



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 PM GMT

PDB ID : 4PL0
Title : Crystal structure of the antibacterial peptide ABC transporter McjD in an outward occluded state
Authors : Choudhury, H.G.; Beis, K.
Deposited on : 2014-05-15
Resolution : 2.70 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

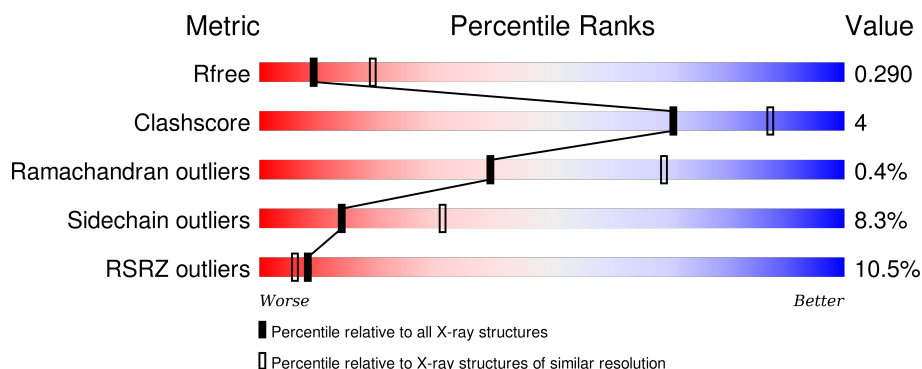
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>12%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	B	580	<div> <div>9%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	602	-	-	-	X
4	BNG	B	603	-	-	-	X

2 Entry composition [i](#)

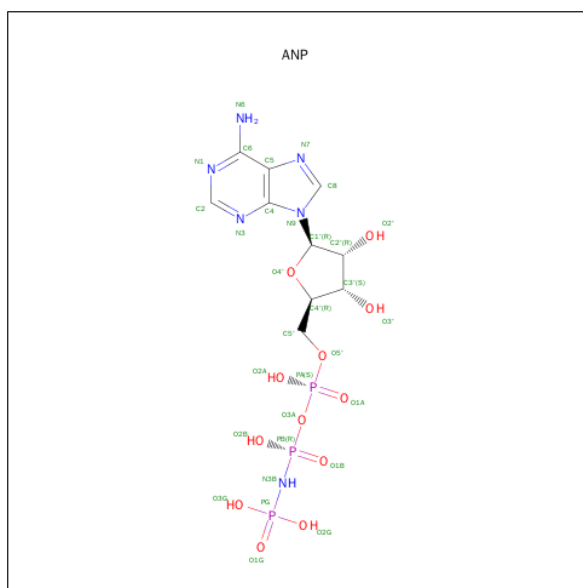
There are 4 unique types of molecules in this entry. The entry contains 9213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

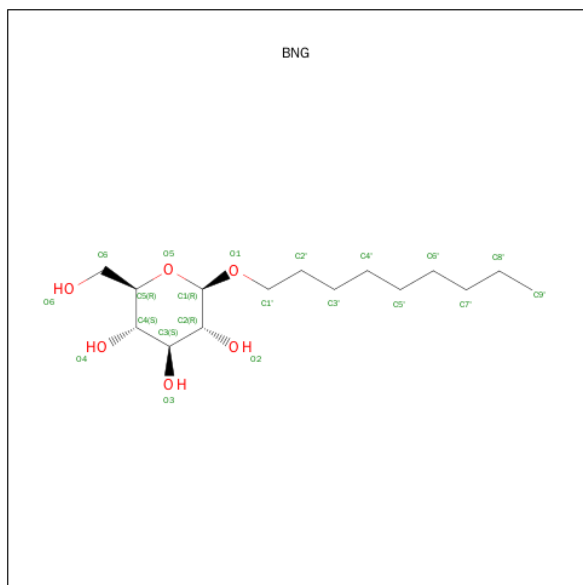


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 4 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: C₁₅H₃₀O₆).

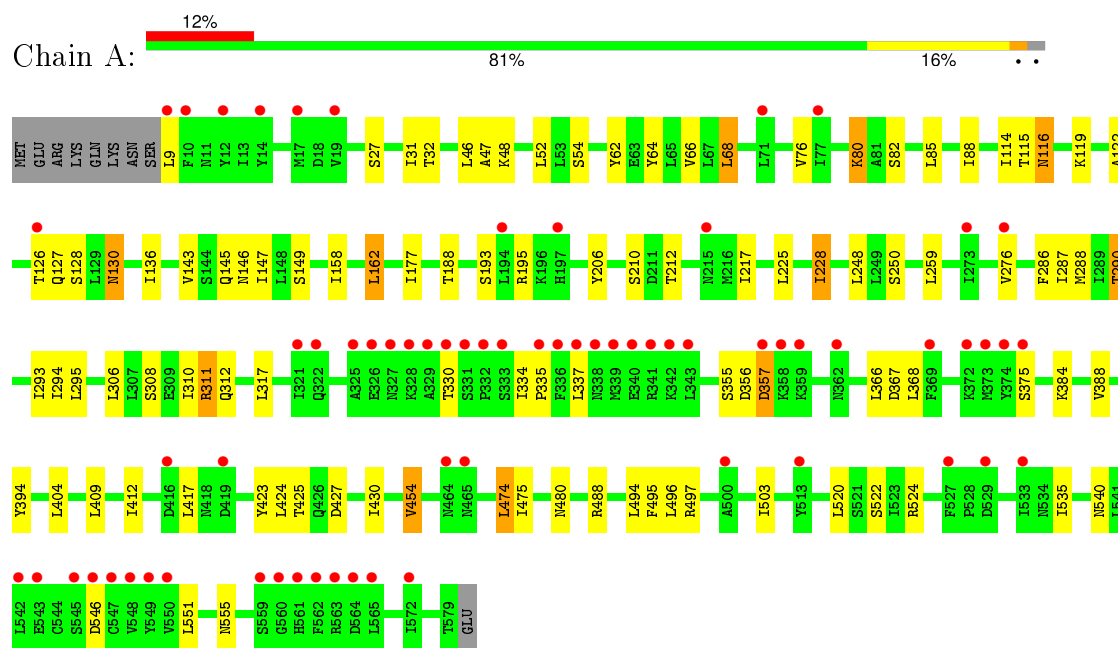


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 21 15 6	0	0
4	B	1	Total C O 21 15 6	0	0

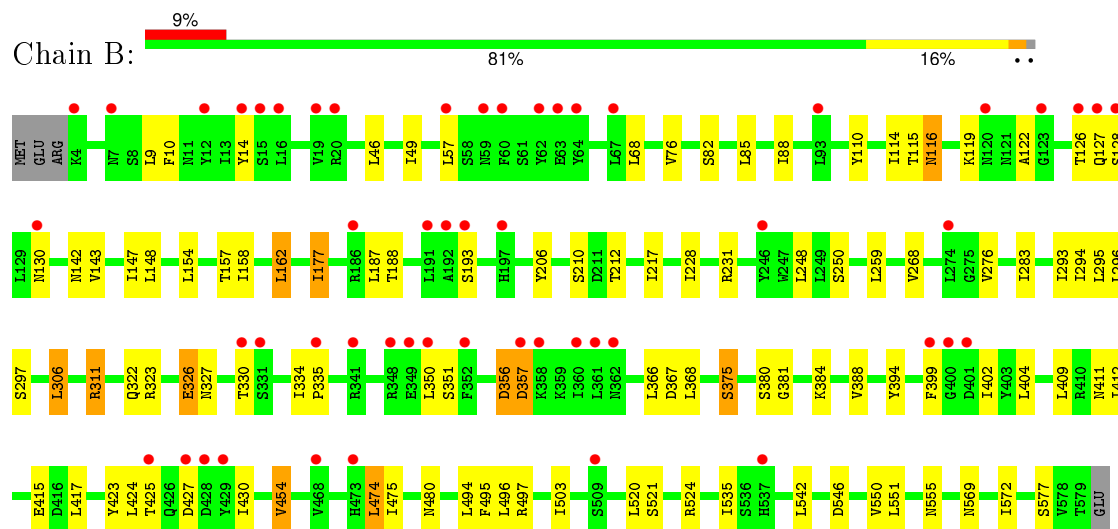
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.83Å 107.92Å 232.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 2.70 48.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.96-2.70) 99.7 (48.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.247 , 0.266 0.267 , 0.290	Depositor DCC
R_{free} test set	2891 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	6 of 56625 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9213	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: BNG, MG, ANP

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	0.50	0/4603	0.64	1/6234 (0.0%)
1	B	0.50	0/4663	0.64	1/6313 (0.0%)
All	All	0.50	0/9266	0.64	2/12547 (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	357	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	357	ASP	CB-CG-OD2	5.17	122.95	118.30

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	4527	0	4638	44	0
1	B	4580	0	4701	46	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	30	0	0
All	All	9213	0	9425	81	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 4.

All (81) 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:48:LYS:HB3	1:A:68:LEU:HD21	1.69	0.75
1:A:143:VAL:HA	1:A:147:ILE:HD12	1.73	0.71
1:B:143:VAL:HA	1:B:147:ILE:HD12	1.75	0.68
1:B:188:THR:HG23	1:B:311:ARG:HE	1.58	0.67
1:A:188:THR:HG23	1:A:308:SER:HA	1.78	0.64
1:A:32:THR:HG21	1:A:145:GLN:HA	1.81	0.62
1:B:454:VAL:HG22	1:B:495:PHE:HB2	1.81	0.62
1:A:454:VAL:HG22	1:A:495:PHE:HB2	1.83	0.61
1:B:212:THR:HG23	1:B:231:ARG:HH21	1.66	0.60
1:B:10:PHE:O	1:B:14:TYR:HD2	1.84	0.59
1:B:409:LEU:HA	1:B:412:ILE:HD12	1.85	0.58
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.86	0.57
1:B:569:ASN:HD22	1:B:572:ILE:H	1.53	0.57
1:A:76:VAL:HG11	1:B:294:ILE:HG12	1.86	0.56
1:A:308:SER:O	1:A:312:GLN:HG2	2.06	0.56
1:B:424:LEU:HD11	1:B:494:LEU:HD22	1.87	0.56
1:B:366:LEU:HD23	1:B:368:LEU:HD11	1.87	0.56
1:A:158:ILE:O	1:A:162:LEU:HB2	2.06	0.56
1:B:384:LYS:HD2	1:B:535:ILE:HG23	1.87	0.56
1:B:351:SER:HB2	1:B:399:PHE:HB2	1.88	0.55
1:A:366:LEU:HD23	1:A:368:LEU:HD11	1.87	0.55
1:A:384:LYS:HD2	1:A:535:ILE:HG23	1.87	0.55
1:B:454:VAL:HG22	1:B:495:PHE:CB	2.36	0.55
1:A:475:ILE:HB	1:A:480:ASN:HB2	1.89	0.54
1:B:454:VAL:HG21	1:B:496:LEU:HG	1.90	0.54
1:B:475:ILE:HB	1:B:480:ASN:HB2	1.89	0.53
1:A:454:VAL:HG21	1:A:496:LEU:HG	1.91	0.52
1:A:430:ILE:HG21	1:A:474:LEU:HD22	1.90	0.52
1:A:188:THR:HG22	1:A:311:ARG:HG2	1.92	0.52
1:A:424:LEU:HD11	1:A:494:LEU:HD22	1.91	0.51
1:B:116:ASN:HA	1:B:119:LYS:HD3	1.92	0.51
1:A:27:SER:O	1:A:31:ILE:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:CE1	1:B:283:ILE:HD11	2.46	0.51
1:B:430:ILE:HG21	1:B:474:LEU:HD22	1.91	0.51
1:A:116:ASN:HA	1:A:119:LYS:HD3	1.92	0.51
1:B:217:ILE:H	1:B:217:ILE:HD12	1.76	0.50
1:A:217:ILE:HD12	1:A:217:ILE:H	1.75	0.50
1:A:454:VAL:HG22	1:A:495:PHE:CB	2.41	0.49
1:A:225:LEU:HB2	1:B:110:TYR:CZ	2.48	0.49
1:B:356:ASP:O	1:B:357:ASP:HB2	2.12	0.48
1:B:375:SER:HB3	1:B:542:LEU:HD23	1.95	0.48
1:A:136:ILE:HG13	1:A:317:LEU:HD21	1.96	0.48
1:A:334:ILE:HG12	1:A:337:LEU:HB2	1.96	0.48
1:A:294:ILE:HG12	1:B:76:VAL:HG11	1.96	0.48
1:A:290:THR:HA	1:A:293:ILE:HD12	1.95	0.48
1:A:210:SER:HB2	1:B:122:ALA:HB1	1.97	0.47
1:B:268:VAL:HG12	1:B:293:ILE:HD11	1.95	0.47
1:A:122:ALA:HB1	1:B:210:SER:HB2	1.97	0.47
1:A:32:THR:HG22	1:A:149:SER:HB2	1.96	0.47
1:A:286:PHE:O	1:A:290:THR:HG23	2.15	0.46
1:A:195:ARG:HD2	1:A:312:GLN:HB2	1.98	0.46
1:B:475:ILE:H	1:B:480:ASN:HD22	1.65	0.45
4:A:603:BNG:H4'1	1:B:46:LEU:HD11	1.97	0.45
1:B:322:GLN:O	1:B:326:GLU:HB2	2.16	0.45
1:A:80:LYS:HE3	1:B:297:SER:HB2	1.99	0.45
1:B:154:LEU:HD22	1:B:177:ILE:HD13	1.99	0.45
1:B:157:THR:HG21	1:B:296:LEU:HD21	1.98	0.45
1:A:146:ASN:O	1:A:306:LEU:HD22	2.16	0.44
1:A:388:VAL:HB	1:A:503:ILE:HD13	2.00	0.44
1:B:158:ILE:O	1:B:162:LEU:HB2	2.18	0.43
1:B:334:ILE:HG12	1:B:411:ASN:O	2.18	0.43
1:B:388:VAL:HB	1:B:503:ILE:HD13	2.00	0.43
1:B:142:ASN:OD1	1:B:306:LEU:HA	2.19	0.43
1:B:114:ILE:HD13	1:B:394:TYR:HA	2.01	0.43
1:A:212:THR:HG21	1:A:228:ILE:HG23	2.01	0.42
1:B:381:GLY:HA2	2:B:601:ANP:H3'	2.00	0.42
1:A:130:ASN:ND2	1:B:206:TYR:OH	2.53	0.42
1:B:49:ILE:HG13	1:B:68:LEU:HB3	2.01	0.42
1:A:114:ILE:HD13	1:A:394:TYR:HA	2.02	0.41
1:A:47:ALA:HB2	1:A:288:MET:HB2	2.03	0.41
1:A:409:LEU:HD22	1:A:417:LEU:HD11	2.02	0.41
1:B:350:LEU:HD22	1:B:402:ILE:HD11	2.01	0.41
1:B:550:VAL:HG11	1:B:569:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD22	1:B:417:LEU:HD11	2.03	0.41
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.89	0.41
1:A:228:ILE:HA	1:A:228:ILE:HD13	1.84	0.41
1:A:127:GLN:HG2	1:A:206:TYR:CD2	2.56	0.41
1:A:355:SER:C	1:A:357:ASP:H	2.24	0.41
1:B:127:GLN:HG2	1:B:206:TYR:CD2	2.56	0.40
1:A:488:ARG:NH2	1:B:380:SER:HB3	2.36	0.40
1:A:52:LEU:HD21	1:A:64:TYR:CD2	2.56	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	569/580 (98%)	531 (93%)	36 (6%)	2 (0%)	39	69
1	B	576/580 (99%)	535 (93%)	38 (7%)	3 (0%)	34	63
All	All	1145/1160 (99%)	1066 (93%)	74 (6%)	5 (0%)	39	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	PRO
1	B	327	ASN
1	A	356	ASP
1	B	323	ARG
1	B	335	PRO

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%)	476 (92%)	44 (8%)	13	30
1	B	527/529 (100%)	484 (92%)	43 (8%)	14	32
All	All	1047/1058 (99%)	960 (92%)	87 (8%)	14	31

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	46	LEU
1	A	54	SER
1	A	66	VAL
1	A	68	LEU
1	A	80	LYS
1	A	82	SER
1	A	85	LEU
1	A	88	ILE
1	A	115	THR
1	A	116	ASN
1	A	126	THR
1	A	128	SER
1	A	130	ASN
1	A	162	LEU
1	A	177	ILE
1	A	193	SER
1	A	228	ILE
1	A	248	LEU
1	A	250	SER
1	A	259	LEU
1	A	276	VAL
1	A	287	ILE
1	A	290	THR
1	A	295	LEU
1	A	310	ILE
1	A	311	ARG

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Mol	Chain	Res	Type
1	A	330	THR
1	A	367	ASP
1	A	375	SER
1	A	404	LEU
1	A	423	TYR
1	A	425	THR
1	A	427	ASP
1	A	454	VAL
1	A	474	LEU
1	A	497	ARG
1	A	520	LEU
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	9	LEU
1	B	57	LEU
1	B	82	SER
1	B	85	LEU
1	B	88	ILE
1	B	115	THR
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	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	326	GLU
1	B	330	THR

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Mol	Chain	Res	Type
1	B	356	ASP
1	B	367	ASP
1	B	375	SER
1	B	404	LEU
1	B	415	GLU
1	B	423	TYR
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	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	96	ASN
1	A	127	GLN
1	A	130	ASN
1	A	153	GLN
1	A	223	ASN
1	A	479	ASN
1	A	487	GLN
1	A	534	ASN
1	B	96	ASN
1	B	127	GLN
1	B	130	ASN
1	B	153	GLN
1	B	223	ASN
1	B	459	ASN
1	B	479	ASN
1	B	480	ASN
1	B	515	ASN
1	B	569	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	ANP	A	601	3	27,33,33	3.08	5 (18%)	30,52,52	2.00	5 (16%)
4	BNG	A	603	-	21,21,21	0.22	0	26,26,26	0.26	0
2	ANP	B	601	3	27,33,33	3.22	5 (18%)	30,52,52	2.06	4 (13%)
4	BNG	B	603	-	21,21,21	0.21	0	26,26,26	0.40	0

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	ANP	A	601	3	-	0/12/38/38	0/3/3/3
4	BNG	A	603	-	-	0/12/32/32	0/1/1/1
2	ANP	B	601	3	-	0/12/38/38	0/3/3/3
4	BNG	B	603	-	-	0/12/32/32	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ANP	PB-O3A	-4.34	1.53	1.59
2	A	601	ANP	PB-O3A	-3.80	1.54	1.59
2	A	601	ANP	PB-O2B	-3.12	1.48	1.56
2	B	601	ANP	PB-O2B	-3.09	1.48	1.56
2	B	601	ANP	PG-O3G	-2.84	1.48	1.56
2	A	601	ANP	PG-O3G	-2.23	1.50	1.56
2	A	601	ANP	PG-O1G	10.13	1.57	1.46
2	B	601	ANP	PG-O1G	10.54	1.58	1.46
2	A	601	ANP	PB-O1B	10.70	1.58	1.46
2	B	601	ANP	PB-O1B	11.03	1.58	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ANP	O2G-PG-O1G	-6.88	95.20	113.49
2	A	601	ANP	O2G-PG-O1G	-6.38	96.53	113.49
2	A	601	ANP	O1B-PB-N3B	-3.44	106.62	111.90
2	B	601	ANP	O1B-PB-N3B	-2.97	107.34	111.90
2	A	601	ANP	O2B-PB-O1B	2.59	115.41	110.00
2	B	601	ANP	O3G-PG-O2G	3.56	118.14	107.58
2	A	601	ANP	O3G-PG-O2G	3.66	118.44	107.58
2	A	601	ANP	PA-O3A-PB	5.33	150.53	132.67
2	B	601	ANP	PA-O3A-PB	5.89	152.41	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	BNG	1	0
2	B	601	ANP	1	0

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	571/580 (98%)	0.66	68 (11%) 6 5	61, 95, 135, 202	0
1	B	576/580 (99%)	0.48	53 (9%) 11 9	63, 92, 134, 184	0
All	All	1147/1160 (98%)	0.57	121 (10%) 8 6	61, 94, 135, 202	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	PHE	18.3
1	A	329	ALA	11.5
1	A	328	LYS	10.1
1	A	335	PRO	10.1
1	A	341	ARG	9.6
1	A	327	ASN	9.2
1	A	330	THR	9.2
1	A	340	GLU	7.6
1	A	562	PHE	7.0
1	A	338	ASN	6.5
1	A	331	SER	5.5
1	A	339	MET	5.3
1	A	326	GLU	5.2
1	A	529	ASP	5.2
1	B	357	ASP	5.0
1	A	500	ALA	4.9
1	A	14	TYR	4.9
1	A	565	LEU	4.9
1	A	564	ASP	4.8
1	B	349	GLU	4.7
1	A	543	GLU	4.6
1	B	63	GLU	4.5
1	A	9	LEU	4.5
1	B	12	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	64	TYR	4.4
1	A	560	GLY	4.4
1	A	548	VAL	4.3
1	A	337	LEU	4.2
1	B	62	TYR	4.1
1	A	332	PRO	3.8
1	A	563	ARG	3.7
1	B	59	ASN	3.7
1	B	193	SER	3.6
1	A	374	TYR	3.6
1	A	549	TYR	3.6
1	B	350	LEU	3.6
1	B	19	VAL	3.5
1	A	333	SER	3.5
1	A	464	ASN	3.5
1	B	16	LEU	3.5
1	A	357	ASP	3.5
1	B	60	PHE	3.4
1	A	561	HIS	3.4
1	B	352	PHE	3.3
1	A	342	LYS	3.3
1	A	17	MET	3.2
1	A	545	SER	3.2
1	B	473	HIS	3.1
1	B	4	LYS	3.0
1	A	343	LEU	3.0
1	B	341	ARG	3.0
1	B	400	GLY	3.0
1	A	547	CYS	2.9
1	A	359	LYS	2.9
1	B	428	ASP	2.9
1	B	126	THR	2.8
1	B	20	ARG	2.8
1	B	331	SER	2.8
1	B	191	LEU	2.8
1	B	246	TYR	2.8
1	A	550	VAL	2.8
1	B	362	ASN	2.8
1	A	419	ASP	2.7
1	B	127	GLN	2.7
1	B	425	THR	2.7
1	B	7	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	362	ASN	2.7
1	B	427	ASP	2.7
1	B	401	ASP	2.7
1	B	14	TYR	2.7
1	A	12	TYR	2.6
1	B	335	PRO	2.6
1	A	19	VAL	2.6
1	A	533	ILE	2.6
1	A	542	LEU	2.6
1	B	330	THR	2.6
1	B	15	SER	2.6
1	A	197	HIS	2.6
1	A	10	PHE	2.6
1	B	274	LEU	2.5
1	A	77	ILE	2.5
1	A	572	ILE	2.5
1	B	537	HIS	2.5
1	B	130	ASN	2.5
1	A	375	SER	2.5
1	B	197	HIS	2.5
1	A	71	LEU	2.4
1	B	429	TYR	2.4
1	A	527	PHE	2.4
1	B	361	LEU	2.4
1	A	559	SER	2.4
1	A	215	ASN	2.4
1	B	399	PHE	2.4
1	A	276	VAL	2.4
1	B	93	LEU	2.3
1	A	322	GLN	2.3
1	B	468	VAL	2.3
1	B	348	ARG	2.3
1	A	372	LYS	2.3
1	A	373	MET	2.3
1	B	360	ILE	2.3
1	A	369	PHE	2.3
1	A	358	LYS	2.3
1	A	325	ALA	2.2
1	B	67	LEU	2.2
1	A	513	TYR	2.2
1	A	546	ASP	2.2
1	A	465	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	ILE	2.1
1	A	126	THR	2.1
1	B	186	ARG	2.1
1	A	416	ASP	2.1
1	B	128	SER	2.1
1	B	57	LEU	2.1
1	B	358	LYS	2.1
1	B	120	ASN	2.1
1	A	194	LEU	2.0
1	B	509	SER	2.1
1	A	273	ILE	2.0
1	B	123	GLY	2.0
1	B	192	ALA	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 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	A	602	1/1	0.94	0.24	5.61	69,69,69,69	0
4	BNG	B	603	21/21	0.90	0.27	2.15	96,111,120,124	0
4	BNG	A	603	21/21	0.85	0.26	1.75	92,123,129,129	0
2	ANP	A	601	31/31	0.96	0.15	-0.30	91,103,107,109	0
2	ANP	B	601	31/31	0.95	0.15	-1.03	81,88,94,94	0
3	MG	B	602	1/1	0.91	0.27	-	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.