



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 08:46 AM EDT

PDB ID : 1MWR
Title : Structure of SeMet Penicillin binding protein 2a from methicillin resistant Staphylococcus aureus strain 27r (trigonal form) at 2.45 Å resolution.
Authors : Lim, D.C.; Strynadka, N.C.J.
Deposited on : 2002-10-01
Resolution : 2.45 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

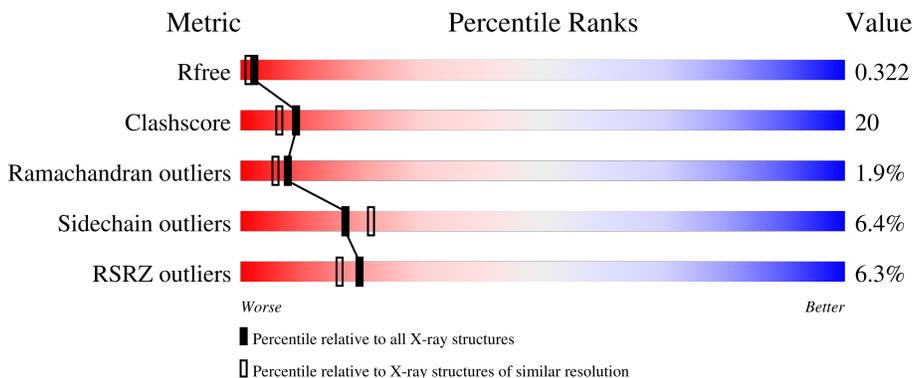
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	646	
1	B	646	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10089 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
			Total	C	N	O	Se			
1	A	624	5019	3169	842	993	15	0	0	0
1	B	629	5054	3188	850	1001	15	0	0	0

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

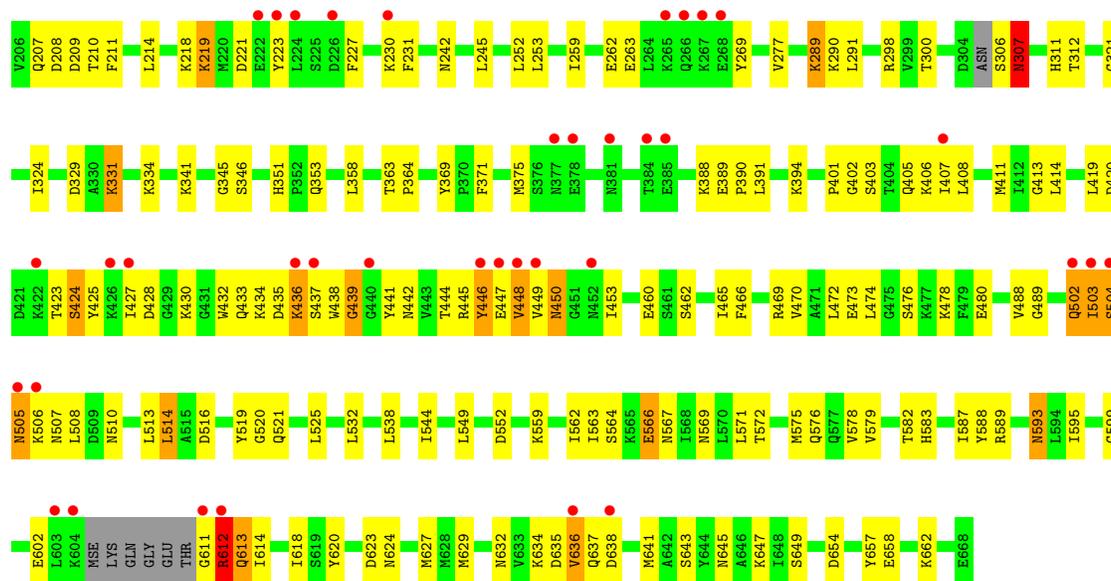
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		
2	B	2	Total	Cd	0	0
			2	2		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.06Å 141.06Å 146.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.89 – 2.45 24.88 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.9 (24.89-2.45) 98.1 (24.88-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.44Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.324 0.269 , 0.322	Depositor DCC
R_{free} test set	3086 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtrriage
Anisotropy	0.491	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10089	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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](#)

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	0.48	4/5086 (0.1%)	0.69	5/6812 (0.1%)
1	B	0.40	0/5122	0.65	0/6861
All	All	0.44	4/10208 (0.0%)	0.67	5/13673 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLU	CD-OE2	-10.92	1.13	1.25
1	A	145	GLU	CD-OE1	-7.97	1.16	1.25
1	A	145	GLU	CG-CD	7.46	1.63	1.51
1	A	145	GLU	CB-CG	6.55	1.64	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	GLU	OE1-CD-OE2	-13.63	106.94	123.30
1	A	145	GLU	CG-CD-OE1	6.66	131.63	118.30
1	A	454	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	454	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	A	144	ILE	N-CA-C	-5.05	97.37	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	5019	0	5005	201	1
1	B	5054	0	5039	207	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
4	A	6	0	0	0	2
4	B	2	0	0	0	0
All	All	10089	0	10044	403	2

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 20.

All (403) 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:HD3	1.18	1.08
1:A:222:GLU:HA	1:A:225:SER:HB3	1.30	1.08
1:A:138:LYS:H	1:A:138:LYS:HD2	1.18	1.04
1:A:145:GLU:OE1	3:A:1207:CL:CL	2.12	1.04
1:B:611:GLY:HA3	1:B:635:ASP:OD1	1.59	1.02
1:A:419:LEU:HD11	1:A:455:LEU:HD22	1.40	1.01
1:A:381:ASN:HA	1:A:384:THR:HG22	1.43	1.00
1:B:87:LYS:H	1:B:87:LYS:HD3	1.30	0.93
1:A:143:HIS:HB3	1:A:145:GLU:HG3	1.50	0.92
1:A:576:GLN:HE21	1:A:593:ASN:HD21	1.16	0.90
1:A:112:VAL:HG11	1:A:134:PRO:HB3	1.54	0.89
1:B:219:LYS:NZ	1:B:219:LYS:H	1.74	0.85
1:A:138:LYS:HD2	1:A:138:LYS:N	1.90	0.85
1:B:87:LYS:HD3	1:B:87:LYS:N	1.91	0.85
1:B:510:ASN:HB3	1:B:513:LEU:HB2	1.58	0.84
1:B:27:ASP:HB2	1:B:30:ILE:HB	1.60	0.83
1:B:602:GLU:HG2	1:B:613:GLN:HE22	1.45	0.82
1:B:300:THR:HG22	1:B:312:THR:HA	1.62	0.82
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.63	0.81
1:A:174:VAL:HB	1:A:177:ASN:HD22	1.47	0.80
1:B:602:GLU:HG2	1:B:613:GLN:NE2	1.97	0.80
1:A:87:LYS:HD3	1:A:87:LYS:N	1.96	0.79
1:A:562:ILE:HG13	1:A:563:ILE:HG22	1.65	0.79
1:B:506:LYS:HE2	1:B:507:ASN:ND2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:HB3	1:A:575:MSE:HE3	1.64	0.78
1:B:230:LYS:HE3	1:B:231:PHE:HE2	1.49	0.77
1:A:51:TYR:HA	1:A:54:LYS:HE2	1.66	0.77
1:B:436:LYS:HD3	1:B:436:LYS:H	1.49	0.77
1:B:419:LEU:HD13	1:B:420:ASP:N	2.00	0.76
1:B:138:LYS:H	1:B:138:LYS:HD2	1.49	0.76
1:B:43:LYS:O	1:B:47:LYS:HG2	1.86	0.76
1:A:146:ASN:ND2	1:A:147:LEU:N	2.33	0.76
1:A:186:ILE:HD13	1:A:233:LEU:HD21	1.67	0.75
1:B:506:LYS:HE2	1:B:507:ASN:HD21	1.51	0.75
1:A:407:ILE:HD12	1:A:575:MSE:HE2	1.68	0.75
1:B:433:GLN:HB3	1:B:442:ASN:ND2	2.02	0.74
1:A:571:LEU:O	1:A:575:MSE:HG3	1.88	0.74
1:A:146:ASN:HD22	1:A:147:LEU:H	1.34	0.74
1:B:94:ARG:HE	1:B:113:GLN:HG3	1.53	0.73
1:A:620:TYR:CD2	1:A:628:MSE:HE3	2.24	0.73
1:B:627:MSE:HE3	1:B:629:MSE:HB2	1.70	0.72
1:B:219:LYS:H	1:B:219:LYS:HZ2	1.36	0.72
1:B:572:THR:HA	1:B:575:MSE:HE2	1.72	0.72
1:A:538:LEU:HD11	1:A:575:MSE:HE1	1.72	0.72
1:A:220:MSE:HA	1:A:220:MSE:HE2	1.71	0.72
1:B:74:GLY:HA3	1:B:104:ASN:ND2	2.04	0.71
1:A:471:ALA:HB1	1:A:514:LEU:CD2	2.22	0.70
1:A:576:GLN:NE2	1:A:593:ASN:HD21	1.87	0.70
1:A:381:ASN:HA	1:A:384:THR:CG2	2.21	0.70
1:B:476:SER:O	1:B:480:GLU:HG3	1.92	0.69
1:A:477:LYS:NZ	1:A:477:LYS:HB3	2.07	0.69
1:B:112:VAL:HG22	1:B:134:PRO:HB3	1.73	0.69
1:A:449:VAL:HG23	1:A:453:ILE:CD1	2.23	0.68
1:A:176:LYS:HG3	1:A:177:ASN:H	1.58	0.68
1:A:217:VAL:HG21	1:A:220:MSE:HE3	1.75	0.68
1:A:384:THR:HG23	1:A:385:GLU:HG3	1.74	0.68
1:A:516:ASP:HA	1:A:519:TYR:CE2	2.28	0.68
1:B:466:PHE:O	1:B:470:VAL:HG23	1.94	0.68
1:A:146:ASN:HD22	1:A:147:LEU:N	1.92	0.68
1:A:260:ASN:OD1	1:A:263:GLU:HG3	1.94	0.68
1:A:180:LYS:NZ	1:A:180:LYS:HA	2.10	0.67
1:A:138:LYS:H	1:A:138:LYS:CD	2.01	0.67
1:B:245:LEU:HD13	1:B:334:LYS:HG3	1.76	0.67
1:B:436:LYS:HD3	1:B:436:LYS:N	2.08	0.67
1:B:99:TYR:HB2	1:B:112:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HB	1:B:163:ALA:HB3	1.76	0.67
1:A:173:ILE:HG12	1:A:178:VAL:HG21	1.76	0.66
1:B:614:ILE:HD11	1:B:634:LYS:HG3	1.77	0.66
1:B:69:ILE:HG23	1:B:142:ILE:HD12	1.78	0.66
1:A:112:VAL:CG1	1:A:134:PRO:HB3	2.24	0.66
1:A:495:ASP:OD1	1:A:548:HIS:HB2	1.96	0.66
1:B:435:ASP:HB2	1:B:436:LYS:HD3	1.77	0.66
1:B:488:VAL:O	1:B:503:ILE:HD11	1.95	0.66
1:A:39:ASP:O	1:A:40:LYS:HB2	1.95	0.65
1:A:137:GLN:HB3	1:A:138:LYS:HD2	1.78	0.65
1:A:307:ASN:ND2	1:B:144:ILE:H	1.93	0.65
1:A:579:VAL:HG13	1:A:587:ILE:HG23	1.78	0.65
1:A:174:VAL:HB	1:A:177:ASN:ND2	2.11	0.65
1:A:407:ILE:O	1:A:411:MSE:HG3	1.97	0.65
1:A:333:GLN:HE22	1:A:360:LEU:H	1.45	0.64
1:A:449:VAL:HG23	1:A:453:ILE:HD11	1.77	0.64
1:B:112:VAL:CG2	1:B:134:PRO:HB3	2.27	0.64
1:A:273:LYS:NZ	1:A:294:GLU:HG3	2.13	0.64
1:A:637:GLN:O	1:A:638:ASP:HB2	1.97	0.64
1:B:306:SER:O	1:B:307:ASN:HB2	1.97	0.64
1:A:28:LYS:HE2	1:A:32:ASN:OD1	1.97	0.64
1:A:79:ASN:HB3	1:A:81:GLN:NE2	2.13	0.64
1:B:129:HIS:HB2	1:B:137:GLN:HA	1.79	0.64
1:A:392:LEU:HD22	1:A:397:ILE:HD13	1.80	0.63
1:B:538:LEU:HD13	1:B:575:MSE:HE1	1.80	0.63
1:B:488:VAL:HG12	1:B:503:ILE:HG12	1.80	0.63
1:A:143:HIS:ND1	1:A:145:GLU:OE2	2.32	0.63
1:A:383:LEU:HB3	1:A:391:LEU:CD1	2.29	0.62
1:B:87:LYS:H	1:B:87:LYS:CD	2.06	0.62
1:B:593:ASN:HB2	1:B:623:ASP:OD2	1.99	0.62
1:A:280:LYS:O	1:A:281:LYS:HG3	1.99	0.62
1:A:580:ASN:O	1:A:584:LYS:HB3	2.00	0.61
1:B:629:MSE:HE1	1:B:649:SER:HA	1.81	0.61
1:B:427:ILE:O	1:B:450:ASN:HA	2.00	0.61
1:B:164:ASN:HD21	1:B:242:ASN:HD22	1.46	0.61
1:B:430:LYS:O	1:B:444:THR:HA	2.00	0.61
1:B:502:GLN:NE2	1:B:525:LEU:HD12	2.16	0.61
1:A:620:TYR:CE2	1:A:628:MSE:HE3	2.36	0.60
1:B:521:GLN:NE2	1:B:602:GLU:O	2.34	0.60
1:B:138:LYS:H	1:B:138:LYS:CD	2.05	0.60
1:A:62:MSE:HE3	1:A:127:TRP:CG	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:NZ	1:A:511:GLU:OE1	2.30	0.60
1:A:408:LEU:HD12	1:A:483:MSE:HE1	1.84	0.60
1:B:138:LYS:HD2	1:B:138:LYS:N	2.16	0.60
1:B:207:GLN:H	1:B:210:THR:HB	1.67	0.60
1:B:329:ASP:OD1	1:B:331:LYS:HG3	2.02	0.60
1:B:27:ASP:OD2	1:B:27:ASP:N	2.34	0.59
1:B:595:ILE:HD11	1:B:620:TYR:CZ	2.37	0.59
1:A:119:GLU:O	1:A:120:ASP:HB2	2.03	0.59
1:A:146:ASN:ND2	1:A:147:LEU:H	1.95	0.59
1:A:477:LYS:HB3	1:A:477:LYS:HZ2	1.67	0.59
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.31	0.59
1:B:430:LYS:HG2	1:B:448:VAL:CG1	2.32	0.59
1:B:230:LYS:HE3	1:B:231:PHE:CE2	2.35	0.59
1:B:504:SER:O	1:B:506:LYS:N	2.36	0.59
1:A:369:TYR:HD2	1:A:372:MSE:HE2	1.67	0.58
1:A:381:ASN:CA	1:A:384:THR:HG22	2.27	0.58
1:A:185:ALA:O	1:A:188:LYS:HG2	2.02	0.58
1:B:184:LYS:HG2	1:B:194:GLU:OE2	2.03	0.58
1:B:407:ILE:O	1:B:411:MSE:HG3	2.04	0.58
1:A:300:THR:HG22	1:A:312:THR:HA	1.86	0.58
1:B:27:ASP:OD1	1:B:30:ILE:HD12	2.03	0.57
1:A:265:LYS:O	1:A:266:GLN:O	2.21	0.57
1:B:158:ASN:O	1:B:159:ASN:HB2	2.05	0.57
1:A:221:ASP:OD2	1:A:223:TYR:HB2	2.04	0.57
1:B:566:GLU:CD	1:B:566:GLU:H	2.07	0.57
1:B:164:ASN:C	1:B:164:ASN:HD22	2.09	0.56
1:B:289:LYS:H	1:B:289:LYS:HD3	1.69	0.56
1:B:94:ARG:NE	1:B:113:GLN:HG3	2.20	0.56
1:B:346:SER:HB3	1:B:394:LYS:HB3	1.88	0.56
1:B:576:GLN:HA	1:B:595:ILE:HG22	1.88	0.56
1:B:69:ILE:CG2	1:B:142:ILE:HD12	2.36	0.56
1:A:158:ASN:O	1:A:159:ASN:HB2	2.06	0.56
1:A:180:LYS:HA	1:A:180:LYS:HZ3	1.71	0.56
1:B:306:SER:O	1:B:307:ASN:CB	2.53	0.55
1:A:189:GLU:HG2	1:A:227:PHE:CE2	2.42	0.55
1:B:413:GLY:HA2	1:B:474:LEU:HD21	1.89	0.55
1:B:187:ALA:HB1	1:B:192:ILE:O	2.07	0.55
1:A:98:GLN:OE1	1:A:111:ASN:HA	2.06	0.55
1:A:383:LEU:HB3	1:A:391:LEU:HD11	1.88	0.55
1:B:502:GLN:CG	1:B:525:LEU:HB2	2.37	0.55
1:B:614:ILE:HD13	1:B:634:LYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LYS:HG2	1:B:448:VAL:HG11	1.88	0.55
1:B:474:LEU:O	1:B:478:LYS:HD2	2.06	0.55
1:B:502:GLN:HE21	1:B:525:LEU:HD12	1.73	0.54
1:A:369:TYR:HB2	1:A:370:PRO:HD3	1.89	0.54
1:A:502:GLN:HG3	1:A:525:LEU:HB2	1.89	0.54
1:A:387:LYS:HA	1:A:387:LYS:HE3	1.89	0.54
1:B:189:GLU:HG2	1:B:227:PHE:CZ	2.42	0.54
1:B:427:ILE:HD12	1:B:453:ILE:HG13	1.88	0.54
1:B:657:TYR:O	1:B:658:GLU:HB2	2.08	0.54
1:B:389:GLU:N	1:B:390:PRO:HD3	2.23	0.54
1:B:145:GLU:HG3	1:B:298:ARG:NH2	2.23	0.54
1:B:658:GLU:OE2	1:B:662:LYS:HE3	2.08	0.54
1:A:157:ARG:HD3	1:A:666:ILE:O	2.08	0.53
1:A:185:ALA:HA	1:A:188:LYS:HG2	1.89	0.53
1:A:176:LYS:HG3	1:A:177:ASN:N	2.21	0.53
1:B:449:VAL:O	1:B:453:ILE:HD11	2.08	0.53
1:B:611:GLY:O	1:B:612:ARG:HB2	2.07	0.53
1:B:645:ASN:HD22	1:B:645:ASN:H	1.56	0.53
1:B:137:GLN:HG3	1:B:138:LYS:HD2	1.90	0.53
1:A:407:ILE:CD1	1:A:575:MSE:HE2	2.36	0.53
1:A:449:VAL:HG23	1:A:449:VAL:O	2.09	0.53
1:B:351:HIS:CE1	1:B:353:GLN:OE1	2.61	0.53
1:B:29:GLU:OE1	1:B:123:TRP:CD1	2.62	0.53
1:B:85:ILE:HG12	1:B:95:VAL:HG22	1.91	0.53
1:B:179:SER:HB2	1:B:181:LYS:HG2	1.91	0.53
1:B:643:SER:O	1:B:647:LYS:HG3	2.09	0.53
1:A:207:GLN:HB2	1:A:210:THR:OG1	2.08	0.53
1:B:480:GLU:HG2	1:B:508:LEU:HD12	1.91	0.52
1:A:189:GLU:C	1:A:191:SER:H	2.12	0.52
1:B:504:SER:C	1:B:506:LYS:N	2.63	0.52
1:A:392:LEU:CD2	1:A:397:ILE:HD13	2.39	0.52
1:A:403:SER:CB	1:A:599:GLY:HA3	2.40	0.52
1:A:502:GLN:HG3	1:A:525:LEU:HD12	1.92	0.52
1:B:436:LYS:H	1:B:436:LYS:CD	2.20	0.52
1:A:130:SER:HA	1:A:133:ILE:O	2.09	0.52
1:A:612:ARG:HH21	1:A:635:ASP:CG	2.12	0.52
1:B:450:ASN:OD1	1:B:450:ASN:N	2.40	0.52
1:A:43:LYS:O	1:A:47:LYS:HG2	2.10	0.52
1:A:95:VAL:O	1:A:113:GLN:HA	2.10	0.52
1:A:143:HIS:ND1	1:A:145:GLU:CD	2.63	0.52
1:B:77:ASP:OD2	1:B:79:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PRO:HG2	1:B:388:LYS:HB3	1.92	0.52
1:A:200:GLN:OE1	1:A:200:GLN:HA	2.11	0.51
1:A:273:LYS:HZ1	1:A:294:GLU:HG3	1.74	0.51
1:B:401:PRO:HB2	1:B:405:GLN:HB2	1.91	0.51
1:A:603:LEU:HD13	1:A:603:LEU:O	2.11	0.51
1:A:589:ARG:HE	1:A:654:ASP:CG	2.14	0.51
1:B:186:ILE:HA	1:B:227:PHE:HZ	1.75	0.51
1:B:363:THR:HA	1:B:364:PRO:C	2.31	0.51
1:A:76:LYS:HG3	1:A:77:ASP:H	1.76	0.51
1:B:460:GLU:O	1:B:582:THR:HG21	2.09	0.51
1:A:52:ILE:O	1:A:55:SER:HB3	2.11	0.51
1:A:145:GLU:CD	1:B:145:GLU:OE1	2.49	0.51
1:B:425:TYR:OH	1:B:473:GLU:HG3	2.11	0.51
1:B:176:LYS:NZ	1:B:176:LYS:HB3	2.26	0.51
1:A:50:SER:O	1:A:54:LYS:HG2	2.11	0.51
1:A:637:GLN:O	1:A:638:ASP:CB	2.58	0.51
1:B:252:LEU:HD13	1:B:253:LEU:HD23	1.92	0.50
1:B:423:THR:O	1:B:424:SER:HB3	2.11	0.50
1:B:432:TRP:CH2	1:B:434:LYS:HA	2.46	0.50
1:A:449:VAL:HG23	1:A:453:ILE:HD12	1.92	0.50
1:B:73:LEU:O	1:B:103:THR:HB	2.11	0.50
1:B:132:ILE:HG22	1:B:133:ILE:HG12	1.92	0.50
1:A:277:VAL:O	1:A:277:VAL:HG23	2.11	0.50
1:A:135:GLY:HA2	1:B:209:ASP:OD2	2.12	0.50
1:B:419:LEU:HD22	1:B:423:THR:HG21	1.93	0.50
1:A:146:ASN:ND2	1:A:296:GLY:O	2.44	0.50
1:A:269:TYR:OH	1:A:278:ILE:HD12	2.11	0.49
1:B:433:GLN:NE2	1:B:442:ASN:HD21	2.10	0.49
1:B:438:TRP:O	1:B:439:GLY:C	2.49	0.49
1:A:350:ILE:HG13	1:A:356:GLU:O	2.12	0.49
1:B:189:GLU:HG2	1:B:227:PHE:CE1	2.47	0.49
1:B:218:LYS:HE2	1:B:369:TYR:CZ	2.48	0.49
1:A:74:GLY:HA3	1:A:104:ASN:ND2	2.27	0.49
1:B:406:LYS:NZ	1:B:462:SER:OG	2.39	0.49
1:A:51:TYR:HA	1:A:54:LYS:CE	2.39	0.49
1:A:263:GLU:O	1:A:265:LYS:N	2.46	0.49
1:A:471:ALA:HB1	1:A:514:LEU:HD21	1.95	0.49
1:A:28:LYS:HE3	1:A:28:LYS:HA	1.95	0.49
1:B:428:ASP:HA	1:B:450:ASN:HB3	1.94	0.48
1:A:586:ASP:OD2	1:A:643:SER:HB2	2.13	0.48
1:B:174:VAL:O	1:B:175:PRO:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:HB3	1:A:391:LEU:HD13	1.94	0.48
1:A:538:LEU:HD22	1:A:568:ILE:HG23	1.94	0.48
1:B:614:ILE:CD1	1:B:634:LYS:HA	2.43	0.48
1:A:595:ILE:HD11	1:A:620:TYR:CE2	2.48	0.48
1:B:289:LYS:HD3	1:B:289:LYS:N	2.26	0.48
1:A:125:LEU:HD13	1:A:127:TRP:N	2.29	0.48
1:A:344:TYR:C	1:A:344:TYR:CD2	2.87	0.48
1:A:54:LYS:HA	1:A:62:MSE:SE	2.64	0.48
1:A:76:LYS:HE2	1:A:102:LYS:HB3	1.94	0.48
1:B:364:PRO:CD	1:B:388:LYS:HB3	2.44	0.48
1:A:65:ARG:HB3	1:A:66:PRO:HD3	1.96	0.48
1:B:566:GLU:N	1:B:566:GLU:OE2	2.45	0.48
1:B:489:GLY:HA3	1:B:503:ILE:HD11	1.96	0.47
1:A:221:ASP:HB2	1:A:223:TYR:HD2	1.77	0.47
1:A:145:GLU:OE2	1:B:145:GLU:OE2	2.32	0.47
1:A:613:GLN:HG3	1:A:637:GLN:HB3	1.95	0.47
1:A:627:MSE:HE3	1:A:629:MSE:HB2	1.97	0.47
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.49	0.47
1:B:441:TYR:C	1:B:442:ASN:HD22	2.17	0.47
1:A:419:LEU:C	1:A:419:LEU:HD13	2.35	0.47
1:A:226:ASP:O	1:A:230:LYS:HG3	2.15	0.47
1:B:176:LYS:HB3	1:B:176:LYS:HZ3	1.79	0.47
1:B:589:ARG:NH2	1:B:654:ASP:OD2	2.42	0.47
1:A:34:ILE:O	1:A:37:ILE:HB	2.15	0.47
1:A:154:ILE:HB	1:A:163:ALA:HB3	1.97	0.47
1:A:290:LYS:HE3	1:A:324:ILE:HG12	1.94	0.47
1:A:333:GLN:NE2	1:A:360:LEU:H	2.10	0.47
1:A:600:THR:OG1	1:A:642:ALA:HB2	2.14	0.47
1:B:406:LYS:HE2	1:B:519:TYR:HB2	1.97	0.47
1:B:472:LEU:HD23	1:B:514:LEU:HD13	1.97	0.47
1:B:516:ASP:HA	1:B:519:TYR:CE2	2.49	0.47
1:A:471:ALA:HB1	1:A:514:LEU:HD22	1.96	0.47
1:B:259:ILE:HG13	1:B:263:GLU:OE2	2.15	0.47
1:B:645:ASN:H	1:B:645:ASN:ND2	2.12	0.47
1:A:403:SER:OG	1:A:599:GLY:HA3	2.15	0.47
1:B:425:TYR:O	1:B:427:ILE:HG13	2.15	0.46
1:B:504:SER:O	1:B:505:ASN:C	2.53	0.46
1:A:438:TRP:HZ3	1:A:443:VAL:HG23	1.81	0.46
1:B:114:PHE:CE2	1:B:131:VAL:HG22	2.50	0.46
1:A:217:VAL:CG2	1:A:220:MSE:HE3	2.42	0.46
1:B:578:VAL:HA	1:B:582:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:HA	1:A:364:PRO:C	2.36	0.46
1:B:427:ILE:HD12	1:B:453:ILE:CG1	2.45	0.46
1:A:634:LYS:O	1:A:635:ASP:HB2	2.16	0.46
1:B:62:MSE:HE3	1:B:127:TRP:HB3	1.98	0.46
1:B:506:LYS:HG2	1:B:507:ASN:N	2.31	0.46
1:A:189:GLU:C	1:A:191:SER:N	2.68	0.46
1:B:502:GLN:NE2	1:B:525:LEU:CD1	2.79	0.46
1:A:346:SER:HB3	1:A:394:LYS:CB	2.46	0.46
1:B:544:ILE:HG13	1:B:562:ILE:HG13	1.97	0.46
1:B:358:LEU:HD12	1:B:627:MSE:HG3	1.97	0.46
1:B:436:LYS:N	1:B:436:LYS:CD	2.79	0.45
1:B:571:LEU:O	1:B:575:MSE:HG3	2.16	0.45
1:B:589:ARG:HH21	1:B:654:ASP:CG	2.19	0.45
1:A:215:LYS:NZ	1:A:373:TYR:O	2.50	0.45
1:B:371:PHE:CZ	1:B:375:MSE:HE1	2.51	0.45
1:A:87:LYS:H	1:A:87:LYS:CD	2.07	0.45
1:B:99:TYR:CB	1:B:112:VAL:HG21	2.46	0.45
1:B:465:ILE:O	1:B:469:ARG:HG2	2.15	0.45
1:B:371:PHE:CE2	1:B:375:MSE:HE1	2.52	0.45
1:A:307:ASN:HD21	1:B:143:HIS:HA	1.81	0.45
1:B:110:ARG:HH21	1:B:135:GLY:HA3	1.81	0.45
1:A:33:THR:O	1:A:36:ALA:HB3	2.17	0.45
1:B:345:GLY:HA3	1:B:632:ASN:O	2.17	0.45
1:B:612:ARG:HG2	1:B:613:GLN:OE1	2.17	0.45
1:B:133:ILE:HG13	1:B:142:ILE:HD11	1.99	0.45
1:B:654:ASP:O	1:B:658:GLU:N	2.49	0.45
1:B:173:ILE:HG23	1:B:178:VAL:HB	1.99	0.44
1:B:446:TYR:CE1	1:B:641:MSE:HE2	2.52	0.44
1:A:186:ILE:HA	1:A:227:PHE:HZ	1.83	0.44
1:A:112:VAL:CG1	1:A:134:PRO:CB	2.95	0.44
1:B:277:VAL:HG23	1:B:277:VAL:O	2.17	0.44
1:B:402:GLY:O	1:B:520:GLY:HA3	2.18	0.44
1:B:506:LYS:CE	1:B:507:ASN:ND2	2.77	0.44
1:A:182:ASP:O	1:A:186:ILE:HG13	2.17	0.44
1:B:179:SER:CB	1:B:181:LYS:HG2	2.48	0.44
1:A:255:TYR:HE2	1:A:281:LYS:HD3	1.83	0.44
1:B:583:HIS:O	1:B:587:ILE:HG22	2.18	0.44
1:A:215:LYS:CG	1:A:216:THR:N	2.80	0.44
1:B:544:ILE:HD12	1:B:559:LYS:HG3	2.00	0.44
1:A:543:ASN:OD1	1:A:560:LYS:HA	2.18	0.43
1:A:598:SER:OG	1:A:599:GLY:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:ILE:CD1	1:B:634:LYS:HG3	2.46	0.43
1:A:619:SER:O	1:A:620:TYR:HB3	2.17	0.43
1:A:186:ILE:O	1:A:189:GLU:HB3	2.19	0.43
1:A:369:TYR:HD2	1:A:372:MSE:CE	2.31	0.43
1:A:389:GLU:HB3	1:A:392:LEU:HB2	2.01	0.43
1:B:414:LEU:HD22	1:B:567:ASN:OD1	2.18	0.43
1:A:355:GLY:O	1:A:547:PRO:HA	2.19	0.43
1:B:174:VAL:HG22	1:B:211:PHE:HA	2.00	0.43
1:B:197:ILE:HG12	1:B:214:LEU:HD22	2.00	0.43
1:B:263:GLU:O	1:B:269:TYR:HD1	2.00	0.43
1:B:612:ARG:NH1	1:B:612:ARG:HG3	2.32	0.43
1:A:173:ILE:HG23	1:A:178:VAL:CG2	2.49	0.43
1:B:364:PRO:CG	1:B:388:LYS:HB3	2.48	0.43
1:A:340:MSE:HE1	1:A:346:SER:C	2.39	0.43
1:A:503:ILE:HG12	1:A:524:ILE:HG12	1.99	0.43
1:B:300:THR:HB	1:B:311:HIS:O	2.18	0.43
1:B:403:SER:CB	1:B:599:GLY:HA3	2.49	0.43
1:A:255:TYR:CE2	1:A:281:LYS:HD3	2.54	0.43
1:A:102:LYS:HE3	1:A:107:ASN:ND2	2.33	0.42
1:B:588:TYR:O	1:B:589:ARG:HD2	2.19	0.42
1:B:138:LYS:O	1:B:140:GLN:HG3	2.18	0.42
1:B:446:TYR:HB3	1:B:447:GLU:H	1.63	0.42
1:B:175:PRO:O	1:B:176:LYS:C	2.58	0.42
1:B:128:ASP:OD2	1:B:130:SER:HB3	2.20	0.42
1:B:636:VAL:O	1:B:638:ASP:N	2.53	0.42
1:A:441:TYR:CE2	1:A:512:ILE:HG23	2.55	0.42
1:A:346:SER:HB3	1:A:394:LYS:HB3	2.02	0.42
1:B:193:SER:OG	1:B:195:ASP:HB3	2.19	0.42
1:A:34:ILE:HA	1:A:37:ILE:HD12	2.01	0.42
1:A:263:GLU:O	1:A:266:GLN:HB2	2.20	0.42
1:A:538:LEU:CD2	1:A:568:ILE:HG23	2.49	0.42
1:B:219:LYS:HD3	1:B:219:LYS:N	2.34	0.42
1:A:122:MSE:H	1:A:122:MSE:HG2	1.60	0.42
1:A:386:ASP:HB3	1:A:390:PRO:CD	2.50	0.42
1:B:618:ILE:HA	1:B:629:MSE:O	2.20	0.42
1:A:174:VAL:O	1:A:175:PRO:C	2.59	0.41
1:A:411:MSE:HE1	1:A:562:ILE:HD11	2.02	0.41
1:B:205:TRP:HZ3	1:B:210:THR:CG2	2.32	0.41
1:B:446:TYR:OH	1:B:641:MSE:HG3	2.20	0.41
1:A:572:THR:HG22	1:A:595:ILE:CD1	2.50	0.41
1:B:175:PRO:O	1:B:177:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HA	1:A:98:GLN:O	2.19	0.41
1:A:129:HIS:C	1:A:131:VAL:H	2.22	0.41
1:A:175:PRO:O	1:A:176:LYS:C	2.58	0.41
1:A:189:GLU:O	1:A:191:SER:N	2.53	0.41
1:B:118:LYS:HD3	1:B:123:TRP:CH2	2.55	0.41
1:B:430:LYS:O	1:B:445:ARG:N	2.52	0.41
1:B:614:ILE:HD13	1:B:614:ILE:HA	1.93	0.41
1:A:111:ASN:HD22	1:A:112:VAL:N	2.19	0.41
1:A:255:TYR:CE1	1:A:280:LYS:HB2	2.54	0.41
1:A:367:ASP:O	1:A:370:PRO:HD2	2.19	0.41
1:A:474:LEU:O	1:A:478:LYS:HD2	2.21	0.41
1:B:128:ASP:OD2	1:B:128:ASP:C	2.59	0.41
1:B:290:LYS:HB2	1:B:290:LYS:HE2	1.68	0.41
1:B:291:LEU:O	1:B:321:GLY:HA3	2.20	0.41
1:A:502:GLN:CG	1:A:525:LEU:HB2	2.50	0.41
1:A:551:LYS:HA	1:A:551:LYS:HD3	1.89	0.41
1:B:173:ILE:CG2	1:B:178:VAL:HB	2.50	0.41
1:B:180:LYS:HA	1:B:183:TYR:CE1	2.55	0.41
1:B:197:ILE:O	1:B:201:MSE:HG2	2.20	0.41
1:B:563:ILE:HG12	1:B:564:SER:N	2.36	0.41
1:A:29:GLU:OE2	1:A:122:MSE:HB3	2.21	0.41
1:A:263:GLU:C	1:A:265:LYS:N	2.74	0.41
1:B:587:ILE:HG12	1:B:587:ILE:O	2.20	0.41
1:A:186:ILE:HG12	1:A:231:PHE:CD1	2.56	0.41
1:A:193:SER:C	1:A:195:ASP:N	2.71	0.41
1:A:221:ASP:O	1:A:223:TYR:N	2.44	0.41
1:A:408:LEU:HD22	1:A:534:ILE:HG21	2.02	0.41
1:B:579:VAL:HG13	1:B:587:ILE:HG23	2.02	0.41
1:A:43:LYS:O	1:A:47:LYS:HE2	2.20	0.41
1:A:192:ILE:O	1:A:193:SER:C	2.59	0.41
1:A:435:ASP:OD1	1:A:437:SER:N	2.48	0.41
1:A:456:LYS:HE3	1:A:456:LYS:HB2	1.86	0.41
1:B:65:ARG:N	1:B:66:PRO:CD	2.84	0.41
1:B:183:TYR:N	1:B:183:TYR:CD1	2.88	0.41
1:B:488:VAL:O	1:B:503:ILE:CD1	2.67	0.41
1:B:569:ASN:HA	1:B:572:THR:OG1	2.21	0.41
1:A:570:LEU:HD12	1:A:570:LEU:HA	1.92	0.41
1:B:183:TYR:N	1:B:183:TYR:HD1	2.19	0.41
1:B:197:ILE:HG23	1:B:214:LEU:HD21	2.02	0.41
1:B:290:LYS:HB3	1:B:324:ILE:HD11	2.03	0.41
1:A:536:SER:HA	1:A:628:MSE:SE	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:THR:HA	1:A:614:ILE:O	2.21	0.40
1:B:502:GLN:HG3	1:B:525:LEU:HB2	2.03	0.40
1:B:506:LYS:HG2	1:B:507:ASN:ND2	2.36	0.40
1:A:142:ILE:CD1	1:A:301:ILE:HG12	2.51	0.40
1:B:50:SER:HA	1:B:124:LYS:HB3	2.03	0.40
1:A:277:VAL:O	1:A:277:VAL:CG2	2.70	0.40
1:A:99:TYR:HB3	1:A:134:PRO:HG3	2.03	0.40
1:A:495:ASP:OD2	1:A:549:LEU:HD12	2.22	0.40
1:A:612:ARG:NH2	1:A:635:ASP:OD2	2.52	0.40
1:B:544:ILE:HB	1:B:559:LYS:HB2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:7:HOH:O	4:A:7:HOH:O[5_555]	0.88	1.32
1:A:509:ASP:OD1	4:A:7:HOH:O[5_555]	2.18	0.02

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	614/646 (95%)	548 (89%)	56 (9%)	10 (2%)	9 8
1	B	621/646 (96%)	569 (92%)	39 (6%)	13 (2%)	7 5
All	All	1235/1292 (96%)	1117 (90%)	95 (8%)	23 (2%)	8 6

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	B	307	ASN

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Mol	Chain	Res	Type
1	B	341	LYS
1	A	175	PRO
1	A	264	LEU
1	A	265	LYS
1	A	269	TYR
1	A	435	ASP
1	B	176	LYS
1	B	437	SER
1	B	446	TYR
1	B	504	SER
1	B	505	ASN
1	B	612	ARG
1	B	637	GLN
1	A	182	ASP
1	A	222	GLU
1	B	424	SER
1	B	204	ASN
1	A	190	LEU
1	A	624	ASN
1	B	439	GLY
1	B	175	PRO

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	557/559 (100%)	523 (94%)	34 (6%)	18	24
1	B	561/559 (100%)	524 (93%)	37 (7%)	16	20
All	All	1118/1118 (100%)	1047 (94%)	71 (6%)	17	21

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	87	LYS

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Mol	Chain	Res	Type
1	A	99	TYR
1	A	111	ASN
1	A	138	LYS
1	A	156	ASP
1	A	175	PRO
1	A	180	LYS
1	A	202	ASP
1	A	222	GLU
1	A	231	PHE
1	A	252	LEU
1	A	262	GLU
1	A	265	LYS
1	A	266	GLN
1	A	269	TYR
1	A	273	LYS
1	A	303	ASP
1	A	333	GLN
1	A	344	TYR
1	A	367	ASP
1	A	387	LYS
1	A	391	LEU
1	A	392	LEU
1	A	446	TYR
1	A	502	GLN
1	A	513	LEU
1	A	514	LEU
1	A	532	LEU
1	A	549	LEU
1	A	551	LYS
1	A	560	LYS
1	A	593	ASN
1	A	662	LYS
1	B	27	ASP
1	B	87	LYS
1	B	99	TYR
1	B	125	LEU
1	B	137	GLN
1	B	138	LYS
1	B	141	SER
1	B	148	LYS
1	B	156	ASP
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	175	PRO
1	B	176	LYS
1	B	208	ASP
1	B	219	LYS
1	B	221	ASP
1	B	223	TYR
1	B	262	GLU
1	B	289	LYS
1	B	307	ASN
1	B	331	LYS
1	B	391	LEU
1	B	408	LEU
1	B	436	LYS
1	B	448	VAL
1	B	450	ASN
1	B	502	GLN
1	B	503	ILE
1	B	514	LEU
1	B	532	LEU
1	B	549	LEU
1	B	552	ASP
1	B	566	GLU
1	B	593	ASN
1	B	612	ARG
1	B	613	GLN
1	B	624	ASN
1	B	636	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	111	ASN
1	A	113	GLN
1	A	146	ASN
1	A	177	ASN
1	A	203	GLN
1	A	207	GLN
1	A	251	HIS
1	A	266	GLN
1	A	307	ASN
1	A	333	GLN

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Mol	Chain	Res	Type
1	A	396	GLN
1	A	433	GLN
1	A	502	GLN
1	A	540	ASN
1	A	545	ASN
1	A	577	GLN
1	A	593	ASN
1	A	661	ASN
1	B	41	ASN
1	B	98	GLN
1	B	104	ASN
1	B	137	GLN
1	B	164	ASN
1	B	207	GLN
1	B	266	GLN
1	B	351	HIS
1	B	433	GLN
1	B	442	ASN
1	B	502	GLN
1	B	507	ASN
1	B	540	ASN
1	B	593	ASN
1	B	624	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 8 ligands modelled in this entry, 8 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	609/646 (94%)	0.37	37 (6%) 21 18	7, 27, 47, 57	0
1	B	614/646 (95%)	0.35	40 (6%) 18 15	5, 26, 47, 56	0
All	All	1223/1292 (94%)	0.36	77 (6%) 20 16	5, 27, 47, 57	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	ASN	7.2
1	A	223	TYR	6.5
1	B	603	LEU	5.8
1	B	611	GLY	5.2
1	A	503	ILE	4.8
1	A	51	TYR	4.6
1	B	604	LYS	4.3
1	A	603	LEU	4.2
1	A	224	LEU	4.1
1	B	504	SER	3.8
1	A	261	SER	3.7
1	B	502	GLN	3.6
1	B	506	LYS	3.6
1	B	381	ASN	3.5
1	B	222	GLU	3.5
1	B	436	LYS	3.4
1	B	384	THR	3.4
1	B	503	ILE	3.3
1	A	121	GLY	3.3
1	B	426	LYS	3.2
1	B	51	TYR	3.1
1	A	268	GLU	3.1
1	A	630	ALA	3.0
1	A	267	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	437	SER	3.0
1	B	446	TYR	2.9
1	A	85	ILE	2.9
1	A	145	GLU	2.8
1	A	612	ARG	2.8
1	B	266	GLN	2.8
1	A	222	GLU	2.8
1	B	638	ASP	2.8
1	B	267	LYS	2.8
1	B	448	VAL	2.8
1	B	223	TYR	2.8
1	A	120	ASP	2.7
1	A	378	GLU	2.7
1	A	232	HIS	2.7
1	B	427	ILE	2.6
1	B	265	LYS	2.6
1	A	188	LYS	2.6
1	B	188	LYS	2.6
1	B	447	GLU	2.6
1	A	231	PHE	2.6
1	A	500	ASN	2.6
1	A	87	LYS	2.5
1	A	193	SER	2.5
1	B	224	LEU	2.5
1	B	452	ASN	2.5
1	A	178	VAL	2.5
1	B	636	VAL	2.4
1	A	264	LEU	2.4
1	B	226	ASP	2.4
1	A	438	TRP	2.4
1	A	349	ALA	2.4
1	A	198	LYS	2.4
1	B	449	VAL	2.3
1	B	612	ARG	2.3
1	A	86	LYS	2.3
1	B	377	ASN	2.3
1	A	454	ASP	2.2
1	A	508	LEU	2.2
1	B	385	GLU	2.2
1	B	268	GLU	2.2
1	B	133	ILE	2.2
1	B	440	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	123	TRP	2.1
1	B	230	LYS	2.1
1	A	618	ILE	2.1
1	A	205	TRP	2.1
1	B	378	GLU	2.1
1	A	179	SER	2.0
1	A	502	GLN	2.0
1	B	422	LYS	2.0
1	A	440	GLY	2.0
1	B	407	ILE	2.0
1	A	613	GLN	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, 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	B-factors(\AA^2)	Q<0.9
3	CL	A	1207	1/1	0.94	0.12	15,15,15,15	0
2	CD	B	1204	1/1	0.99	0.08	21,21,21,21	0
3	CL	A	1205	1/1	0.99	0.05	16,16,16,16	0
2	CD	B	1201	1/1	0.99	0.12	19,19,19,19	0
3	CL	B	1206	1/1	0.99	0.10	24,24,24,24	0
3	CL	B	1208	1/1	0.99	0.06	10,10,10,10	0
2	CD	A	1202	1/1	1.00	0.07	17,17,17,17	0
2	CD	A	1203	1/1	1.00	0.07	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.