OE1	1.79	0.82
1:A:87:LYS:H	1:A:87:LYS:HD3	1.42	0.82
1:B:604:LYS:HA	1:B:604:LYS:HE3	1.59	0.82
1:B:267:LYS:HA	1:B:270:LYS:HG3	1.59	0.81
1:B:138:LYS:H	1:B:138:LYS:CD	1.93	0.80
1:A:112:VAL:HG11	1:A:134:PRO:HB3	1.62	0.79
1:A:658:GLU:HG3	1:A:662:LYS:HD3	1.65	0.78
1:A:176:LYS:HG3	1:A:208:ASP:O	1.84	0.78
1:A:133:ILE:HB	1:A:136:MET:HE2	1.65	0.78
1:A:112:VAL:CG1	1:A:134:PRO:HB3	2.15	0.77
1:A:603:LEU:HD22	1:A:613:GLN:N	2.00	0.77
1:A:179:SER:OG	1:A:181:LYS:HB3	1.86	0.75
1:A:576:GLN:HG2	4:A:1154:HOH:O	1.87	0.75
1:A:480:GLU:HG3	1:A:508:LEU:HD12	1.69	0.74
1:A:176:LYS:HD2	1:B:113:GLN:NE2	2.02	0.73
1:A:602:GLU:HG2	1:A:613:GLN:HE22	1.54	0.72
1:B:86:LYS:HG2	1:B:87:LYS:H	1.54	0.72
1:B:220:MET:HE1	1:B:224:LEU:HD23	1.72	0.71
1:B:87:LYS:O	1:B:88:VAL:HG13	1.91	0.70
1:B:88:VAL:HG23	1:B:92:LYS:O	1.92	0.70
1:B:579:VAL:HG13	1:B:587:ILE:HG23	1.74	0.69
1:A:138:LYS:HE3	4:A:1151:HOH:O	1.91	0.69
1:B:138:LYS:HD2	1:B:138:LYS:N	1.98	0.69
1:A:187:ALA:HB1	1:A:192:ILE:O	1.93	0.69
1:B:29:GLU:OE1	1:B:123:TRP:HD1	1.77	0.66
1:A:176:LYS:HB2	1:A:176:LYS:NZ	2.11	0.65
1:A:516:ASP:HA	1:A:519:TYR:CE2	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:HB3	1:A:92:LYS:HB3	1.80	0.64
1:B:99:TYR:HB2	1:B:112:VAL:HG22	1.79	0.64
1:A:138:LYS:N	1:A:138:LYS:HD2	2.11	0.64
1:A:268:GLU:HG3	1:A:269:TYR:CD1	2.33	0.63
1:B:627:MET:O	1:B:627:MET:HG3	1.97	0.63
1:A:403:NC1:O31	1:A:403:NC1:H4	1.98	0.63
1:A:658:GLU:CG	1:A:662:LYS:HD3	2.29	0.63
1:A:554:LYS:HD3	1:A:554:LYS:H	1.63	0.62
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.82	0.61
1:B:186:ILE:HA	1:B:227:PHE:HZ	1.65	0.61
1:B:449:VAL:HG23	1:B:449:VAL:O	2.01	0.61
1:A:91:ASN:ND2	1:A:118:LYS:HB3	2.14	0.61
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.30	0.61
1:B:614:ILE:HD11	1:B:634:LYS:HG3	1.84	0.60
1:B:318:LYS:HE3	1:B:320:ASP:OD2	2.02	0.60
1:B:251:HIS:HE1	1:B:390:PRO:O	1.84	0.60
1:B:171:ILE:HD11	1:B:220:MET:HE3	1.84	0.59
1:B:536:SER:HA	1:B:628:MET:CE	2.32	0.59
1:A:46:TYR:O	1:A:54:LYS:HD3	2.02	0.58
1:A:112:VAL:CG1	1:A:134:PRO:CB	2.81	0.58
1:A:180:LYS:HA	1:A:183:TYR:CE1	2.38	0.58
1:A:432:TRP:CH2	1:A:469:ARG:HD3	2.39	0.57
1:B:108:ILE:HD13	1:B:313:LEU:HD13	1.87	0.57
1:A:383:LEU:HB3	1:A:391:LEU:HD11	1.85	0.57
1:B:38:GLU:OE1	1:B:83:ARG:NH2	2.38	0.57
1:A:602:GLU:HG2	1:A:613:GLN:NE2	2.19	0.57
1:B:85:ILE:HG12	1:B:95:VAL:HG22	1.87	0.57
1:A:557:VAL:HG11	1:A:560:LYS:HG2	1.85	0.57
1:A:87:LYS:H	1:A:87:LYS:CD	2.15	0.57
1:B:614:ILE:HD13	1:B:634:LYS:HA	1.86	0.57
1:A:184:LYS:HB3	1:A:194:GLU:CD	2.25	0.56
1:A:37:ILE:HD13	1:A:131:VAL:HG13	1.86	0.56
1:A:300:THR:HG22	1:A:312:THR:HA	1.87	0.56
1:A:179:SER:C	1:A:181:LYS:H	2.08	0.56
1:B:96:ASP:OD1	1:B:113:GLN:HG2	2.06	0.56
1:A:352:PRO:HA	1:A:536:SER:HB2	1.87	0.56
1:A:81:GLN:NE2	1:A:100:LYS:NZ	2.55	0.55
1:A:137:GLN:HB3	1:A:138:LYS:HD2	1.88	0.55
1:B:294:GLU:OE2	1:B:319:LYS:NZ	2.40	0.55
1:A:176:LYS:HD2	1:B:113:GLN:HE21	1.72	0.54
1:B:220:MET:CE	1:B:224:LEU:HD23	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:HB3	1:A:75:VAL:CG2	2.37	0.54
1:A:93:LYS:HG3	1:A:123:TRP:CH2	2.42	0.54
1:B:220:MET:HA	1:B:220:MET:HE2	1.89	0.54
1:B:267:LYS:H	1:B:267:LYS:HD3	1.73	0.54
1:A:108:ILE:HD13	1:A:313:LEU:HD13	1.90	0.53
1:B:256:VAL:HG22	4:B:1161:HOH:O	2.07	0.53
1:B:86:LYS:C	1:B:87:LYS:HG2	2.28	0.53
1:A:77:ASP:HB2	1:A:102:LYS:HE2	1.89	0.53
1:B:93:LYS:HG3	1:B:123:TRP:CZ2	2.44	0.53
1:A:261:SER:O	1:A:265:LYS:HG2	2.08	0.53
1:B:86:LYS:NZ	1:B:86:LYS:HB2	2.23	0.53
1:A:577:GLN:NE2	1:A:581:LYS:HE2	2.24	0.53
1:B:87:LYS:C	1:B:88:VAL:HG22	2.29	0.53
1:B:595:ILE:HD11	1:B:620:TYR:CZ	2.44	0.53
1:A:460:GLU:OE1	1:A:581:LYS:HE3	2.09	0.53
1:B:614:ILE:CD1	1:B:634:LYS:HA	2.38	0.52
1:A:432:TRP:CZ2	1:A:469:ARG:HD3	2.44	0.52
1:B:476:SER:HB3	1:B:508:LEU:O	2.10	0.52
1:A:387:LYS:NZ	1:A:387:LYS:HB3	2.25	0.52
1:B:48:ASP:O	1:B:124:LYS:HD2	2.10	0.51
1:B:86:LYS:HZ2	1:B:86:LYS:HB2	1.75	0.51
1:A:138:LYS:H	1:A:138:LYS:CE	2.24	0.51
1:B:50:SER:O	1:B:54:LYS:HG3	2.11	0.51
1:B:406:LYS:HG2	1:B:467:PHE:CD1	2.46	0.51
1:B:267:LYS:HA	1:B:270:LYS:CG	2.36	0.50
1:A:603:LEU:HD23	1:A:603:LEU:N	2.26	0.50
1:A:407:ILE:O	1:A:411:MET:HG3	2.11	0.50
1:B:502:GLN:NE2	1:B:502:GLN:HA	2.26	0.50
1:A:91:ASN:HD22	1:A:118:LYS:HB3	1.74	0.50
1:B:87:LYS:HD2	1:B:93:LYS:HG2	1.93	0.50
1:A:551:LYS:HB2	4:A:1121:HOH:O	2.12	0.49
1:B:637:GLN:HA	1:B:641:MET:SD	2.52	0.49
1:B:251:HIS:CD2	1:B:362:SER:HB3	2.47	0.49
1:A:305:ASN:O	1:B:72:SER:HB2	2.12	0.49
1:A:179:SER:C	1:A:181:LYS:N	2.66	0.49
1:A:603:LEU:HD23	1:A:603:LEU:H	1.78	0.49
1:B:643:SER:O	1:B:647:LYS:HG3	2.12	0.48
1:A:344:TYR:CD1	1:A:344:TYR:C	2.87	0.48
1:B:41:ASN:HB3	4:B:1030:HOH:O	2.12	0.48
1:A:77:ASP:HB2	1:A:102:LYS:CE	2.44	0.48
1:A:584:LYS:NZ	4:A:1180:HOH:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:N	1:A:111:ASN:OD1	2.47	0.48
1:A:382:LYS:C	1:A:382:LYS:HD3	2.34	0.47
1:A:527:ASN:OD1	1:A:529:VAL:HB	2.13	0.47
1:A:93:LYS:HE2	1:A:123:TRP:CE2	2.49	0.47
1:A:30:ILE:HD11	1:A:93:LYS:HE3	1.96	0.47
1:B:604:LYS:CE	1:B:604:LYS:HA	2.39	0.47
1:B:46:TYR:O	1:B:54:LYS:HD3	2.15	0.47
1:B:624:ASN:CG	1:B:663:LYS:HE3	2.35	0.47
1:B:190:LEU:O	1:B:192:ILE:HG23	2.15	0.47
1:A:543:ASN:OD1	1:A:560:LYS:HA	2.15	0.47
1:A:298:ARG:HD3	1:A:315:GLU:OE1	2.15	0.47
1:A:269:TYR:CE2	1:A:278:ILE:HD12	2.50	0.47
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.49	0.47
1:A:217:VAL:HG21	1:A:224:LEU:HD13	1.96	0.46
1:B:474:LEU:O	1:B:478:LYS:HB2	2.15	0.46
1:B:220:MET:HE1	1:B:224:LEU:CD2	2.44	0.46
1:A:30:ILE:HG23	1:A:116:PHE:CE1	2.50	0.46
1:B:513:LEU:HD13	1:B:513:LEU:O	2.15	0.46
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.50	0.46
1:A:298:ARG:HG2	1:A:300:THR:HG23	1.97	0.46
1:B:187:ALA:HB1	1:B:192:ILE:O	2.16	0.46
1:B:302:VAL:CG1	1:B:307:ASN:HA	2.46	0.46
1:A:471:ALA:HB1	1:A:514:LEU:CD2	2.46	0.46
1:A:176:LYS:HD2	1:B:113:GLN:HE22	1.79	0.46
1:A:182:ASP:O	1:A:186:ILE:HG13	2.15	0.46
1:A:498:PHE:CE2	1:A:529:VAL:HG21	2.51	0.45
1:A:77:ASP:CB	1:A:102:LYS:HE2	2.46	0.45
1:B:167:THR:HG23	1:B:237:GLU:HG3	1.97	0.45
1:B:86:LYS:CB	1:B:86:LYS:NZ	2.78	0.45
1:A:72:SER:HB2	1:B:305:ASN:O	2.16	0.45
1:A:41:ASN:ND2	1:A:44:GLN:HB2	2.30	0.45
1:A:363:THR:HA	1:A:364:PRO:C	2.36	0.45
1:B:428:ASP:HA	1:B:450:ASN:OD1	2.17	0.45
1:B:86:LYS:HG2	1:B:87:LYS:N	2.27	0.45
1:B:603:LEU:HD11	1:B:634:LYS:HE2	1.97	0.45
1:B:48:ASP:C	1:B:124:LYS:HD2	2.37	0.45
1:A:158:ASN:OD1	1:B:551:LYS:NZ	2.40	0.45
1:B:119:GLU:O	1:B:120:ASP:C	2.55	0.45
1:B:35:ASP:OD1	1:B:83:ARG:NH1	2.38	0.45
1:A:70:TYR:HB3	1:A:75:VAL:HG22	1.99	0.45
1:A:72:SER:HB3	1:B:305:ASN:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:HA	1:A:98:GLN:OE1	2.16	0.45
1:A:613:GLN:N	4:A:1088:HOH:O	2.50	0.45
1:A:179:SER:HB3	1:A:182:ASP:OD1	2.17	0.45
1:B:86:LYS:O	1:B:87:LYS:HG2	2.16	0.45
1:B:82:ASP:O	1:B:82:ASP:OD1	2.34	0.45
1:A:577:GLN:HE21	1:A:581:LYS:HE2	1.82	0.44
1:A:521:GLN:CA	1:A:521:GLN:HE21	2.29	0.44
1:A:436:LYS:HG2	1:A:436:LYS:H	1.49	0.44
1:A:70:TYR:HB3	1:A:75:VAL:HG21	1.98	0.44
1:B:327:THR:OG1	1:B:549:LEU:HA	2.18	0.44
1:B:391:LEU:HB2	4:B:1066:HOH:O	2.17	0.44
1:A:369:TYR:HB2	1:A:370:PRO:HD3	1.99	0.44
1:B:138:LYS:CD	1:B:138:LYS:N	2.69	0.44
1:A:327:THR:OG1	1:A:549:LEU:HA	2.16	0.44
1:A:603:LEU:H	1:A:603:LEU:CD2	2.31	0.44
1:B:484:LYS:HB2	1:B:484:LYS:HE3	1.62	0.44
1:B:93:LYS:HG3	1:B:123:TRP:CH2	2.52	0.44
1:A:260:ASN:O	1:A:263:GLU:HB2	2.18	0.44
1:A:614:ILE:CD1	1:A:634:LYS:HG3	2.48	0.43
1:A:180:LYS:HA	1:A:183:TYR:CD1	2.54	0.43
1:A:81:GLN:NE2	1:A:100:LYS:HZ2	2.14	0.43
1:A:566:GLU:HG3	1:A:567:ASN:N	2.33	0.43
1:B:353:GLN:N	1:B:353:GLN:OE1	2.45	0.43
1:A:425:TYR:OH	1:A:473:GLU:HG3	2.18	0.43
1:A:129:HIS:HB3	1:A:136:MET:HG2	1.99	0.43
1:B:112:VAL:HG13	1:B:134:PRO:HB3	1.99	0.43
1:B:251:HIS:CE1	1:B:390:PRO:O	2.70	0.43
1:A:428:ASP:HA	1:A:450:ASN:OD1	2.18	0.43
1:B:516:ASP:HA	1:B:519:TYR:CE2	2.53	0.43
1:B:269:TYR:HA	1:B:272:TYR:CD1	2.54	0.43
1:A:112:VAL:HG12	1:A:134:PRO:CB	2.48	0.43
1:B:369:TYR:HB2	1:B:370:PRO:HD3	2.01	0.43
1:B:33:THR:O	1:B:36:ALA:HB3	2.19	0.43
1:B:363:THR:HA	1:B:364:PRO:C	2.39	0.43
1:B:112:VAL:HG13	1:B:134:PRO:CB	2.50	0.42
1:A:270:LYS:HB3	1:A:270:LYS:HE2	1.90	0.42
1:B:490:GLU:OE1	1:B:559:LYS:NZ	2.47	0.42
1:A:474:LEU:O	1:A:478:LYS:HB2	2.19	0.42
1:A:620:TYR:HB3	1:A:628:MET:HG2	2.01	0.42
1:B:614:ILE:CD1	1:B:634:LYS:HG3	2.50	0.42
1:A:668:GLU:OE2	1:B:554:LYS:HD3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:MET:HG2	1:B:379:GLU:HB2	2.01	0.42
1:A:102:LYS:HA	1:A:107:ASN:OD1	2.20	0.42
1:A:614:ILE:HD13	1:A:634:LYS:HA	2.01	0.42
1:A:521:GLN:HA	1:A:521:GLN:NE2	2.35	0.42
1:A:184:LYS:HB3	1:A:194:GLU:OE2	2.19	0.42
1:A:100:LYS:HA	1:A:108:ILE:O	2.19	0.42
1:A:81:GLN:HE22	1:A:100:LYS:HZ2	1.68	0.42
1:A:304:ASP:O	1:A:305:ASN:HB2	2.20	0.42
1:B:289:LYS:HB2	1:B:289:LYS:NZ	2.35	0.42
1:A:228:ALA:HA	1:A:233:LEU:HB2	2.02	0.41
1:A:28:LYS:HD3	4:A:1183:HOH:O	2.19	0.41
1:A:536:SER:HA	1:A:628:MET:CE	2.50	0.41
1:B:259:ILE:HG22	1:B:276:ALA:O	2.21	0.41
1:A:352:PRO:HD2	1:A:353:GLN:OE1	2.20	0.41
1:A:81:GLN:NE2	1:A:100:LYS:HZ1	2.18	0.41
1:A:658:GLU:CD	1:A:662:LYS:HD3	2.41	0.41
1:A:267:LYS:O	1:A:270:LYS:HG3	2.21	0.41
1:A:383:LEU:HB3	1:A:391:LEU:CD1	2.49	0.41
1:A:93:LYS:HE2	1:A:123:TRP:CZ2	2.55	0.41
1:A:331:LYS:HE3	1:A:668:GLU:OXT	2.20	0.41
1:A:219:LYS:HD2	1:A:219:LYS:H	1.86	0.41
1:B:74:GLY:HA3	1:B:104:ASN:ND2	2.36	0.41
1:A:476:SER:O	1:A:477:LYS:C	2.58	0.41
1:B:77:ASP:HB3	1:B:102:LYS:HD3	2.02	0.41
1:A:209:ASP:OD1	1:B:135:GLY:HA2	2.21	0.41
1:A:176:LYS:HB2	1:A:176:LYS:HZ1	1.84	0.41
1:A:268:GLU:HG3	1:A:269:TYR:CE1	2.56	0.41
1:A:403:NC1:C25	1:A:641:MET:HG3	2.51	0.41
1:A:302:VAL:CG1	1:A:307:ASN:HA	2.50	0.41
1:A:579:VAL:HG13	1:A:587:ILE:HG23	2.03	0.40
1:A:171:ILE:HD11	1:A:217:VAL:HG11	2.03	0.40
1:B:406:LYS:NZ	1:B:446:TYR:OH	2.54	0.40
1:B:551:LYS:HD2	1:B:551:LYS:O	2.22	0.40
1:B:658:GLU:HB2	1:B:661:ASN:HB2	2.04	0.40
1:B:587:ILE:HG12	1:B:587:ILE:O	2.21	0.40
1:B:532:LEU:HD21	1:B:628:MET:HB3	2.03	0.40
1:A:618:ILE:HA	1:A:629:MET:O	2.22	0.40
1:A:43:LYS:HE2	1:A:59:GLU:OE2	2.22	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	629/646 (97%)	607 (96%)	22 (4%)	0	100	100
1	B	620/646 (96%)	596 (96%)	23 (4%)	1 (0%)	52	48
All	All	1249/1292 (97%)	1203 (96%)	45 (4%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	MET

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	566/575 (98%)	541 (96%)	25 (4%)	35	30
1	B	560/575 (97%)	537 (96%)	23 (4%)	37	32
All	All	1126/1150 (98%)	1078 (96%)	48 (4%)	35	30

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	76	LYS
1	A	77	ASP
1	A	87	LYS
1	A	89	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	94	ARG
1	A	98	GLN
1	A	99	TYR
1	A	111	ASN
1	A	125	LEU
1	A	130	SER
1	A	138	LYS
1	A	156	ASP
1	A	208	ASP
1	A	219	LYS
1	A	226	ASP
1	A	252	LEU
1	A	344	TYR
1	A	382	LYS
1	A	419	LEU
1	A	514	LEU
1	A	521	GLN
1	A	549	LEU
1	A	554	LYS
1	A	663	LYS
1	B	32	ASN
1	B	88	VAL
1	B	99	TYR
1	B	102	LYS
1	B	111	ASN
1	B	112	VAL
1	B	120	ASP
1	B	125	LEU
1	B	138	LYS
1	B	156	ASP
1	B	252	LEU
1	B	267	LYS
1	B	367	ASP
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	603	LEU
1	B	622	LYS
1	B	627	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	662	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	41	ASN
1	A	81	GLN
1	A	91	ASN
1	A	177	ASN
1	A	207	GLN
1	A	266	GLN
1	A	457	GLN
1	A	521	GLN
1	A	540	ASN
1	A	577	GLN
1	A	593	ASN
1	A	613	GLN
1	A	632	ASN
1	A	645	ASN
1	B	32	ASN
1	B	41	ASN
1	B	44	GLN
1	B	199	GLN
1	B	251	HIS
1	B	305	ASN
1	B	351	HIS
1	B	433	GLN
1	B	502	GLN
1	B	645	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	NC1	A	403	1	31,43,44	2.83	8 (25%)	30,59,61	1.72	6 (20%)
1	NC1	B	403	1	4,5,44	0.74	0	2,5,61	1.67	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NC1	A	403	1	-	0/27/53/55	0/2/3/3
1	NC1	B	403	1	-	0/2/4/55	0/0/0/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	NC1	OG-C7	2.21	1.38	1.33
1	A	403	NC1	C9-N10	2.26	1.50	1.45
1	A	403	NC1	C26-C25	4.60	1.48	1.39
1	A	403	NC1	C29-C24	4.75	1.49	1.41
1	A	403	NC1	C28-C27	5.08	1.49	1.38
1	A	403	NC1	C11-N10	5.85	1.45	1.34
1	A	403	NC1	O32-N30	7.09	1.36	1.22
1	A	403	NC1	O35-N33	7.53	1.37	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	NC1	C26-C25-C24	-3.46	119.02	122.98
1	A	403	NC1	C17-C16-S15	-3.38	109.49	113.23
1	A	403	NC1	C24-C23-C22	-2.73	121.44	126.87
1	A	403	NC1	CB-OG-C7	-2.51	111.52	116.94
1	B	403	NC1	O-C-CA	-2.34	119.39	125.49
1	A	403	NC1	O-C-CA	-2.11	119.99	125.49
1	A	403	NC1	C6-S1-C2	4.75	103.52	94.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	403	NC1	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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, 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	633/646 (97%)	0.33	31 (4%) 33 35	19, 34, 56, 75	0
1	B	628/646 (97%)	0.42	47 (7%) 17 18	22, 35, 60, 72	0
All	All	1261/1292 (97%)	0.38	78 (6%) 24 25	19, 35, 58, 75	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	TYR	5.8
1	B	267	LYS	5.3
1	A	204	ASN	5.0
1	A	121	GLY	4.9
1	A	223	TYR	4.8
1	B	261	SER	4.6
1	A	604	LYS	4.6
1	B	204	ASN	4.4
1	B	28	LYS	4.1
1	A	90	LYS	4.0
1	B	603	LEU	3.7
1	B	120	ASP	3.6
1	B	121	GLY	3.6
1	A	222	GLU	3.6
1	B	131	VAL	3.5
1	B	51	TYR	3.5
1	A	603	LEU	3.4
1	A	122	MET	3.4
1	A	181	LYS	3.3
1	A	91	ASN	3.2
1	A	205	TRP	3.2
1	A	407	ILE	3.0
1	B	532	LEU	3.0
1	A	409	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	88	VAL	2.9
1	B	222	GLU	2.9
1	B	618	ILE	2.8
1	B	133	ILE	2.8
1	B	441	TYR	2.7
1	B	407	ILE	2.7
1	A	274	ASP	2.7
1	B	123	TRP	2.7
1	B	270	LYS	2.7
1	B	86	LYS	2.6
1	A	378	GLU	2.6
1	B	268	GLU	2.6
1	B	94	ARG	2.6
1	A	262	GLU	2.5
1	B	85	ILE	2.5
1	A	85	ILE	2.5
1	B	132	ILE	2.5
1	B	404	THR	2.5
1	A	506	LYS	2.5
1	B	274	ASP	2.5
1	A	267	LYS	2.4
1	B	360	LEU	2.4
1	B	446	TYR	2.4
1	A	554	LYS	2.4
1	A	133	ILE	2.4
1	A	87	LYS	2.4
1	B	205	TRP	2.4
1	B	272	TYR	2.4
1	B	408	LEU	2.4
1	B	229	LYS	2.4
1	A	186	ILE	2.3
1	B	531	ILE	2.3
1	B	202	ASP	2.3
1	B	252	LEU	2.3
1	B	273	LYS	2.3
1	B	422	LYS	2.3
1	A	470	VAL	2.2
1	B	513	LEU	2.2
1	A	273	LYS	2.2
1	B	436	LYS	2.2
1	B	442	ASN	2.2
1	A	408	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	SER	2.2
1	B	122	MET	2.1
1	B	426	LYS	2.1
1	A	422	LYS	2.1
1	B	585	GLU	2.1
1	B	87	LYS	2.1
1	A	84	LYS	2.1
1	B	37	ILE	2.1
1	B	357	LEU	2.1
1	A	602	GLU	2.0
1	A	132	ILE	2.0
1	B	199	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
1	NC1	B	403	6/42	0.96	0.18	-	26,27,29,32	0
1	NC1	A	403	41/42	0.87	0.17	-	25,39,57,61	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
3	CL	A	1010	1/1	0.99	0.12	0.44	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CD	A	1001	1/1	1.00	0.10	-0.71	26,26,26,26	0
2	CD	A	1005	1/1	1.00	0.09	-1.19	28,28,28,28	0
2	CD	B	1002	1/1	1.00	0.09	-1.23	26,26,26,26	0
2	CD	A	1003	1/1	1.00	0.10	-1.37	30,30,30,30	0
3	CL	B	1012	1/1	0.98	0.08	-1.60	31,31,31,31	0
3	CL	B	1009	1/1	0.99	0.06	-2.28	24,24,24,24	0
3	CL	A	1011	1/1	0.98	0.06	-2.36	31,31,31,31	0
2	CD	A	1004	1/1	0.99	0.03	-3.47	50,50,50,50	0
2	CD	B	1006	1/1	0.93	0.05	-	65,65,65,65	0
2	CD	A	1008	1/1	0.87	0.07	-	100,100,100,100	0
2	CD	B	1007	1/1	0.98	0.04	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.