



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2017 – 06:19 AM EST

PDB ID : 5OFR
Title : Structure of the antibacterial peptide ABC transporter McjD in a high energy outward occluded intermediate state
Authors : Beis, K.; Bountra, K.
Deposited on : unknown
Resolution : 3.40 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

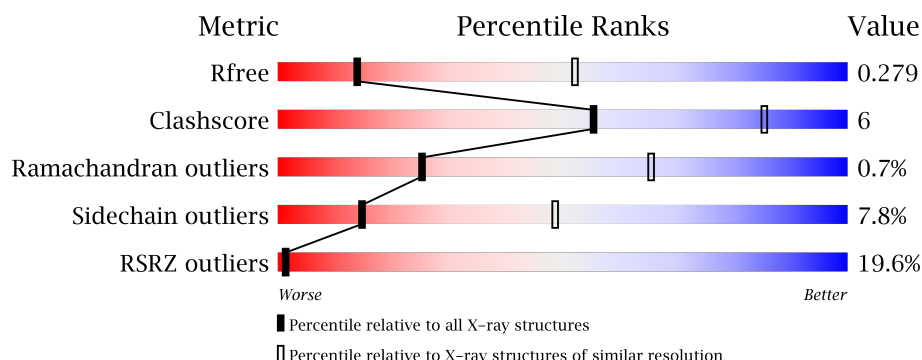
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	580	<div> <div>16%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
1	B	580	<div> <div>23%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9173 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 Microcin-J25 export ATP-binding/permease protein McjD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4527	2920	739	850	18			
1	B	576	Total	C	N	O	S	0	2	0
			4580	2954	750	858	18			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

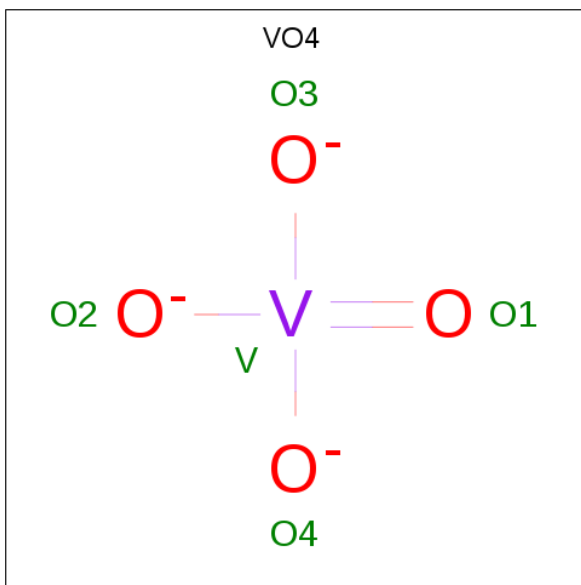


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is VANADATE ION (three-letter code: VO4) (formula: O₄V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	V	0	0
			5	4	1		
4	B	1	Total	O	V	0	0
			5	4	1		

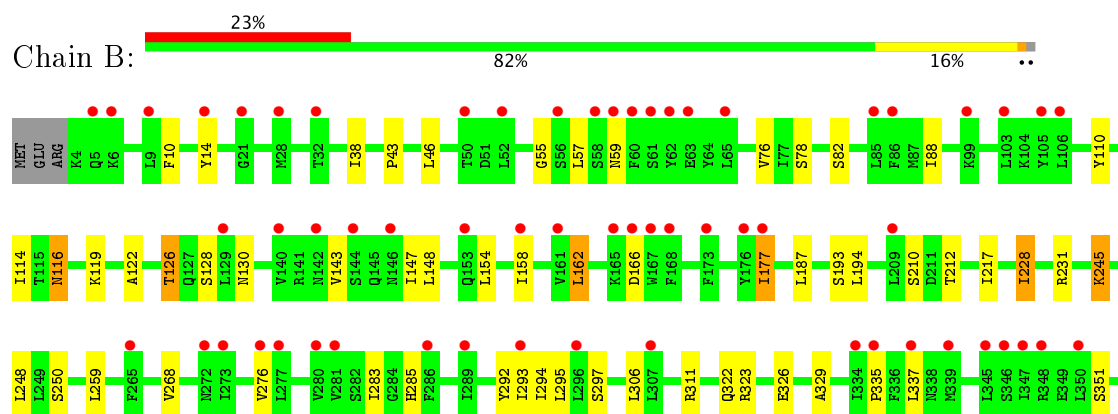
3 Residue-property plots [i](#)

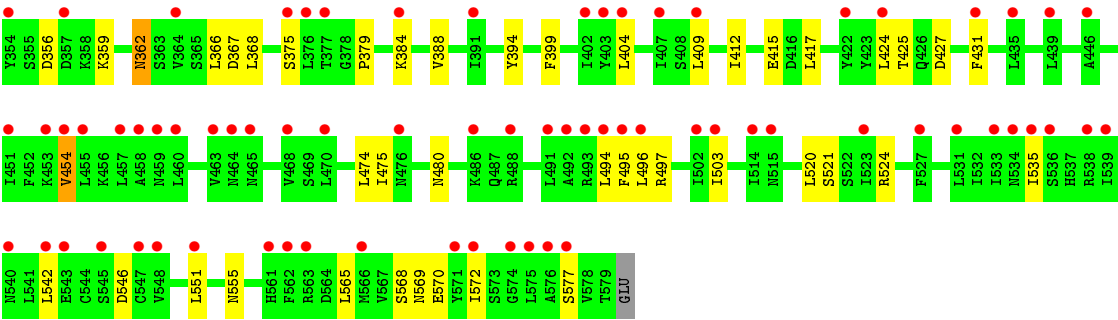
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Microcin-J25 export ATP-binding/permease protein McjD



- Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.29Å 105.04Å 117.37Å 90.00° 105.55° 90.00°	Depositor
Resolution (Å)	95.30 – 3.40 95.30 – 3.40	Depositor EDS
% Data completeness (in resolution range)	58.6 (95.30-3.40) 58.6 (95.30-3.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.257 , 0.260 0.277 , 0.279	Depositor DCC
R_{free} test set	1068 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	9173	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, MG, ADP

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	0.52	0/4603	0.68	0/6234
1	B	0.49	0/4663	0.65	0/6313
All	All	0.51	0/9266	0.67	0/12547

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4527	0	4638	74	0
1	B	4580	0	4701	44	2
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
All	All	9173	0	9363	109	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 6.

All (109) 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:333:SER:HB2	1:A:411:ASN:HA	1.56	0.86
1:B:359:LYS:HD3	1:B:362:ASN:HA	1.65	0.79
1:A:339:MET:HG2	1:A:343:LEU:HD21	1.66	0.77
1:A:339:MET:HE2	1:A:404:LEU:HB3	1.66	0.76
1:A:516:GLU:O	1:A:520:LEU:HD12	1.88	0.73
1:A:338:ASN:HB3	1:A:339:MET:HE1	1.70	0.73
1:A:339:MET:HE2	1:A:404:LEU:CB	2.20	0.72
1:B:143:VAL:HA	1:B:147:ILE:HD12	1.73	0.70
1:A:333:SER:CB	1:A:411:ASN:HA	2.22	0.69
1:A:343:LEU:HB2	1:A:500:ALA:HB1	1.75	0.68
1:A:143:VAL:HA	1:A:147:ILE:HD12	1.75	0.68
1:A:306:LEU:HD12	1:A:310:ILE:HG13	1.77	0.66
1:A:32:THR:HG21	1:A:145:GLN:HA	1.78	0.66
1:A:188:THR:HG23	1:A:308:SER:HA	1.80	0.64
1:A:45:ILE:HG23	1:A:68:LEU:CD1	2.28	0.64
1:A:339:MET:HG2	1:A:343:LEU:CD2	2.29	0.63
1:A:116:ASN:HA	1:A:119:LYS:HD2	1.83	0.61
1:A:335:PRO:HD2	1:A:411:ASN:O	2.00	0.60
1:A:454:VAL:HG22	1:A:495:PHE:HB2	1.83	0.60
1:B:454:VAL:HG22	1:B:495:PHE:HB2	1.84	0.59
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.86	0.58
1:A:217:ILE:HD12	1:A:217:ILE:H	1.69	0.57
1:B:212:THR:HG23	1:B:231:ARG:HH21	1.69	0.57
1:A:338:ASN:HB3	1:A:339:MET:CE	2.33	0.57
1:A:424:LEU:HD11	1:A:494:LEU:HD22	1.86	0.57
1:A:430:ILE:HG21	1:A:474:LEU:HD22	1.87	0.57
1:A:45:ILE:HG23	1:A:68:LEU:HD12	1.86	0.56
1:A:475:ILE:HB	1:A:480:ASN:HB2	1.87	0.56
1:A:343:LEU:HD12	1:A:500:ALA:HB3	1.88	0.56
1:B:424:LEU:HD11	1:B:494:LEU:HD22	1.88	0.56
1:A:158:ILE:O	1:A:162:LEU:HB2	2.06	0.55
1:B:57:LEU:H	1:B:59:ASN:ND2	2.05	0.55
1:A:384:LYS:HD2	1:A:535:ILE:HG23	1.89	0.55
1:A:80:LYS:HE3	1:B:297:SER:HB2	1.88	0.55
1:A:366:LEU:HD23	1:A:368:LEU:HD11	1.89	0.54
1:B:569:ASN:HD22	1:B:572:ILE:H	1.55	0.54
1:B:384:LYS:HD2	1:B:535:ILE:HG23	1.89	0.54
1:B:409:LEU:HA	1:B:412:ILE:HD12	1.90	0.53
1:B:454:VAL:HG21	1:B:496:LEU:HG	1.91	0.53
1:A:308:SER:O	1:A:312:GLN:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:CB	1:A:339:MET:HE1	2.39	0.53
1:B:366:LEU:HD23	1:B:368:LEU:HD11	1.91	0.53
1:A:58:SER:H	1:A:61:SER:HB3	1.74	0.52
1:A:512:ASP:OD2	1:B:379:PRO:HA	2.09	0.52
1:B:375:SER:HB3	1:B:542:LEU:HD23	1.91	0.52
1:B:454:VAL:HG22	1:B:495:PHE:CB	2.39	0.52
1:A:52:LEU:O	1:A:57:LEU:HG	2.10	0.51
1:B:475:ILE:HB	1:B:480:ASN:HB2	1.91	0.51
1:B:116:ASN:HA	1:B:119:LYS:HD3	1.93	0.51
1:B:217:ILE:H	1:B:217:ILE:HD12	1.76	0.51
1:A:146:ASN:O	1:A:306:LEU:HD22	2.13	0.49
1:A:32:THR:HG22	1:A:149:SER:HB2	1.94	0.49
1:B:268:VAL:HG12	1:B:293:ILE:HD11	1.94	0.49
1:A:76:VAL:HG11	1:B:294:ILE:HG12	1.94	0.49
1:A:45:ILE:HG23	1:A:68:LEU:HD13	1.93	0.48
1:A:338:ASN:ND2	1:A:412:ILE:HG23	2.28	0.48
1:B:158:ILE:O	1:B:162:LEU:HB2	2.14	0.48
1:A:286:PHE:O	1:A:290:THR:HG23	2.14	0.48
1:B:565:LEU:HA	1:B:568:SER:OG	2.14	0.48
1:A:290:THR:HA	1:A:293:ILE:HD12	1.96	0.47
1:B:351:SER:HB2	1:B:399:PHE:HB2	1.95	0.47
1:A:454:VAL:HG21	1:A:496:LEU:HG	1.97	0.47
1:A:58:SER:N	1:A:61:SER:HB3	2.30	0.47
1:A:339:MET:HG2	1:A:343:LEU:CG	2.45	0.46
1:A:504:ILE:HG23	1:A:507:ALA:HB3	1.97	0.46
1:B:154:LEU:HD22	1:B:177:ILE:HD13	1.96	0.46
1:A:195:ARG:HD2	1:A:312:GLN:HB2	1.96	0.46
1:A:339:MET:HE2	1:A:404:LEU:HB2	1.94	0.46
1:A:188:THR:HG21	1:A:311:ARG:HH11	1.80	0.46
1:A:337:LEU:HG	1:A:337:LEU:O	2.16	0.45
1:B:322:GLN:O	1:B:326:GLU:HG2	2.17	0.45
1:B:194:LEU:HD22	1:B:245:LYS:HB3	1.97	0.44
1:A:46:LEU:HD12	1:A:291:SER:OG	2.17	0.44
1:A:306:LEU:CD1	1:A:310:ILE:HG13	2.46	0.44
1:A:454:VAL:HG22	1:A:495:PHE:CB	2.46	0.44
1:B:10:PHE:O	1:B:14:TYR:HD2	2.00	0.44
1:B:57:LEU:H	1:B:59:ASN:HD22	1.66	0.44
1:A:225:LEU:HB2	1:B:110:TYR:CZ	2.53	0.44
1:B:212:THR:HG22	1:B:228:ILE:HD12	2.00	0.43
1:A:122:ALA:HB1	1:B:210:SER:HB2	1.99	0.43
1:A:136:ILE:HG13	1:A:317:LEU:HD21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD22	1:B:417:LEU:HD11	2.01	0.43
1:A:294:ILE:HG12	1:B:76:VAL:HG11	2.02	0.42
1:A:409:LEU:HD22	1:A:417:LEU:HD11	2.00	0.42
1:A:62:TYR:CE1	1:B:283:ILE:HD11	2.55	0.42
1:A:52:LEU:HD21	1:A:64:TYR:HD2	1.85	0.42
1:B:114:ILE:HD13	1:B:394:TYR:HA	2.02	0.42
1:A:210:SER:HB2	1:B:122:ALA:HB1	2.01	0.42
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.87	0.41
1:B:475:ILE:H	1:B:480:ASN:HD22	1.67	0.41
1:A:350:LEU:HD22	1:A:402:ILE:HD11	2.02	0.41
1:B:166:ASP:OD2	1:B:285:HIS:HE1	2.04	0.41
1:A:317:LEU:O	1:A:321:ILE:HG12	2.21	0.41
1:B:43:PRO:HG2	1:B:292:TYR:CE1	2.56	0.41
1:A:212:THR:HG21	1:A:228:ILE:HG23	2.03	0.41
1:A:333:SER:HB2	1:A:411:ASN:CA	2.40	0.41
1:B:388:VAL:HB	1:B:503:ILE:HD13	2.01	0.41
1:B:38:ILE:HG21	1:B:78:SER:OG	2.20	0.41
1:A:27:SER:O	1:A:31:ILE:HD12	2.20	0.41
1:A:13:ILE:HA	1:A:16:LEU:HD12	2.03	0.41
1:A:334:ILE:O	1:A:335:PRO:C	2.59	0.41
1:A:162:LEU:HA	1:A:162:LEU:HD12	1.98	0.40
1:A:342:LYS:HB2	1:A:370:THR:HG21	2.02	0.40
1:A:38:ILE:HG21	1:A:78:SER:OG	2.21	0.40
1:A:228:ILE:HD11	1:B:431:PHE:CE2	2.57	0.40
1:A:45:ILE:HD13	1:A:71:LEU:HB3	2.04	0.40
1:A:289:ILE:HD13	1:A:289:ILE:HA	1.95	0.40
1:A:351:SER:HB2	1:A:399:PHE:HB2	2.03	0.40
1:B:122:ALA:O	1:B:126:THR:HB	2.22	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)
1:B:55:GLY:O	1:B:55:GLY:O 2_558	1.02	1.18
1:B:55:GLY:C	1:B:55:GLY:O 2_558	1.99	0.21

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	569/580 (98%)	531 (93%)	33 (6%)	5 (1%)	20	61
1	B	576/580 (99%)	538 (93%)	35 (6%)	3 (0%)	32	71
All	All	1145/1160 (99%)	1069 (93%)	68 (6%)	8 (1%)	25	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	334	ILE
1	B	335	PRO
1	A	337	LEU
1	A	341	ARG
1	B	329	ALA
1	A	333	SER
1	B	323	ARG

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	520/529 (98%)	478 (92%)	42 (8%)	14	47
1	B	527/529 (100%)	488 (93%)	39 (7%)	16	51
All	All	1047/1058 (99%)	966 (92%)	81 (8%)	15	49

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	54	SER
1	A	66	VAL
1	A	68	LEU
1	A	80	LYS
1	A	82	SER
1	A	88	ILE
1	A	115	THR
1	A	116	ASN
1	A	126	THR
1	A	130	ASN
1	A	133	SER
1	A	162	LEU
1	A	177	ILE
1	A	193	SER
1	A	228	ILE
1	A	248	LEU
1	A	259	LEU
1	A	276	VAL
1	A	287	ILE
1	A	295	LEU
1	A	339	MET
1	A	340	GLU
1	A	341	ARG
1	A	343	LEU
1	A	344	ASN
1	A	367	ASP
1	A	375	SER
1	A	407	ILE
1	A	425	THR
1	A	427	ASP
1	A	452	PHE
1	A	454	VAL
1	A	466	GLU
1	A	474	LEU
1	A	497	ARG
1	A	522	SER
1	A	524	ARG
1	A	540	ASN
1	A	546	ASP
1	A	551	LEU
1	A	555	ASN
1	B	82	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	88	ILE
1	B	116	ASN
1	B	126	THR
1	B	128	SER
1	B	130	ASN
1	B	148	LEU
1	B	162	LEU
1	B	177	ILE
1	B	187	LEU
1	B	193	SER
1	B	228	ILE
1	B	245	LYS
1	B	248	LEU
1	B	250	SER
1	B	259	LEU
1	B	276	VAL
1	B	295	LEU
1	B	306	LEU
1	B	311	ARG
1	B	337	LEU
1	B	356	ASP
1	B	362	ASN
1	B	367	ASP
1	B	404	LEU
1	B	415	GLU
1	B	425	THR
1	B	427	ASP
1	B	454	VAL
1	B	474	LEU
1	B	497	ARG
1	B	520	LEU
1	B	521	SER
1	B	524	ARG
1	B	546	ASP
1	B	551	LEU
1	B	555	ASN
1	B	570	GLU
1	B	577	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	130	ASN
1	A	153	GLN
1	A	223	ASN
1	A	464	ASN
1	A	487	GLN
1	B	59	ASN
1	B	127	GLN
1	B	130	ASN
1	B	153	GLN
1	B	362	ASN
1	B	426	GLN
1	B	459	ASN
1	B	479	ASN
1	B	480	ASN
1	B	515	ASN
1	B	555	ASN
1	B	569	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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
2	ADP	A	601	3,4	25,29,29	0.66	0	24,45,45	0.71	0
4	VO4	A	603	3,2	1,4,4	4.76	1 (100%)	0,6,6	0.00	-
2	ADP	B	601	3,4	25,29,29	0.55	0	24,45,45	1.09	2 (8%)
4	VO4	B	603	3,2	1,4,4	4.57	1 (100%)	0,6,6	0.00	-

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
2	ADP	A	601	3,4	-	0/12/32/32	0/3/3/3
4	VO4	A	603	3,2	-	0/0/0/0	0/0/0/0
2	ADP	B	601	3,4	-	0/12/32/32	0/3/3/3
4	VO4	B	603	3,2	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	VO4	O1-V	4.57	1.90	1.63
4	A	603	VO4	O1-V	4.76	1.91	1.63

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C4'-O4'-C1'	2.06	111.96	109.77
2	B	601	ADP	O3'-C3'-C2'	2.31	119.24	111.83

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	571/580 (98%)	1.11	94 (16%) 2 2	47, 101, 158, 202	0
1	B	576/580 (99%)	1.32	131 (22%) 1 1	40, 110, 164, 188	0
All	All	1147/1160 (98%)	1.22	225 (19%) 1 1	40, 106, 162, 202	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	11.4
1	A	59	ASN	10.9
1	B	539	ILE	8.8
1	A	58	SER	7.2
1	A	62	TYR	7.0
1	B	458	ALA	6.9
1	B	56	SER	6.7
1	A	60	PHE	6.6
1	B	63	GLU	6.4
1	B	463	VAL	6.3
1	B	575	LEU	6.3
1	B	337	LEU	6.3
1	B	495	PHE	6.1
1	B	457	LEU	6.0
1	B	5	GLN	5.9
1	B	542	LEU	5.7
1	B	562	PHE	5.7
1	A	65	LEU	5.6
1	A	274	LEU	5.6
1	A	562	PHE	5.6
1	B	60	PHE	5.3
1	B	335	PRO	5.2
1	B	59	ASN	5.1
1	B	464	ASN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	569	ASN	5.0
1	A	324	HIS	5.0
1	B	334	ILE	4.9
1	B	488	ARG	4.8
1	A	173	PHE	4.8
1	B	460	LEU	4.7
1	A	550	VAL	4.6
1	B	58	SER	4.6
1	B	276	VAL	4.6
1	A	513	TYR	4.5
1	B	62	TYR	4.5
1	A	339	MET	4.4
1	B	492	ALA	4.4
1	A	559	SER	4.4
1	A	542	LEU	4.3
1	A	61	SER	4.3
1	B	533	ILE	4.3
1	B	491	LEU	4.3
1	A	265	PHE	4.2
1	A	558	ALA	4.1
1	B	168	PHE	4.1
1	B	534	ASN	4.1
1	A	375	SER	4.0
1	B	465	ASN	4.0
1	B	166	ASP	4.0
1	B	494	LEU	3.9
1	B	451	ILE	3.9
1	A	549	TYR	3.9
1	B	402	ILE	3.9
1	A	571	TYR	3.8
1	B	339	MET	3.8
1	B	439	LEU	3.7
1	B	454	VAL	3.7
1	B	61	SER	3.7
1	B	273	ILE	3.6
1	B	548	VAL	3.6
1	B	167	TRP	3.6
1	A	52	LEU	3.6
1	B	496	LEU	3.6
1	A	144	SER	3.6
1	A	232	TYR	3.6
1	A	295	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	376	LEU	3.6
1	A	576	ALA	3.6
1	A	347	ILE	3.5
1	A	142	ASN	3.5
1	B	281	VAL	3.5
1	A	177	ILE	3.5
1	B	52	LEU	3.4
1	B	435	LEU	3.4
1	B	572	ILE	3.4
1	B	14	TYR	3.4
1	A	572	ILE	3.4
1	B	265	PHE	3.3
1	A	168	PHE	3.3
1	A	548	VAL	3.3
1	A	49	ILE	3.3
1	B	177	ILE	3.3
1	B	470	LEU	3.3
1	B	375	SER	3.2
1	B	144	SER	3.2
1	A	561	HIS	3.2
1	B	272	ASN	3.2
1	B	277	LEU	3.2
1	B	32	THR	3.2
1	B	407	ILE	3.1
1	B	502	ILE	3.1
1	B	577	SER	3.1
1	B	566	MET	3.1
1	B	523	ILE	3.1
1	B	161	VAL	3.1
1	A	63	GLU	3.1
1	A	565	LEU	3.1
1	A	533	ILE	3.1
1	B	576	ALA	3.0
1	B	468	VAL	3.0
1	B	173	PHE	3.0
1	B	571	TYR	3.0
1	B	99	LYS	3.0
1	A	39	ILE	3.0
1	A	536	SER	3.0
1	A	579	THR	3.0
1	B	350	LEU	3.0
1	B	545	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	493	ARG	2.9
1	A	45	ILE	2.9
1	B	455	LEU	2.9
1	A	503	ILE	2.9
1	A	338	ASN	2.9
1	B	142	ASN	2.9
1	B	146	ASN	2.9
1	A	535	ILE	2.9
1	B	527	PHE	2.9
1	A	161	VAL	2.8
1	B	535	ILE	2.8
1	A	44	LEU	2.8
1	B	307	LEU	2.8
1	A	208	LEU	2.8
1	B	409	LEU	2.8
1	B	536	SER	2.8
1	B	503	ILE	2.8
1	B	293	ILE	2.8
1	B	453	LYS	2.8
1	A	272	ASN	2.8
1	A	9	LEU	2.8
1	A	14	TYR	2.8
1	B	105	TYR	2.8
1	B	286	PHE	2.7
1	A	362	ASN	2.7
1	A	364	VAL	2.7
1	B	563	ARG	2.7
1	A	534	ASN	2.7
1	B	514	ILE	2.7
1	B	384	LYS	2.7
1	B	515	ASN	2.7
1	B	547	CYS	2.7
1	A	32	THR	2.7
1	A	254	LEU	2.7
1	B	158	ILE	2.7
1	A	387	LEU	2.6
1	B	165	LYS	2.6
1	A	346	SER	2.6
1	A	242	ALA	2.6
1	B	21	GLY	2.6
1	A	76	VAL	2.6
1	B	65	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	2.6
1	A	566	MET	2.6
1	A	495	PHE	2.6
1	A	577	SER	2.6
1	A	502	ILE	2.6
1	A	246	TYR	2.5
1	B	296	LEU	2.5
1	A	276	VAL	2.5
1	B	289	ILE	2.5
1	A	129	LEU	2.5
1	A	560	GLY	2.5
1	A	79	ASN	2.5
1	B	574	GLY	2.5
1	B	543	GLU	2.5
1	B	103	LEU	2.4
1	B	357	ASP	2.4
1	B	348	ARG	2.4
1	A	243	GLN	2.4
1	B	540	ASN	2.4
1	A	286	PHE	2.4
1	A	539	ILE	2.4
1	B	476	ASN	2.4
1	A	293	ILE	2.4
1	B	28	MET	2.4
1	B	129	LEU	2.4
1	B	6	LYS	2.4
1	A	404	LEU	2.4
1	B	486	LYS	2.4
1	A	551	LEU	2.4
1	A	67	LEU	2.3
1	B	377	THR	2.3
1	B	403	TYR	2.3
1	B	422	TYR	2.3
1	A	106	LEU	2.3
1	B	561	HIS	2.3
1	B	106	LEU	2.2
1	B	404	LEU	2.2
1	B	531	LEU	2.2
1	B	153	GLN	2.2
1	B	551	LEU	2.2
1	A	192	ALA	2.2
1	A	460	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	245	LYS	2.2
1	A	281	VAL	2.2
1	A	64	TYR	2.2
1	B	459	ASN	2.2
1	B	538	ARG	2.2
1	B	50	THR	2.2
1	B	86	PHE	2.1
1	B	280	VAL	2.1
1	A	361	LEU	2.1
1	B	431	PHE	2.1
1	A	402	ILE	2.1
1	A	567	VAL	2.1
1	B	347	ILE	2.1
1	B	424	LEU	2.1
1	B	209	LEU	2.1
1	A	219	ALA	2.1
1	B	364	VAL	2.1
1	A	313	SER	2.1
1	B	391	ILE	2.1
1	A	312	GLN	2.1
1	A	457	LEU	2.1
1	B	376	LEU	2.1
1	A	126	THR	2.1
1	B	9	LEU	2.1
1	A	25	PHE	2.0
1	B	354	TYR	2.0
1	A	188	THR	2.0
1	B	345	LEU	2.0
1	A	390	ILE	2.0
1	B	346	SER	2.0
1	B	85	LEU	2.0
1	B	446	ALA	2.0
1	B	176	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	MG	B	602	1/1	0.97	0.24	-0.48	37,37,37,37	0
2	ADP	B	601	27/27	0.98	0.24	-0.69	60,64,68,70	0
2	ADP	A	601	27/27	0.93	0.19	-0.80	116,122,125,126	0
4	VO4	A	603	5/5	0.98	0.18	-0.81	103,105,106,107	0
4	VO4	B	603	5/5	0.98	0.18	-0.95	87,91,91,93	0
3	MG	A	602	1/1	0.93	0.17	-1.97	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.