



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:34 PM GMT

PDB ID : 5D92
Title : Structure of a phosphatidylinositolphosphate (PIP) synthase from Renibacterium Salmoninarum
Authors : Clarke, O.B.; Tomasek, D.T.; Jorge, C.D.; Belcher Dufrisne, M.; Kim, M.; Banerjee, S.; Rajashankar, K.R.; Hendrickson, W.A.; Santos, H.; Mancina, F.
Deposited on : 2015-08-18
Resolution : 3.62 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

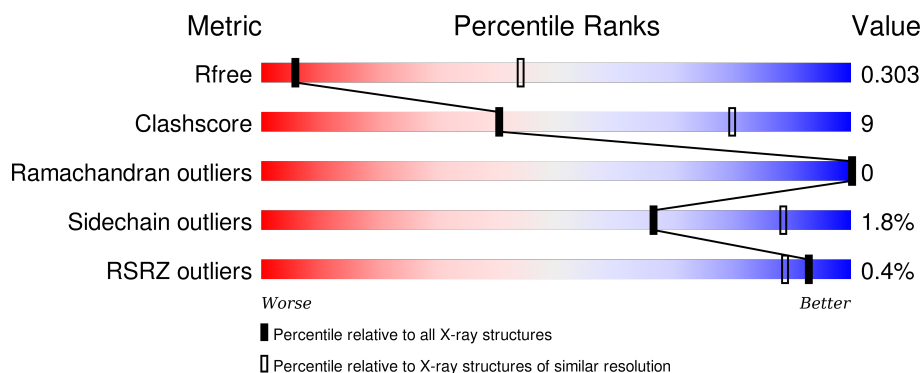
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	342	 77% 22% .
1	B	342	 81% 18%
1	C	342	 79% 18% ..
1	D	342	 76% 23% .

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	8K6	A	301	-	-	-	X
2	8K6	A	303	-	-	-	X
2	8K6	A	305	-	-	-	X
2	8K6	B	301	-	-	-	X
2	8K6	C	303	-	-	-	X
2	8K6	D	306	-	-	-	X
2	8K6	D	307	-	-	-	X
2	8K6	D	311	-	-	-	X
4	58A	B	309	-	-	-	X
4	58A	C	310	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10844 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 AF2299 protein, Phosphatidylinositol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	342	Total	C	N	O	S	0	0	0
			2605	1716	414	470	5			
1	A	340	Total	C	N	O	S	0	0	0
			2591	1707	414	465	5			
1	B	342	Total	C	N	O	S	0	0	0
			2602	1715	413	469	5			
1	C	334	Total	C	N	O	S	0	0	0
			2551	1683	405	458	5			

There are 40 discrepancies between the modelled and reference sequences:

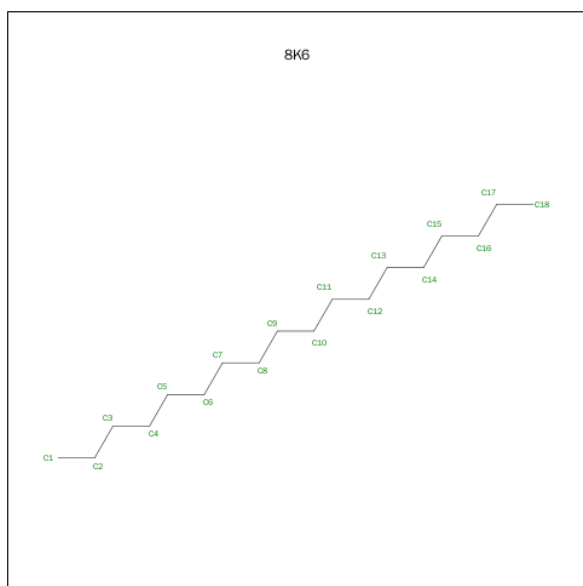
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	linker	UNP O27985
D	-1	SER	-	linker	UNP O27985
D	0	GLY	-	linker	UNP O27985
D	1	SER	-	linker	UNP O27985
D	15	LEU	MET	conflict	UNP A9WSF5
D	22	ALA	VAL	conflict	UNP A9WSF5
D	23	ASP	ARG	conflict	UNP A9WSF5
D	75	LEU	GLN	conflict	UNP A9WSF5
D	77	PHE	ASP	conflict	UNP A9WSF5
D	79	GLU	PRO	conflict	UNP A9WSF5
A	-2	GLY	-	linker	UNP O27985
A	-1	SER	-	linker	UNP O27985
A	0	GLY	-	linker	UNP O27985
A	1	SER	-	linker	UNP O27985
A	15	LEU	MET	conflict	UNP A9WSF5
A	22	ALA	VAL	conflict	UNP A9WSF5
A	23	ASP	ARG	conflict	UNP A9WSF5
A	75	LEU	GLN	conflict	UNP A9WSF5
A	77	PHE	ASP	conflict	UNP A9WSF5
A	79	GLU	PRO	conflict	UNP A9WSF5
B	-2	GLY	-	linker	UNP O27985

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	linker	UNP O27985
B	0	GLY	-	linker	UNP O27985
B	1	SER	-	linker	UNP O27985
B	15	LEU	MET	conflict	UNP A9WSF5
B	22	ALA	VAL	conflict	UNP A9WSF5
B	23	ASP	ARG	conflict	UNP A9WSF5
B	75	LEU	GLN	conflict	UNP A9WSF5
B	77	PHE	ASP	conflict	UNP A9WSF5
B	79	GLU	PRO	conflict	UNP A9WSF5
C	-2	GLY	-	linker	UNP O27985
C	-1	SER	-	linker	UNP O27985
C	0	GLY	-	linker	UNP O27985
C	1	SER	-	linker	UNP O27985
C	15	LEU	MET	conflict	UNP A9WSF5
C	22	ALA	VAL	conflict	UNP A9WSF5
C	23	ASP	ARG	conflict	UNP A9WSF5
C	75	LEU	GLN	conflict	UNP A9WSF5
C	77	PHE	ASP	conflict	UNP A9WSF5
C	79	GLU	PRO	conflict	UNP A9WSF5

- Molecule 2 is Octadecane (three-letter code: 8K6) (formula: C₁₈H₃₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0

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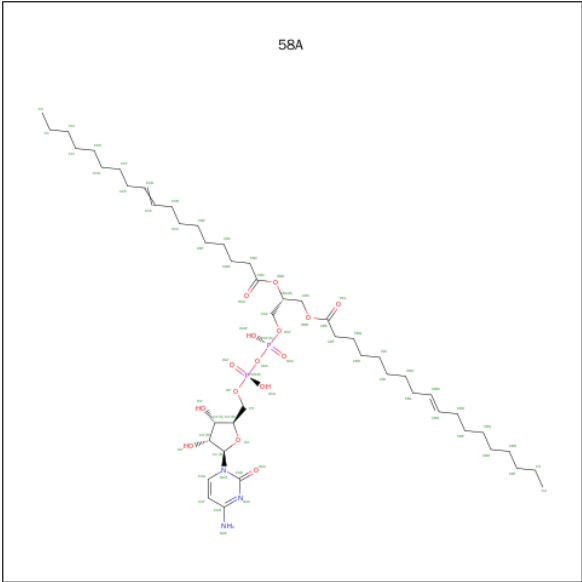
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is 5'-O-[(R)-{[(S)-{(2R)-2,3-bis[(9E)-octadec-9-enoyloxy]propoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]cytidine (three-letter code: 58A) (formula: C₄₈H₈₅N₃O₁₅P₂).

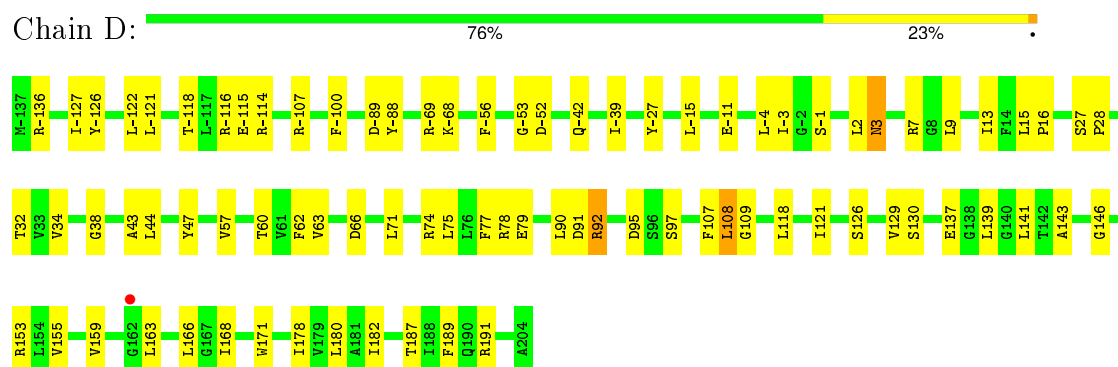


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	A	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	B	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	C	1	Total	C	N	O	P	0	0
			64	44	3	15	2		

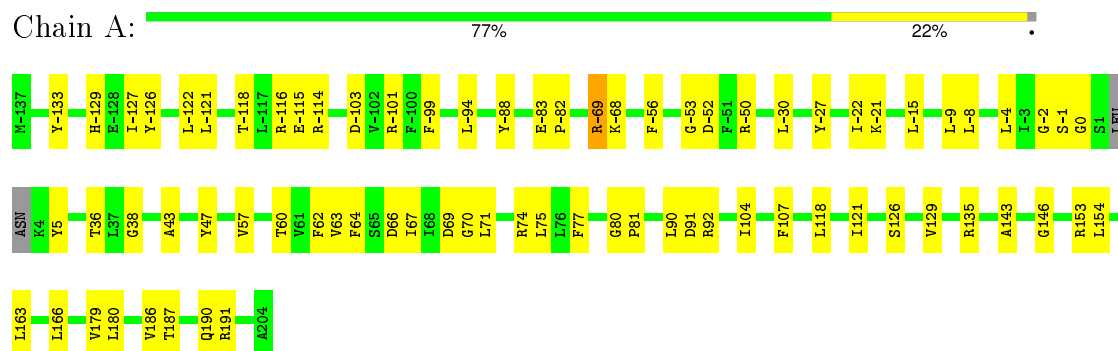
3 Residue-property plots

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

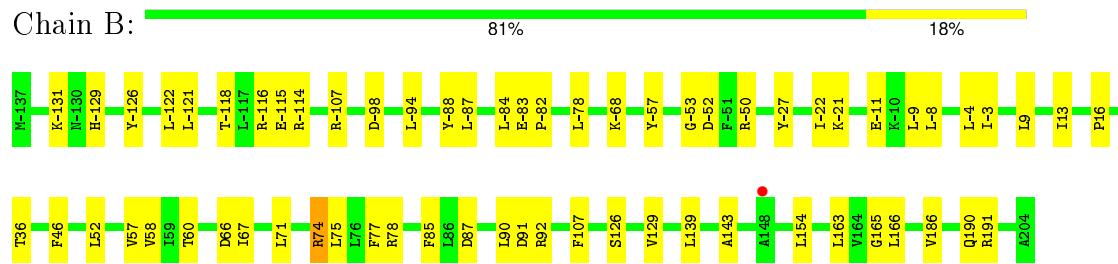
- Molecule 1: AF2299 protein, Phosphatidylinositol synthase



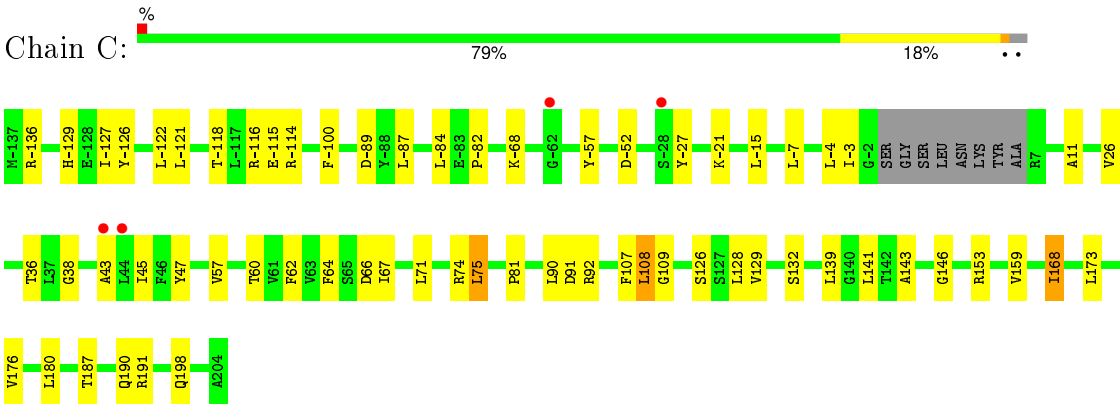
- Molecule 1: AF2299 protein, Phosphatidylinositol synthase



- Molecule 1: AF2299 protein, Phosphatidylinositol synthase



- Molecule 1: AF2299 protein, Phosphatidylinositol synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.00 Å 62.49 Å 169.76 Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	166.97 – 3.62 167.30 – 3.61	Depositor EDS
% Data completeness (in resolution range)	98.4 (166.97-3.62) 98.6 (167.30-3.61)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.58 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.300 0.282 , 0.303	Depositor DCC
R_{free} test set	1043 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 21263 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10844	wwPDB-VP
Average B, all atoms (Å ²)	76.0	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 20.91 % 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 7.8532e-03. 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, 0.375 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: MG, 8K6, 58A

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	0.27	0/2641	0.55	1/3596 (0.0%)
1	B	0.26	0/2653	0.55	0/3616
1	C	0.27	0/2600	0.54	0/3542
1	D	0.27	0/2656	0.54	0/3620
All	All	0.27	0/10550	0.55	1/14374 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLY	N-CA-C	5.84	127.71	113.10

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	2591	0	2635	54	0
1	B	2602	0	2646	41	0
1	C	2551	0	2603	42	0
1	D	2605	0	2650	52	0
2	A	56	0	80	2	0
2	B	42	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	49	0	70	3	0
2	D	84	0	120	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	64	0	68	5	0
4	B	64	0	68	1	0
4	C	64	0	68	5	0
4	D	64	0	68	7	0
All	All	10844	0	11136	191	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 9.

The worst 5 of 191 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)
4:C:310:58A:O4'	4:C:310:58A:C1'	1.65	1.29
4:A:311:58A:C1'	4:A:311:58A:O4'	1.65	1.27
4:B:309:58A:O4'	4:B:309:58A:C1'	1.65	1.21
4:D:315:58A:O4'	4:D:315:58A:C1'	1.65	1.15
1:D:66:ASP:OD1	4:D:315:58A:OAW	1.62	1.14

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	336/342 (98%)	329 (98%)	7 (2%)	0	100	100
1	B	340/342 (99%)	334 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/342 (96%)	324 (98%)	6 (2%)	0	100	100
1	D	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
All	All	1346/1368 (98%)	1321 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	268/283 (95%)	265 (99%)	3 (1%)	80	92
1	B	270/283 (95%)	267 (99%)	3 (1%)	80	92
1	C	266/283 (94%)	261 (98%)	5 (2%)	65	87
1	D	271/283 (96%)	263 (97%)	8 (3%)	48	81
All	All	1075/1132 (95%)	1056 (98%)	19 (2%)	66	88

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-69	ARG
1	A	107	PHE
1	C	75	LEU
1	D	189	PHE
1	C	107	PHE

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

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 45 ligands modelled in this entry, 8 are monoatomic - leaving 37 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	8K6	A	301	-	6,6,17	0.31	0	5,5,16	0.64	0
2	8K6	A	302	-	6,6,17	0.30	0	5,5,16	0.65	0
2	8K6	A	303	-	6,6,17	0.31	0	5,5,16	0.67	0
2	8K6	A	304	-	6,6,17	0.31	0	5,5,16	0.68	0
2	8K6	A	305	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	A	306	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	A	307	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	A	308	-	6,6,17	0.30	0	5,5,16	0.66	0
4	58A	A	311	3	60,65,69	3.26	14 (23%)	66,82,86	1.39	6 (9%)
2	8K6	B	301	-	6,6,17	0.31	0	5,5,16	0.63	0
2	8K6	B	302	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	B	303	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	B	304	-	6,6,17	0.30	0	5,5,16	0.69	0
2	8K6	B	305	-	6,6,17	0.31	0	5,5,16	0.67	0
2	8K6	B	306	-	6,6,17	0.31	0	5,5,16	0.65	0
4	58A	B	309	3	60,65,69	3.27	14 (23%)	66,82,86	1.33	6 (9%)
2	8K6	C	301	-	6,6,17	0.31	0	5,5,16	0.64	0
2	8K6	C	302	-	6,6,17	0.31	0	5,5,16	0.62	0
2	8K6	C	303	-	6,6,17	0.32	0	5,5,16	0.66	0
2	8K6	C	304	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	C	305	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	C	306	-	6,6,17	0.30	0	5,5,16	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	8K6	C	307	-	6,6,17	0.30	0	5,5,16	0.70	0
4	58A	C	310	3	60,65,69	3.26	14 (23%)	66,82,86	1.40	6 (9%)
2	8K6	D	301	-	6,6,17	0.31	0	5,5,16	0.64	0
2	8K6	D	302	-	6,6,17	0.31	0	5,5,16	0.65	0
2	8K6	D	303	-	6,6,17	0.31	0	5,5,16	0.63	0
2	8K6	D	304	-	6,6,17	0.31	0	5,5,16	0.67	0
2	8K6	D	305	-	6,6,17	0.32	0	5,5,16	0.62	0
2	8K6	D	306	-	6,6,17	0.31	0	5,5,16	0.64	0
2	8K6	D	307	-	6,6,17	0.31	0	5,5,16	0.64	0
2	8K6	D	308	-	6,6,17	0.32	0	5,5,16	0.66	0
2	8K6	D	309	-	6,6,17	0.32	0	5,5,16	0.60	0
2	8K6	D	310	-	6,6,17	0.31	0	5,5,16	0.66	0
2	8K6	D	311	-	6,6,17	0.30	0	5,5,16	0.67	0
2	8K6	D	312	-	6,6,17	0.32	0	5,5,16	0.67	0
4	58A	D	315	3	60,65,69	3.27	14 (23%)	66,82,86	1.34	6 (9%)

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	8K6	A	301	-	-	0/4/4/15	0/0/0/0
2	8K6	A	302	-	-	0/4/4/15	0/0/0/0
2	8K6	A	303	-	-	0/4/4/15	0/0/0/0
2	8K6	A	304	-	-	0/4/4/15	0/0/0/0
2	8K6	A	305	-	-	0/4/4/15	0/0/0/0
2	8K6	A	306	-	-	0/4/4/15	0/0/0/0
2	8K6	A	307	-	-	0/4/4/15	0/0/0/0
2	8K6	A	308	-	-	0/4/4/15	0/0/0/0
4	58A	A	311	3	-	0/57/77/81	0/2/2/2
2	8K6	B	301	-	-	0/4/4/15	0/0/0/0
2	8K6	B	302	-	-	0/4/4/15	0/0/0/0
2	8K6	B	303	-	-	0/4/4/15	0/0/0/0
2	8K6	B	304	-	-	0/4/4/15	0/0/0/0
2	8K6	B	305	-	-	0/4/4/15	0/0/0/0
2	8K6	B	306	-	-	0/4/4/15	0/0/0/0
4	58A	B	309	3	-	0/57/77/81	0/2/2/2
2	8K6	C	301	-	-	0/4/4/15	0/0/0/0
2	8K6	C	302	-	-	0/4/4/15	0/0/0/0
2	8K6	C	303	-	-	0/4/4/15	0/0/0/0
2	8K6	C	304	-	-	0/4/4/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8K6	C	305	-	-	0/4/4/15	0/0/0/0
2	8K6	C	306	-	-	0/4/4/15	0/0/0/0
2	8K6	C	307	-	-	0/4/4/15	0/0/0/0
4	58A	C	310	3	-	0/57/77/81	0/2/2/2
2	8K6	D	301	-	-	0/4/4/15	0/0/0/0
2	8K6	D	302	-	-	0/4/4/15	0/0/0/0
2	8K6	D	303	-	-	0/4/4/15	0/0/0/0
2	8K6	D	304	-	-	0/4/4/15	0/0/0/0
2	8K6	D	305	-	-	0/4/4/15	0/0/0/0
2	8K6	D	306	-	-	0/4/4/15	0/0/0/0
2	8K6	D	307	-	-	0/4/4/15	0/0/0/0
2	8K6	D	308	-	-	0/4/4/15	0/0/0/0
2	8K6	D	309	-	-	0/4/4/15	0/0/0/0
2	8K6	D	310	-	-	0/4/4/15	0/0/0/0
2	8K6	D	311	-	-	0/4/4/15	0/0/0/0
2	8K6	D	312	-	-	0/4/4/15	0/0/0/0
4	58A	D	315	3	-	0/57/77/81	0/2/2/2

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	309	58A	C2'-C1'	-12.61	1.33	1.53
4	D	315	58A	C2'-C1'	-12.54	1.33	1.53
4	C	310	58A	C2'-C1'	-12.44	1.33	1.53
4	A	311	58A	C2'-C1'	-12.36	1.34	1.53
4	C	310	58A	O4'-C4'	-6.27	1.30	1.45

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	58A	C4'-O4'-C1'	-5.77	103.53	109.64
4	C	310	58A	C4'-O4'-C1'	-5.53	103.78	109.64
4	D	315	58A	C4'-O4'-C1'	-4.60	104.77	109.64
4	B	309	58A	C4'-O4'-C1'	-4.16	105.23	109.64
4	C	310	58A	CAF-CAD-NAC	-3.03	117.94	121.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	8K6	1	0
2	A	306	8K6	1	0
4	A	311	58A	5	0
2	B	306	8K6	1	0
4	B	309	58A	1	0
2	C	301	8K6	1	0
2	C	302	8K6	1	0
2	C	304	8K6	1	0
2	C	306	8K6	1	0
4	C	310	58A	5	0
2	D	307	8K6	1	0
4	D	315	58A	7	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	340/342 (99%)	-0.16	0 100 100	38, 68, 106, 154	0
1	B	342/342 (100%)	-0.10	1 (0%) 94 90	37, 69, 119, 151	0
1	C	334/342 (97%)	-0.06	4 (1%) 81 69	44, 87, 149, 176	0
1	D	342/342 (100%)	-0.18	1 (0%) 94 90	35, 66, 127, 152	0
All	All	1358/1368 (99%)	-0.12	6 (0%) 93 89	35, 70, 134, 176	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-62	GLY	3.9
1	B	148	ALA	2.8
1	C	43	ALA	2.7
1	C	-28	SER	2.6
1	C	44	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. 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	8K6	A	305	7/18	0.71	0.91	13.60	45,48,50,56	0
2	8K6	B	301	7/18	0.83	0.64	6.15	37,39,41,42	0
2	8K6	D	311	7/18	0.84	0.50	3.86	61,62,69,84	0
2	8K6	D	306	7/18	0.84	0.53	3.37	40,41,46,47	0
2	8K6	A	303	7/18	0.86	0.46	2.85	35,37,40,41	0
2	8K6	D	307	7/18	0.88	0.28	2.42	38,40,44,44	0
2	8K6	A	301	7/18	0.89	0.42	2.18	40,40,44,46	0
4	58A	C	310	64/68	0.88	0.38	2.04	59,73,101,139	0
4	58A	A	311	64/68	0.91	0.37	1.65	48,63,91,113	0
2	8K6	C	307	7/18	0.91	0.25	1.61	46,50,56,60	0
2	8K6	B	306	7/18	0.82	0.40	1.61	47,51,52,53	0
4	58A	D	315	64/68	0.90	0.40	1.38	56,67,84,126	0
2	8K6	C	303	7/18	0.77	0.59	1.32	44,47,54,56	0
2	8K6	D	304	7/18	0.83	0.22	1.10	60,74,85,91	0
4	58A	B	309	64/68	0.90	0.42	0.97	55,75,116,127	0
2	8K6	C	306	7/18	0.84	0.26	0.76	63,65,70,79	0
2	8K6	D	302	7/18	0.84	0.29	-0.63	40,45,48,48	0
3	MG	D	314	1/1	0.93	0.11	-2.08	63,63,63,63	0
3	MG	A	310	1/1	0.99	0.04	-2.68	61,61,61,61	0
3	MG	B	308	1/1	0.85	0.09	-2.69	63,63,63,63	0
3	MG	C	309	1/1	0.92	0.06	-3.11	69,69,69,69	0
2	8K6	B	302	7/18	0.85	0.58	-	27,28,29,29	0
2	8K6	D	305	7/18	0.80	0.65	-	26,28,31,34	0
3	MG	B	307	1/1	0.89	0.21	-	63,63,63,63	0
2	8K6	D	309	7/18	0.83	0.40	-	55,57,64,76	0
2	8K6	B	305	7/18	0.45	1.36	-	57,68,77,90	0
2	8K6	D	312	7/18	0.74	0.42	-	51,52,54,61	0
2	8K6	C	301	7/18	0.46	0.48	-	61,69,83,92	0
2	8K6	C	305	7/18	0.78	0.73	-	63,66,71,71	0
2	8K6	C	302	7/18	0.76	0.62	-	44,51,58,60	0
3	MG	A	309	1/1	0.92	0.21	-	59,59,59,59	0
2	8K6	A	302	7/18	0.83	0.40	-	46,49,54,65	0
2	8K6	C	304	7/18	0.85	0.82	-	51,53,55,57	0
2	8K6	D	301	7/18	0.86	0.62	-	36,36,40,43	0
2	8K6	B	304	7/18	0.85	0.60	-	36,37,39,42	0
2	8K6	A	306	7/18	0.84	0.92	-	44,48,54,63	0
2	8K6	A	308	7/18	0.83	0.54	-	35,36,37,37	0
2	8K6	A	304	7/18	0.91	1.05	-	36,38,41,44	0
3	MG	D	313	1/1	0.65	0.16	-	64,64,64,64	0
2	8K6	D	310	7/18	0.69	0.78	-	63,73,75,90	0
2	8K6	A	307	7/18	0.88	0.45	-	33,35,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	8K6	D	303	7/18	0.88	0.23	-	37,38,40,40	0
2	8K6	D	308	7/18	0.80	0.57	-	32,33,41,44	0
3	MG	C	308	1/1	0.74	0.13	-	70,70,70,70	0
2	8K6	B	303	7/18	0.67	0.51	-	50,51,57,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.