



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2018 – 02:40 PM EST

PDB ID : 5X6F
Title : Crystal structure of Phosphopantetheine adenylyltransferase from *Pseudomonas aeruginosa*
Authors : Mondal, A.; Chatterjee, R.; Datta, S.
Deposited on : 2017-02-21
Resolution : 2.59 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-20030736
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-20030736

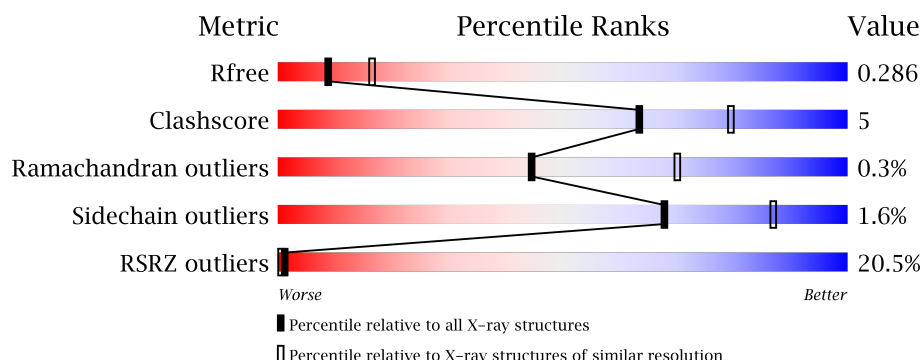
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	159	<div> <div>34%</div> <div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	159	<div> <div>5%</div> <div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
1	C	159	<div> <div>36%</div> <div> <div>86%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	159	<div> <div>5%</div> <div> <div>89%</div> <div>11%</div> <div>.</div> </div> </div>
1	E	159	<div> <div>36%</div> <div> <div>82%</div> <div>17%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	159	

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
2	IPA	F	201	-	-	-	X

2 Entry composition [i](#)

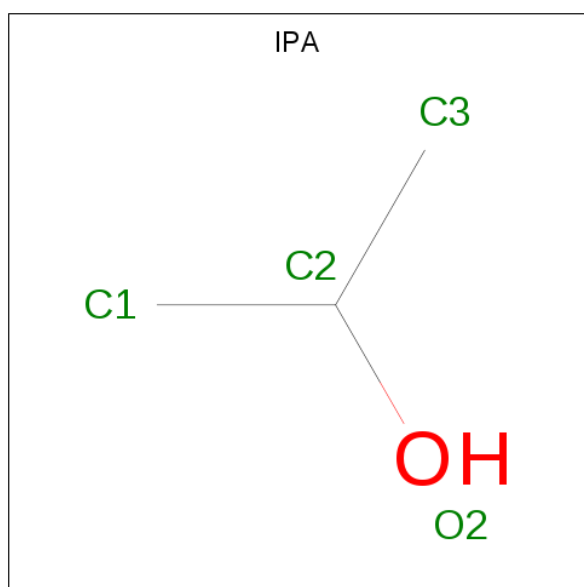
There are 4 unique types of molecules in this entry. The entry contains 7525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1244	801	215	225	3			
1	B	158	Total	C	N	O	S	0	0	0
			1244	801	215	225	3			
1	C	158	Total	C	N	O	S	0	0	0
			1244	801	215	225	3			
1	D	158	Total	C	N	O	S	0	0	0
			1244	801	215	225	3			
1	E	158	Total	C	N	O	S	0	0	0
			1244	801	215	225	3			
1	F	158	Total	C	N	O	S	0	0	0
			1244	801	215	225	3			

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	3	1		
2	F	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	8	Total	O	0	0
			8	8		
4	D	8	Total	O	0	0
			8	8		

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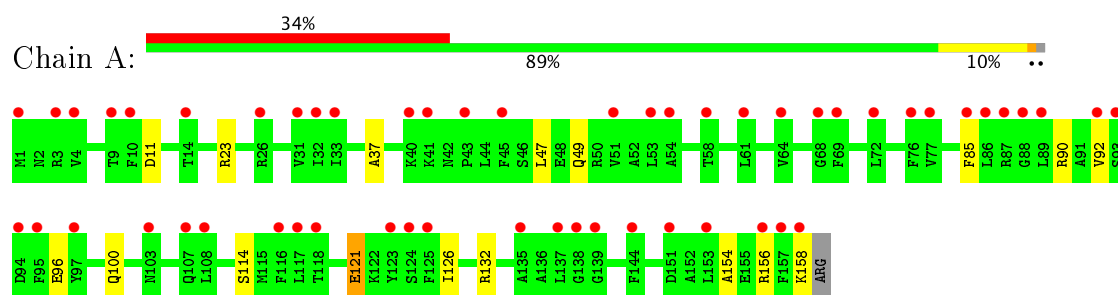
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	O	0	0
			1	1		
4	F	5	Total	O	0	0
			5	5		

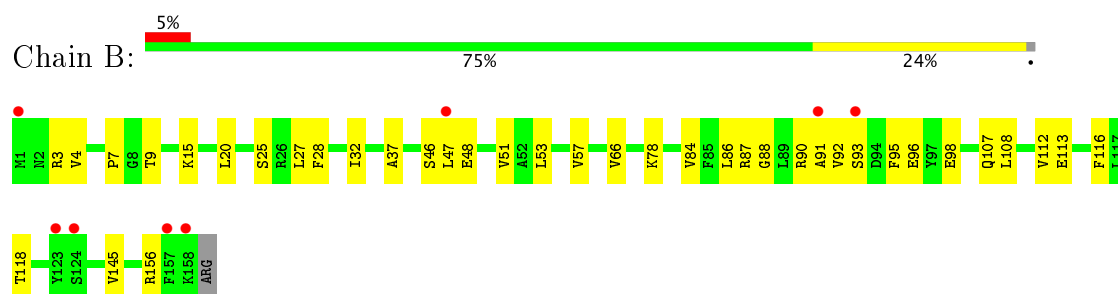
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

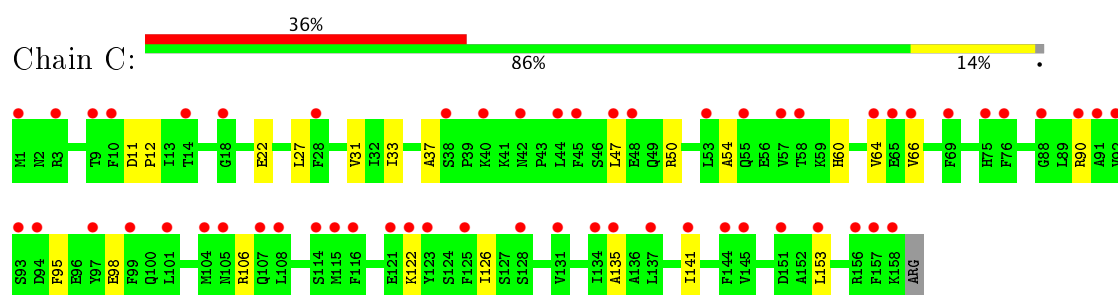
• Molecule 1: Phosphopantetheine adenylyltransferase



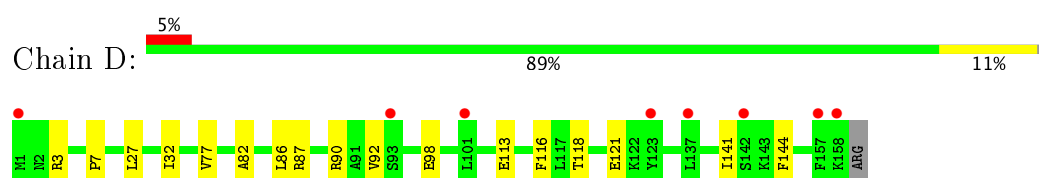
• Molecule 1: Phosphopantetheine adenylyltransferase



• Molecule 1: Phosphopantetheine adenylyltransferase

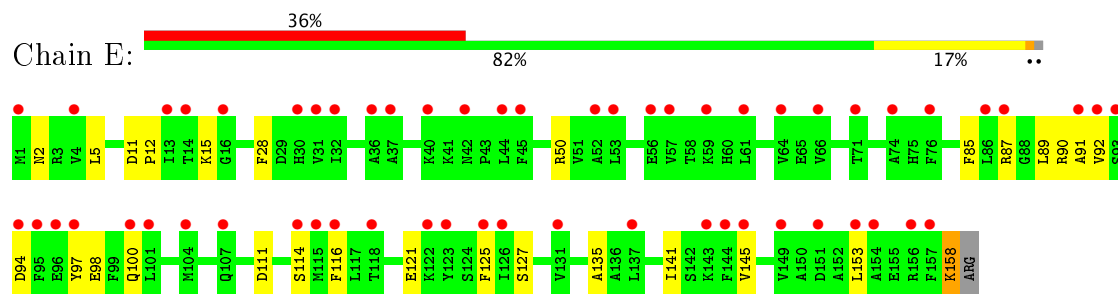


• Molecule 1: Phosphopantetheine adenylyltransferase



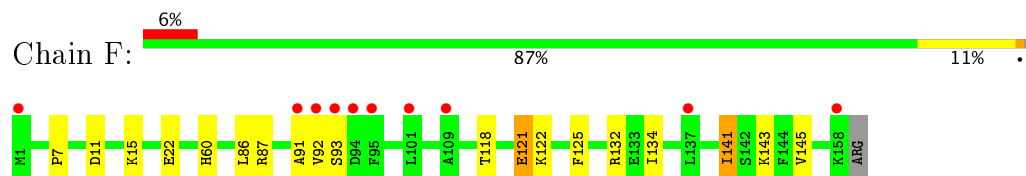
● Molecule 1: Phosphopantetheine adenylyltransferase

Chain E:



● Molecule 1: Phosphopantetheine adenylyltransferase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.69Å 65.03Å 124.98Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	32.39 – 2.59 49.17 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.2 (32.39-2.59) 90.1 (49.17-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.265 , 0.291 0.254 , 0.286	Depositor DCC
R_{free} test set	1893 reflections (7.57%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7525	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.05 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5490e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, IPA

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	0.25	0/1271	0.40	0/1720
1	B	0.33	0/1271	0.48	0/1720
1	C	0.25	0/1271	0.39	0/1720
1	D	0.30	0/1271	0.45	0/1720
1	E	0.25	0/1271	0.40	0/1720
1	F	0.30	0/1271	0.46	0/1720
All	All	0.28	0/7626	0.43	0/10320

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	92	VAL	Peptide

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	1244	0	1261	14	0
1	B	1244	0	1261	26	0
1	C	1244	0	1261	11	0
1	D	1244	0	1261	11	0
1	E	1244	0	1261	16	0
1	F	1244	0	1261	11	0
2	B	4	0	8	0	0
2	F	4	0	8	1	0
3	B	6	0	8	1	0
3	D	18	0	24	1	0
3	F	6	0	8	0	0
4	A	1	0	0	0	0
4	B	8	0	0	0	0
4	D	8	0	0	0	0
4	E	1	0	0	0	0
4	F	5	0	0	0	0
All	All	7525	0	7622	74	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 5.

All (74) 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:90:ARG:NH2	1:A:126:ILE:O	2.22	0.72
1:C:31:VAL:HB	1:C:64:VAL:HG22	1.74	0.69
1:C:12:PRO:HG3	1:C:153:LEU:HD11	1.77	0.66
1:F:87:ARG:HH22	2:F:201:IPA:H11	1.60	0.66
1:B:107:GLN:O	1:F:143:LYS:NZ	2.27	0.66
1:E:12:PRO:HG3	1:E:153:LEU:HD11	1.82	0.61
1:F:22:GLU:OE2	1:F:60:HIS:NE2	2.29	0.61
1:B:27:LEU:HD11	1:D:113:GLU:HG2	1.82	0.61
1:B:108:LEU:HD11	1:F:134:ILE:HD13	1.83	0.60
1:B:15:LYS:NZ	1:B:145:VAL:O	2.36	0.58
1:B:90:ARG:C	1:B:92:VAL:H	2.07	0.58
1:F:121:GLU:OE2	1:F:122:LYS:N	2.38	0.57
1:E:89:LEU:HD13	1:E:116:PHE:HB3	1.87	0.55
1:E:135:ALA:HB2	1:E:141:ILE:HD13	1.88	0.55
1:E:15:LYS:NZ	1:E:145:VAL:O	2.39	0.55
1:B:116:PHE:HB2	1:D:116:PHE:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:HG3	1:E:92:VAL:HB	1.89	0.55
1:E:94:ASP:HB3	1:E:97:TYR:HB3	1.89	0.55
1:B:87:ARG:NE	1:B:98:GLU:OE2	2.39	0.55
1:E:87:ARG:NE	1:E:98:GLU:OE2	2.29	0.55
1:B:37:ALA:HB2	1:B:47:LEU:HD22	1.88	0.54
1:C:37:ALA:HB2	1:C:47:LEU:HD22	1.88	0.54
1:A:37:ALA:HB2	1:A:47:LEU:HD22	1.90	0.54
1:C:54:ALA:HB3	1:C:66:VAL:HG11	1.91	0.53
1:C:22:GLU:OE2	1:C:60:HIS:NE2	2.38	0.53
1:B:91:ALA:HA	1:B:95:PHE:HE1	1.74	0.52
1:D:3:ARG:HH11	1:D:32:ILE:HD11	1.74	0.52
1:D:87:ARG:NE	1:D:98:GLU:OE2	2.42	0.51
1:F:11:ASP:O	1:F:132:ARG:NH1	2.37	0.51
1:C:90:ARG:NH2	1:C:126:ILE:O	2.39	0.51
1:E:90:ARG:HH22	1:E:127:SER:HA	1.77	0.50
1:A:154:ALA:O	1:A:158:LYS:HB2	2.12	0.49
1:D:7:PRO:HD2	1:D:86:LEU:O	2.12	0.48
1:F:141:ILE:HD13	1:F:141:ILE:H	1.79	0.48
1:A:23:ARG:NH2	1:C:106:ARG:HD2	2.29	0.48
1:C:122:LYS:HA	1:E:121:GLU:HG3	1.94	0.48
1:C:135:ALA:HB2	1:C:141:ILE:HD13	1.94	0.48
1:D:141:ILE:HG22	1:D:144:PHE:HD2	1.78	0.48
1:D:87:ARG:NH2	3:D:203:GOL:O3	2.47	0.48
1:A:156:ARG:NH1	1:B:46:SER:HB3	2.29	0.47
1:E:97:TYR:HA	1:E:100:GLN:HG2	1.96	0.47
1:B:113:GLU:HG2	1:D:27:LEU:HD11	1.97	0.47
1:A:92:VAL:HG12	1:A:92:VAL:O	2.15	0.47
1:E:85:PHE:HB2	1:E:114:SER:HA	1.98	0.46
1:B:20:LEU:HD21	1:B:88:GLY:HA2	1.97	0.45
1:D:90:ARG:C	1:D:92:VAL:H	2.20	0.45
1:F:15:LYS:NZ	1:F:145:VAL:O	2.44	0.45
1:A:49:GLN:OE1	1:B:156:ARG:NE	2.50	0.45
1:E:11:ASP:HB2	1:E:50:ARG:HD3	1.98	0.45
1:B:7:PRO:HD2	1:B:86:LEU:O	2.17	0.45
1:B:4:VAL:HG22	1:B:84:VAL:HB	1.98	0.45
1:E:111:ASP:N	1:E:111:ASP:OD1	2.39	0.44
1:B:87:ARG:NH2	3:B:202:GOL:O2	2.51	0.44
1:D:121:GLU:HB2	1:F:125:PHE:CE2	2.53	0.44
1:F:7:PRO:HD2	1:F:86:LEU:O	2.18	0.43
1:A:121:GLU:HG3	1:A:121:GLU:H	1.50	0.43
1:C:11:ASP:HB2	1:C:50:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ASN:HB3	1:E:28:PHE:HD1	1.83	0.43
1:B:3:ARG:HH11	1:B:32:ILE:HD11	1.84	0.42
1:B:78:LYS:HZ1	1:B:112:VAL:HG23	1.84	0.42
1:B:96:GLU:HG3	1:F:93:SER:HB2	2.01	0.42
1:E:158:LYS:HE3	1:E:158:LYS:HA	2.03	0.41
1:A:85:PHE:HB2	1:A:114:SER:HA	2.02	0.41
1:A:158:LYS:HA	1:B:48:GLU:OE2	2.21	0.41
1:C:33:ILE:HB	1:C:66:VAL:HG22	2.01	0.41
1:B:4:VAL:HG21	1:B:28:PHE:CE2	2.55	0.41
1:A:100:GLN:HG2	1:E:125:PHE:HA	2.03	0.41
1:B:53:LEU:O	1:B:57:VAL:HG23	2.21	0.41
1:B:20:LEU:HD12	1:B:20:LEU:HA	1.87	0.40
1:B:51:VAL:HG13	1:B:66:VAL:HG12	2.02	0.40
1:A:11:ASP:O	1:A:132:ARG:NH1	2.44	0.40
1:A:156:ARG:HD2	1:B:46:SER:HB3	2.04	0.40
1:B:4:VAL:HG21	1:B:28:PHE:CZ	2.56	0.40
1:D:77:VAL:HG23	1:D:82:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	B	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	28	53
1	C	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	D	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
1	E	156/159 (98%)	150 (96%)	5 (3%)	1 (1%)	28	53
1	F	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	28	53
All	All	936/954 (98%)	896 (96%)	37 (4%)	3 (0%)	44	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	91	ALA
1	B	93	SER
1	F	91	ALA

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	134/135 (99%)	133 (99%)	1 (1%)	87	96
1	B	134/135 (99%)	131 (98%)	3 (2%)	57	81
1	C	134/135 (99%)	131 (98%)	3 (2%)	57	81
1	D	134/135 (99%)	133 (99%)	1 (1%)	87	96
1	E	134/135 (99%)	132 (98%)	2 (2%)	70	88
1	F	134/135 (99%)	131 (98%)	3 (2%)	57	81
All	All	804/810 (99%)	791 (98%)	13 (2%)	68	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	GLU
1	B	9	THR
1	B	25	SER
1	B	118	THR
1	C	27	LEU
1	C	95	PHE
1	C	98	GLU
1	D	118	THR
1	E	5	LEU
1	E	158	LYS
1	F	118	THR
1	F	121	GLU
1	F	141	ILE

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 [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IPA	B	201	-	3,3,3	0.54	0	3,3,3	0.26	0
3	GOL	B	202	-	5,5,5	0.39	0	5,5,5	0.17	0
3	GOL	D	201	-	5,5,5	0.29	0	5,5,5	0.37	0
3	GOL	D	202	-	5,5,5	0.39	0	5,5,5	0.24	0
3	GOL	D	203	-	5,5,5	0.36	0	5,5,5	0.17	0
2	IPA	F	201	-	3,3,3	0.52	0	3,3,3	0.27	0
3	GOL	F	202	-	5,5,5	0.34	0	5,5,5	0.23	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	IPA	B	201	-	-	0/0/0/0	0/0/0/0
3	GOL	B	202	-	-	0/4/4/4	0/0/0/0
3	GOL	D	201	-	-	0/4/4/4	0/0/0/0
3	GOL	D	202	-	-	0/4/4/4	0/0/0/0
3	GOL	D	203	-	-	0/4/4/4	0/0/0/0
2	IPA	F	201	-	-	0/0/0/0	0/0/0/0
3	GOL	F	202	-	-	0/4/4/4	0/0/0/0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	GOL	1	0
3	D	203	GOL	1	0
2	F	201	IPA	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	158/159 (99%)	1.72	54 (34%) 0 0	83, 99, 113, 119	0
1	B	158/159 (99%)	0.61	8 (5%) 29 22	38, 49, 65, 71	0
1	C	158/159 (99%)	2.04	57 (36%) 0 0	94, 103, 121, 138	0
1	D	158/159 (99%)	0.58	8 (5%) 29 22	38, 47, 66, 71	0
1	E	158/159 (99%)	1.84	57 (36%) 0 0	88, 100, 116, 121	0
1	F	158/159 (99%)	0.65	10 (6%) 21 15	37, 46, 62, 77	0
All	All	948/954 (99%)	1.24	194 (20%) 1 0	37, 77, 111, 138	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	PHE	8.8
1	F	93	SER	8.1
1	F	92	VAL	7.8
1	C	92	VAL	7.6
1	A	144	PHE	7.1
1	C	145	VAL	7.1
1	A	88	GLY	6.5
1	C	1	MET	6.4
1	D	158	LYS	6.3
1	C	44	LEU	6.0
1	A	158	LYS	5.9
1	C	158	LYS	5.9
1	C	125	PHE	5.7
1	C	122	LYS	5.6
1	C	151	ASP	5.6
1	C	76	PHE	5.5
1	E	95	PHE	5.5
1	C	69	PHE	5.3
1	C	66	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	153	LEU	5.0
1	E	37	ALA	4.9
1	A	53	LEU	4.9
1	C	131	VAL	4.9
1	E	40	LYS	4.7
1	D	1	MET	4.6
1	F	91	ALA	4.5
1	A	31	VAL	4.5
1	E	1	MET	4.5
1	A	86	LEU	4.4
1	C	42	ASN	4.3
1	A	95	PHE	4.3
1	C	53	LEU	4.2
1	C	123	TYR	4.2
1	C	91	ALA	4.2
1	E	32	ILE	4.2
1	A	1	MET	4.1
1	A	4	VAL	4.0
1	A	125	PHE	4.0
1	C	104	MET	4.0
1	C	144	PHE	3.9
1	E	137	LEU	3.9
1	C	134	ILE	3.9
1	E	74	ALA	3.8
1	E	114	SER	3.8
1	C	101	LEU	3.8
1	C	141	ILE	3.8
1	C	45	PHE	3.8
1	E	154	ALA	3.7
1	E	104	MET	3.7
1	A	3	ARG	3.7
1	C	75	HIS	3.7
1	C	3	ARG	3.6
1	E	149	VAL	3.6
1	C	93	SER	3.6
1	A	9	THR	3.6
1	C	14	THR	3.6
1	C	115	MET	3.6
1	E	4	VAL	3.6
1	E	126	ILE	3.5
1	C	57	VAL	3.5
1	D	101	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	92	VAL	3.5
1	A	10	PHE	3.4
1	A	123	TYR	3.4
1	A	97	TYR	3.4
1	E	36	ALA	3.4
1	E	151	ASP	3.4
1	C	65	GLU	3.4
1	E	45	PHE	3.4
1	E	122	LYS	3.4
1	A	93	SER	3.4
1	E	96	GLU	3.3
1	E	42	ASN	3.3
1	C	156	ARG	3.3
1	A	135	ALA	3.2
1	E	86	LEU	3.2
1	A	54	ALA	3.2
1	C	114	SER	3.2
1	A	151	ASP	3.2
1	B	93	SER	3.2
1	A	64	VAL	3.1
1	C	28	PHE	3.1
1	D	93	SER	3.1
1	C	137	LEU	3.1
1	C	105	ASN	3.0
1	E	145	VAL	3.0
1	B	158	LYS	3.0
1	C	94	ASP	3.0
1	A	118	THR	3.0
1	E	123	TYR	3.0
1	E	71	THR	3.0
1	C	18	GLY	2.9
1	C	121	GLU	2.9
1	C	157	PHE	2.9
1	E	94	ASP	2.9
1	E	87	ARG	2.9
1	C	116	PHE	2.9
1	B	123	TYR	2.9
1	E	97	TYR	2.9
1	C	38	SER	2.9
1	C	10	PHE	2.9
1	C	48	GLU	2.9
1	C	55	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	14	THR	2.8
1	E	59	LYS	2.8
1	A	14	THR	2.8
1	C	128	SER	2.8
1	E	115	MET	2.8
1	D	123	TYR	2.8
1	E	76	PHE	2.8
1	A	92	VAL	2.8
1	F	95	PHE	2.8
1	A	137	LEU	2.8
1	E	44	LEU	2.7
1	E	101	LEU	2.7
1	E	64	VAL	2.7
1	C	9	THR	2.7
1	C	135	ALA	2.7
1	D	137	LEU	2.7
1	E	53	LEU	2.7
1	B	157	PHE	2.7
1	A	89	LEU	2.7
1	C	64	VAL	2.6
1	C	97	TYR	2.6
1	E	107	GLN	2.6
1	F	1	MET	2.6
1	E	56	GLU	2.6
1	E	116	PHE	2.6
1	A	107	GLN	2.6
1	A	156	ARG	2.6
1	D	157	PHE	2.6
1	D	142	SER	2.6
1	E	16	GLY	2.6
1	A	45	PHE	2.6
1	C	99	PHE	2.6
1	B	124	SER	2.6
1	A	153	LEU	2.5
1	A	103	ASN	2.5
1	A	61	LEU	2.5
1	A	94	ASP	2.5
1	B	91	ALA	2.5
1	E	30	HIS	2.5
1	B	1	MET	2.5
1	A	87	ARG	2.4
1	C	108	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	77	VAL	2.4
1	C	47	LEU	2.4
1	E	157	PHE	2.4
1	E	118	THR	2.4
1	C	40	LYS	2.4
1	E	144	PHE	2.4
1	C	58	THR	2.4
1	E	143	LYS	2.4
1	F	94	ASP	2.4
1	A	108	LEU	2.4
1	A	26	ARG	2.4
1	A	33	ILE	2.4
1	A	85	PHE	2.4
1	A	43	PRO	2.4
1	F	158	LYS	2.3
1	F	101	LEU	2.3
1	E	57	VAL	2.3
1	E	131	VAL	2.3
1	C	90	ARG	2.3
1	A	138	GLY	2.3
1	E	93	SER	2.3
1	E	31	VAL	2.2
1	E	125	PHE	2.2
1	A	124	SER	2.2
1	A	76	PHE	2.2
1	A	68	GLY	2.2
1	A	69	PHE	2.2
1	A	139	GLY	2.2
1	E	91	ALA	2.2
1	E	61	LEU	2.2
1	F	109	ALA	2.2
1	A	51	VAL	2.1
1	E	66	VAL	2.1
1	A	32	ILE	2.1
1	B	47	LEU	2.1
1	A	58	THR	2.1
1	A	117	LEU	2.1
1	F	137	LEU	2.1
1	E	100	GLN	2.1
1	A	116	PHE	2.1
1	C	153	LEU	2.1
1	A	41	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	13	ILE	2.1
1	C	88	GLY	2.1
1	E	52	ALA	2.0
1	C	107	GLN	2.0
1	A	40	LYS	2.0
1	A	72	LEU	2.0
1	E	156	ARG	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
2	IPA	F	201	4/4	0.74	0.29	3.42	47,47,47,47	0
3	GOL	B	202	6/6	0.85	0.21	1.19	46,48,50,51	0
3	GOL	D	202	6/6	0.86	0.28	0.81	51,51,52,53	0
3	GOL	F	202	6/6	0.73	0.23	0.16	44,48,49,50	0
3	GOL	D	203	6/6	0.92	0.12	-1.01	47,47,47,47	0
2	IPA	B	201	4/4	0.82	0.25	-	51,52,52,53	0
3	GOL	D	201	6/6	0.72	0.42	-	47,47,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.