



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:20 am BST

PDB ID : 6SJ9
Title : Proteasome accessory factor B/C (PafBC) of *Arthrobacter aurescens*
Authors : Mueller, A.U.; Leibundgut, M.; Ban, N.; Weber-Ban, E.
Deposited on : 2019-08-13
Resolution : 2.20 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 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 : 2.11
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) : 2.11

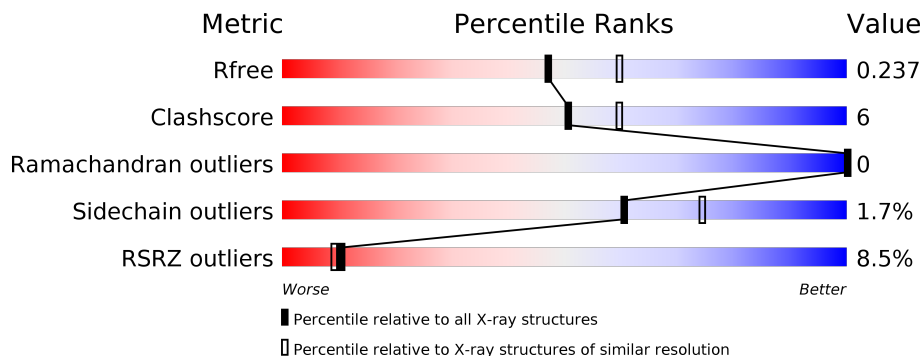
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	664	
1	B	664	

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
4	PG4	A	703	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10249 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.

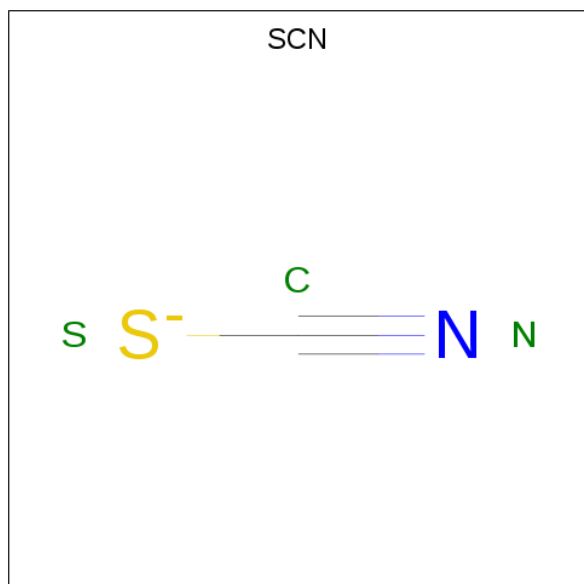
- Molecule 1 is a protein called Proteasome accessory factor B/C (PafBC).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	642	4978	3124	898	946	3	7	0	1	0
1	B	637	4958	3113	895	940	3	7	0	1	0

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

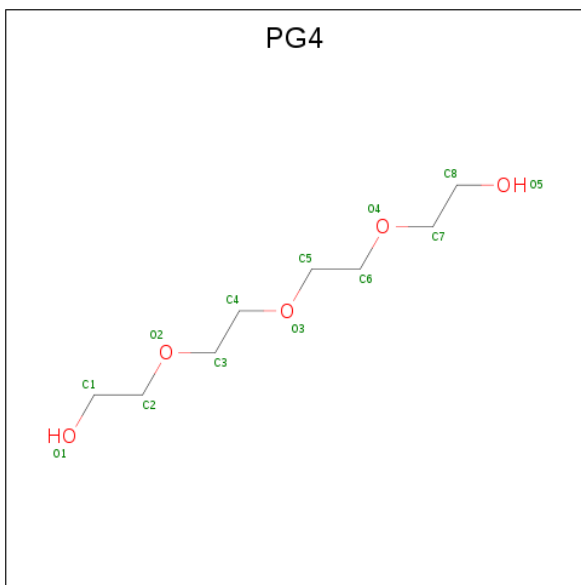
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	K 1	0	0
2	A	1	Total 1	K 1	0	0

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



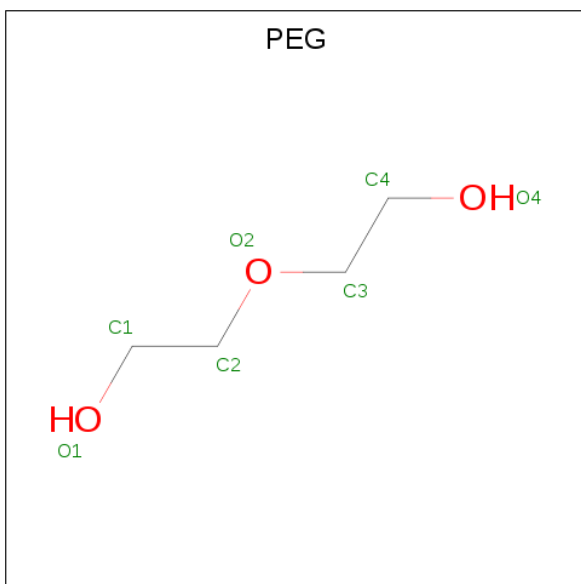
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

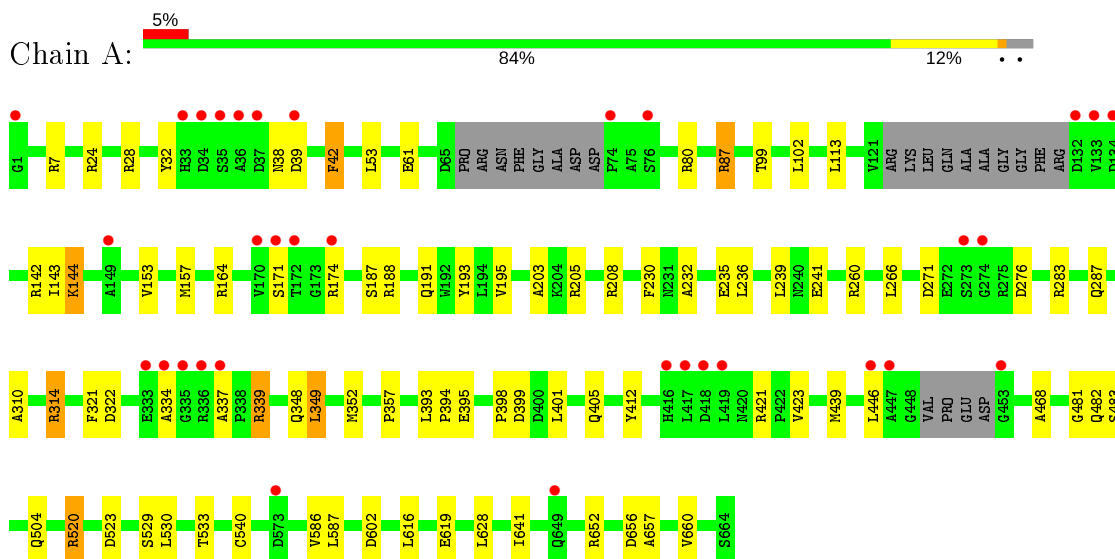
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	170	Total O 170 170	0	0
6	B	94	Total O 94 94	0	0

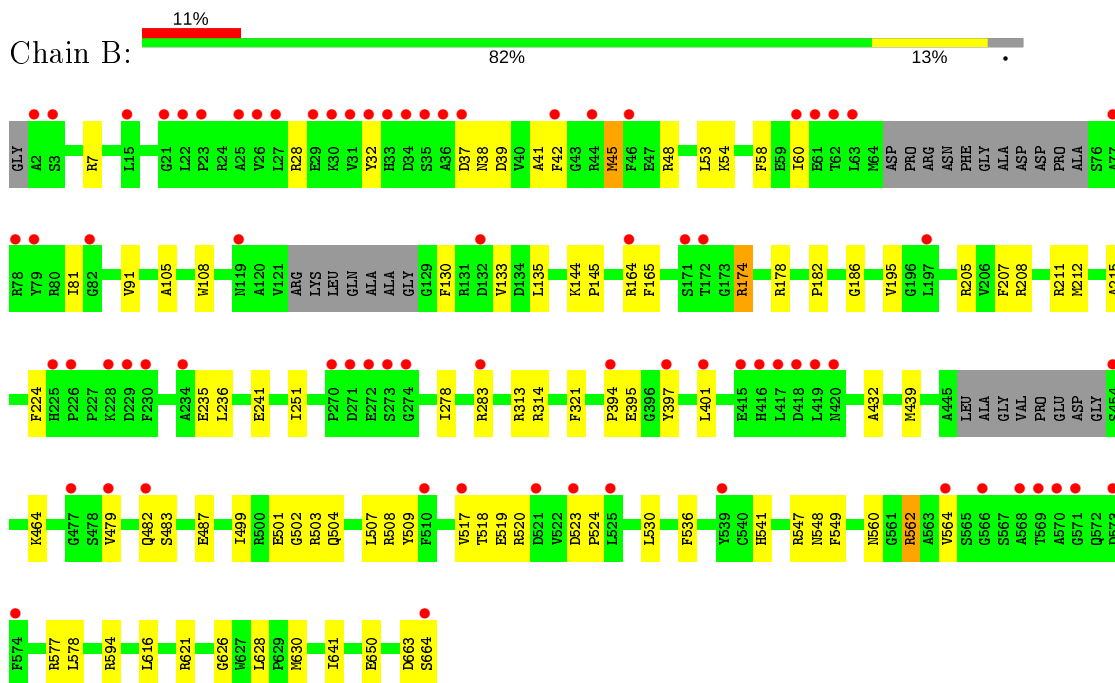
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Proteasome accessory factor B/C (PafBC)



- Molecule 1: Proteasome accessory factor B/C (PafBC)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.88Å 119.03Å 160.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 2.20 48.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.73-2.20) 99.9 (48.72-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.203 , 0.237 0.203 , 0.237	Depositor DCC
R_{free} test set	4361 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage'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, 0.333 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: PG4, K, PEG, SCN

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	0.61	0/5071	0.76	4/6863 (0.1%)
1	B	0.52	0/5050	0.69	2/6832 (0.0%)
All	All	0.57	0/10121	0.73	6/13695 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	621	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	520	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	349	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	B	314	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	314	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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	4978	0	4929	53	0
1	B	4958	0	4910	61	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	13	0	18	1	0
5	A	21	0	30	1	0
5	B	7	0	10	0	0
6	A	170	0	0	1	0
6	B	94	0	0	3	0
All	All	10249	0	9897	114	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 6.

All (114) 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:105:ALA:HB1	1:B:394:PRO:HB3	1.70	0.72
1:A:241:GLU:OE1	1:A:283:ARG:NH1	2.22	0.72
1:B:241:GLU:OE2	1:B:283:ARG:NH2	2.23	0.71
1:B:547:ARG:O	6:B:801:HOH:O	2.10	0.70
1:A:334:ALA:O	1:A:339:ARG:NH1	2.25	0.69
1:B:91:VAL:HG21	1:B:464:LYS:HB3	1.76	0.67
1:B:501:GLU:OE1	1:B:503:ARG:NE	2.20	0.65
1:A:260:ARG:NH2	1:A:276:ASP:OD2	2.18	0.63
1:A:401:LEU:HA	1:A:421:ARG:HD3	1.82	0.61
1:A:195:VAL:HG21	1:A:235:GLU:HG2	1.84	0.60
1:A:337:ALA:O	1:A:339:ARG:NH2	2.29	0.60
1:A:520:ARG:HD3	1:A:540:CYS:SG	2.42	0.60
1:B:105:ALA:CB	1:B:394:PRO:HB3	2.31	0.60
1:B:28:ARG:NH1	1:B:38:ASN:HA	2.17	0.60
1:B:439:MSE:HE3	1:B:530:LEU:HD13	1.84	0.60
1:B:313:ARG:NH2	6:B:803:HOH:O	2.28	0.58
1:B:215:ALA:HB1	1:B:594:ARG:HH11	1.68	0.57
1:B:38:ASN:HD22	1:B:39:ASP:H	1.54	0.56
1:A:188:ARG:NH2	1:A:405:GLN:OE1	2.39	0.56
1:B:208:ARG:HB2	1:B:211:ARG:HG2	1.87	0.56
1:A:587:LEU:HD21	1:A:619:GLU:HG2	1.88	0.55
1:B:186:GLY:HA3	1:B:236:LEU:HD11	1.87	0.55
1:B:394:PRO:HG2	1:B:397:TYR:CB	2.37	0.55
1:A:144:LYS:HE3	1:A:602:ASP:OD2	2.08	0.54
1:A:322:ASP:OD1	1:A:652:ARG:NH1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG21	1:B:626:GLY:O	2.08	0.53
1:A:142:ARG:NH2	1:A:394:PRO:HG3	2.24	0.53
1:B:397:TYR:OH	1:B:401:LEU:HD13	2.08	0.53
1:A:446:LEU:HD23	1:A:446:LEU:H	1.74	0.52
1:A:628:LEU:HG	1:A:641:ILE:HD11	1.92	0.52
1:A:142:ARG:CZ	1:A:394:PRO:HG3	2.39	0.52
1:B:205:ARG:HD3	1:B:207:PHE:CZ	2.45	0.52
1:B:130:PHE:HA	1:B:650:GLU:HG3	1.91	0.52
1:A:481:GLY:HA3	4:A:703:PG4:H41	1.92	0.52
1:B:523:ASP:OD1	1:B:541:HIS:NE2	2.43	0.51
1:B:38:ASN:ND2	1:B:39:ASP:H	2.09	0.50
1:B:394:PRO:HG2	1:B:397:TYR:HB2	1.91	0.50
1:B:508:ARG:HA	1:B:518:THR:O	2.11	0.50
1:A:348:GLN:HG2	1:A:352:MSE:HE2	1.93	0.50
1:B:144:LYS:HB2	1:B:145:PRO:HD2	1.94	0.50
1:B:182:PRO:HD2	1:B:224:PHE:CZ	2.47	0.50
1:A:349:LEU:HA	1:A:352:MSE:HE3	1.92	0.50
1:B:482:GLN:HG3	1:B:483:SER:O	2.10	0.50
1:A:482:GLN:HG3	1:A:483:SER:O	2.13	0.49
1:A:412:TYR:HB2	6:A:932:HOH:O	2.12	0.49
1:A:24:ARG:HD3	1:A:42:PHE:HE2	1.77	0.48
1:B:135:LEU:HD21	1:B:630:MSE:HE1	1.96	0.48
1:A:349:LEU:HD23	1:A:352:MSE:HE3	1.94	0.48
1:A:310:ALA:O	1:A:314:ARG:HG3	2.13	0.48
1:B:37:ASP:HB2	1:B:41:ALA:HB3	1.96	0.48
1:A:393:LEU:CD1	1:A:399:ASP:HA	2.44	0.47
1:B:195:VAL:HG21	1:B:235:GLU:HG2	1.96	0.47
1:B:518:THR:OG1	1:B:520:ARG:NH2	2.28	0.47
1:B:60:ILE:HG12	1:B:81:ILE:HD11	1.96	0.47
1:B:439:MSE:HE2	1:B:479:VAL:CG1	2.44	0.47
1:B:502:GLY:C	1:B:564:VAL:HG13	2.34	0.47
1:A:504:GLN:HG3	1:A:523:ASP:OD1	2.15	0.47
1:A:188:ARG:HH11	1:A:188:ARG:HG3	1.80	0.47
1:B:439:MSE:CE	1:B:530:LEU:HD13	2.45	0.47
1:A:349:LEU:HD23	1:A:352:MSE:CE	2.46	0.46
1:A:628:LEU:HA	1:A:628:LEU:HD12	1.60	0.46
1:B:165:PHE:CD2	1:B:212:MSE:HG2	2.50	0.46
1:B:507:LEU:O	1:B:519:GLU:HA	2.15	0.46
1:B:520:ARG:NH1	6:B:811:HOH:O	2.47	0.46
1:B:628:LEU:HG	1:B:641:ILE:HD11	1.98	0.46
1:A:24:ARG:HD3	1:A:42:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLY:HA3	1:B:236:LEU:CD1	2.45	0.46
1:B:487:GLU:H	1:B:487:GLU:CD	2.19	0.46
1:B:663:ASP:OD1	1:B:664:SER:N	2.46	0.46
1:B:504:GLN:HG2	1:B:523:ASP:OD2	2.16	0.46
1:A:61:GLU:OE2	1:A:80:ARG:NE	2.30	0.45
1:A:87:ARG:HD2	1:A:468:ALA:O	2.16	0.45
1:B:499:ILE:HG13	1:B:524:PRO:HB2	1.98	0.45
1:A:398:PRO:HG3	1:A:423:VAL:HG11	1.99	0.45
1:A:657:ALA:O	1:A:660:VAL:HG22	2.17	0.45
1:B:54:LYS:HA	1:B:58:PHE:O	2.16	0.45
1:B:108:TRP:CE2	1:B:432:ALA:HB1	2.51	0.45
1:B:164:ARG:HA	1:B:178:ARG:O	2.17	0.45
1:B:241:GLU:HG2	1:B:283:ARG:HD2	1.99	0.45
1:A:339:ARG:HD3	1:A:339:ARG:HA	1.82	0.45
1:A:439:MSE:SE	1:A:530:LEU:HD21	2.67	0.44
1:B:7:ARG:HD2	1:B:32:TYR:CE1	2.53	0.44
1:A:357:PRO:HB2	5:A:704:PEG:H21	2.00	0.44
1:A:656:ASP:O	1:A:660:VAL:HG13	2.18	0.44
1:B:536:PHE:CE1	1:B:549:PHE:HB2	2.53	0.44
1:A:191:GLN:HG3	1:A:208:ARG:HH12	1.82	0.43
1:B:401:LEU:O	1:B:401:LEU:HD23	2.18	0.43
1:A:38:ASN:HB3	1:A:39:ASP:H	1.61	0.43
1:A:230:PHE:CZ	1:A:232:ALA:HB2	2.53	0.43
1:B:182:PRO:HD2	1:B:224:PHE:CE1	2.53	0.43
1:A:7:ARG:HD2	1:A:32:TYR:CE2	2.53	0.43
1:A:28:ARG:NH2	1:A:38:ASN:HA	2.33	0.43
1:A:153:VAL:O	1:A:157:MSE:HG3	2.19	0.43
1:A:171:SER:O	1:A:171:SER:OG	2.30	0.43
1:A:203:ALA:HB3	1:A:205:ARG:HH12	1.82	0.42
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.88	0.42
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.85	0.42
1:B:548:ASN:ND2	1:B:577:ARG:O	2.52	0.42
1:A:99:THR:O	1:A:102:LEU:HB3	2.19	0.42
1:A:236:LEU:O	1:A:239:LEU:HB2	2.20	0.42
1:A:529:SER:HA	1:A:533:THR:O	2.20	0.42
1:B:251:ILE:HD13	1:B:278:ILE:HD13	2.01	0.42
1:B:509:TYR:O	1:B:517:VAL:HA	2.20	0.42
1:A:143:ILE:HG21	1:A:287:GLN:HG3	2.02	0.41
1:B:174:ARG:H	1:B:174:ARG:CD	2.33	0.41
1:B:523:ASP:CG	1:B:541:HIS:HE2	2.23	0.41
1:A:187:SER:O	1:A:188:ARG:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.84	0.41
1:B:439:MSE:HE3	1:B:530:LEU:HD22	2.01	0.41
1:A:193:TYR:OH	1:A:208:ARG:NH2	2.53	0.41
1:B:502:GLY:O	1:B:564:VAL:N	2.47	0.41
1:B:45:MSE:HA	1:B:48:ARG:NH2	2.36	0.40
1:B:560:ASN:CG	1:B:562:ARG:HD3	2.42	0.40
1:B:530:LEU:HD23	1:B:578:LEU:HD21	2.04	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	635/664 (96%)	623 (98%)	12 (2%)	0	100	100
1	B	630/664 (95%)	618 (98%)	12 (2%)	0	100	100
All	All	1265/1328 (95%)	1241 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/524 (98%)	505 (98%)	11 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	515/524 (98%)	508 (99%)	7 (1%)	67	80
All	All	1031/1048 (98%)	1013 (98%)	18 (2%)	60	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	PHE
1	A	144	LYS
1	A	164	ARG
1	A	174	ARG
1	A	266	LEU
1	A	271	ASP
1	A	321	PHE
1	A	339	ARG
1	A	395	GLU
1	A	586	VAL
1	A	616	LEU
1	B	42	PHE
1	B	45	MSE
1	B	174	ARG
1	B	321	PHE
1	B	395	GLU
1	B	562	ARG
1	B	616	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
5	PEG	A	704	-	6,6,6	0.50	0	5,5,5	0.40	0
5	PEG	A	705	-	6,6,6	0.47	0	5,5,5	0.30	0
5	PEG	B	703	-	6,6,6	0.48	0	5,5,5	0.31	0
4	PG4	A	703	-	12,12,12	0.54	0	11,11,11	0.42	0
3	SCN	A	702	-	1,2,2	0.30	0	0,1,1	0.00	-
5	PEG	A	706	-	6,6,6	0.49	0	5,5,5	0.40	0
3	SCN	B	702	-	1,2,2	0.58	0	0,1,1	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
5	PEG	A	704	-	-	3/4/4/4	-
5	PEG	A	705	-	-	1/4/4/4	-
5	PEG	A	706	-	-	3/4/4/4	-
5	PEG	B	703	-	-	2/4/4/4	-
4	PG4	A	703	-	-	8/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	PG4	C5-C6-O4-C7
4	A	703	PG4	O2-C3-C4-O3
5	A	704	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	705	PEG	O1-C1-C2-O2
5	A	706	PEG	O2-C3-C4-O4
4	A	703	PG4	O4-C7-C8-O5
5	A	706	PEG	O1-C1-C2-O2
5	A	704	PEG	C1-C2-O2-C3
5	B	703	PEG	C1-C2-O2-C3
5	B	703	PEG	C4-C3-O2-C2
5	A	706	PEG	C1-C2-O2-C3
5	A	704	PEG	C4-C3-O2-C2
4	A	703	PG4	C6-C5-O3-C4
4	A	703	PG4	O1-C1-C2-O2
4	A	703	PG4	C1-C2-O2-C3
4	A	703	PG4	O3-C5-C6-O4
4	A	703	PG4	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	PEG	1	0
4	A	703	PG4	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	635/664 (95%)	0.18	33 (5%) 27 26	34, 58, 130, 203	0
1	B	630/664 (94%)	0.59	75 (11%) 4 4	34, 76, 147, 198	0
All	All	1265/1328 (95%)	0.39	108 (8%) 10 9	34, 67, 141, 203	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	11.4
1	B	419	LEU	9.4
1	A	170	VAL	8.5
1	B	566	GLY	7.9
1	B	664	SER	7.5
1	A	447	ALA	7.3
1	B	570	ALA	7.3
1	A	172	THR	7.3
1	B	415	GLU	6.6
1	B	569	THR	6.4
1	B	35	SER	6.3
1	B	36	ALA	6.1
1	B	63	LEU	6.1
1	B	225	HIS	6.1
1	B	420	ASN	5.6
1	A	336	ARG	5.0
1	A	37	ASP	4.9
1	B	32	TYR	4.9
1	B	42	PHE	4.9
1	B	172	THR	4.8
1	A	174	ARG	4.7
1	B	564	VAL	4.7
1	A	39	ASP	4.6
1	B	228	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	453	GLY	4.6
1	A	337	ALA	4.6
1	B	62	THR	4.5
1	A	446	LEU	4.5
1	A	334	ALA	4.5
1	B	226	PRO	4.5
1	A	34	ASP	4.4
1	B	573	ASP	4.4
1	B	37	ASP	4.3
1	A	133	VAL	4.2
1	B	523	ASP	4.0
1	B	3	SER	4.0
1	B	77	ALA	4.0
1	A	171	SER	4.0
1	B	61	GLU	3.9
1	B	171	SER	3.9
1	B	78	ARG	3.9
1	B	539	TYR	3.9
1	B	2	ALA	3.9
1	B	27	LEU	3.9
1	A	416	HIS	3.7
1	B	30	LYS	3.6
1	A	649	GLN	3.6
1	A	274	GLY	3.6
1	B	273	SER	3.6
1	A	36	ALA	3.6
1	B	31	VAL	3.6
1	B	34	ASP	3.5
1	A	273	SER	3.4
1	A	418	ASP	3.3
1	B	517	VAL	3.3
1	B	33	HIS	3.3
1	B	271	ASP	3.2
1	B	79	TYR	3.2
1	B	234	ALA	3.1
1	B	283	ARG	3.1
1	B	26	VAL	3.0
1	B	394	PRO	3.0
1	B	274	GLY	3.0
1	B	164	ARG	2.9
1	B	22	LEU	2.9
1	B	418	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	23	PRO	2.8
1	A	1	GLY	2.8
1	B	29	GLU	2.8
1	A	335	GLY	2.8
1	A	573	ASP	2.8
1	B	229	ASP	2.8
1	B	416	HIS	2.8
1	B	119	ASN	2.8
1	B	568	ALA	2.7
1	B	132	ASP	2.7
1	B	25	ALA	2.7
1	B	46	PHE	2.7
1	B	21	GLY	2.7
1	B	270	PRO	2.7
1	B	574	PHE	2.7
1	B	272	GLU	2.7
1	B	482	GLN	2.7
1	B	15	LEU	2.6
1	A	333	GLU	2.6
1	B	521	ASP	2.6
1	A	74	PRO	2.6
1	B	44	ARG	2.6
1	B	477	GLY	2.5
1	B	82	GLY	2.5
1	B	479	VAL	2.5
1	B	230	PHE	2.5
1	B	454	SER	2.5
1	A	134	ASP	2.5
1	A	33	HIS	2.4
1	B	60	ILE	2.4
1	B	510	PHE	2.4
1	B	571	GLY	2.4
1	A	132	ASP	2.3
1	A	419	LEU	2.2
1	B	397	TYR	2.2
1	B	197	LEU	2.2
1	A	149	ALA	2.1
1	A	35	SER	2.1
1	B	401	LEU	2.0
1	B	525	LEU	2.0
1	A	76	SER	2.0
1	A	417	LEU	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. 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(Å ²)	Q<0.9
4	PG4	A	703	13/13	0.48	0.54	97,107,112,112	0
5	PEG	B	703	7/7	0.60	0.34	88,90,92,92	0
2	K	B	701	1/1	0.78	0.05	98,98,98,98	0
5	PEG	A	705	7/7	0.84	0.32	88,91,93,93	0
5	PEG	A	704	7/7	0.87	0.23	75,77,81,83	0
5	PEG	A	706	7/7	0.87	0.20	95,95,98,98	0
3	SCN	B	702	3/3	0.94	0.09	57,57,60,61	0
2	K	A	701	1/1	0.98	0.12	52,52,52,52	0
3	SCN	A	702	3/3	0.99	0.15	32,32,34,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.