



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:17 PM UTC

PDB ID : 5D92 / pdb_00005d92
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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

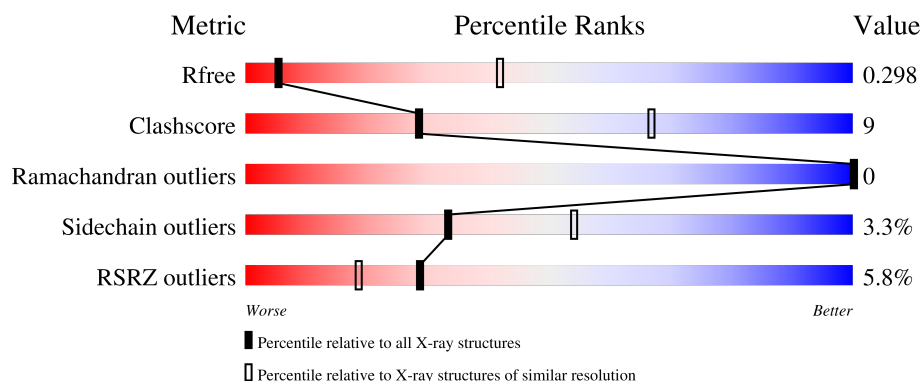
1 Overall quality at a glance

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}	180053	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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 of 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	342	4% 75% 23% ..
1	B	342	9% 79% 20% .
1	C	342	8% 75% 21% ..
1	D	342	3% 74% 25% .

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	D	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:

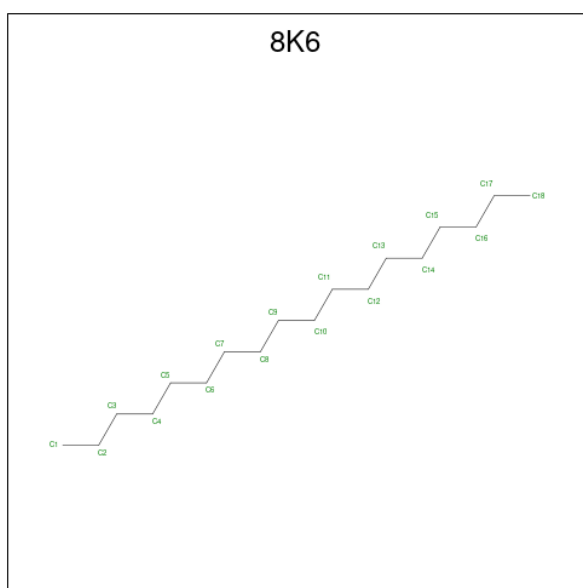
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	linker	UNP O27985
D	-1	SER	-	linker	UNP O27985
D	0	GLY	-	linker	UNP O27985
D	1	SER	-	linker	UNP O27985
D	15	LEU	MET	conflict	UNP A9WSF5
D	22	ALA	VAL	conflict	UNP A9WSF5
D	23	ASP	ARG	conflict	UNP A9WSF5
D	75	LEU	GLN	conflict	UNP A9WSF5
D	77	PHE	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 (CCD ID: 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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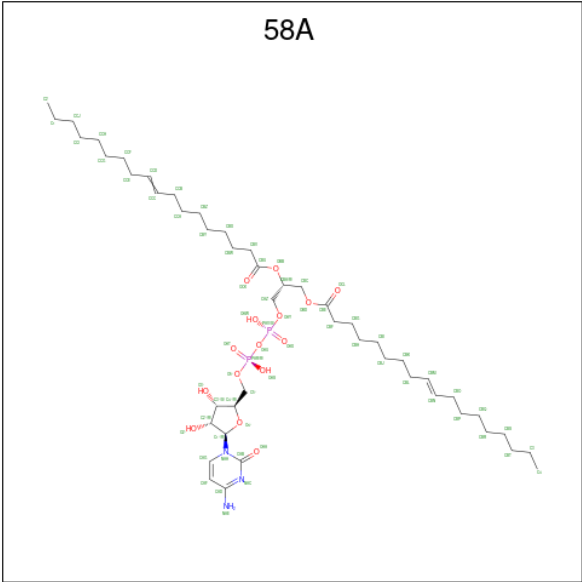
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	B	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 (CCD ID: 58A) (formula: C₄₈H₈₅N₃O₁₅P₂).

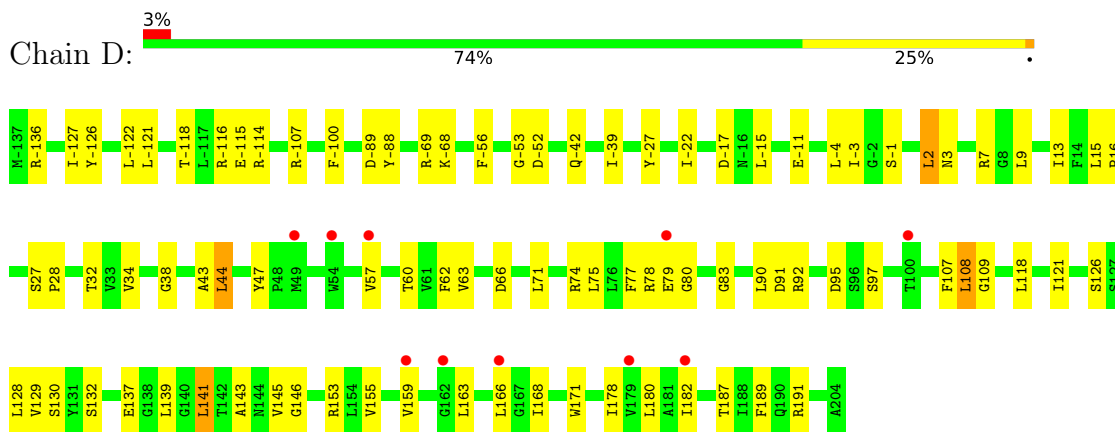


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	A	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	B	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
4	C	1	Total	C	N	O	P	0	0
			64	44	3	15	2		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

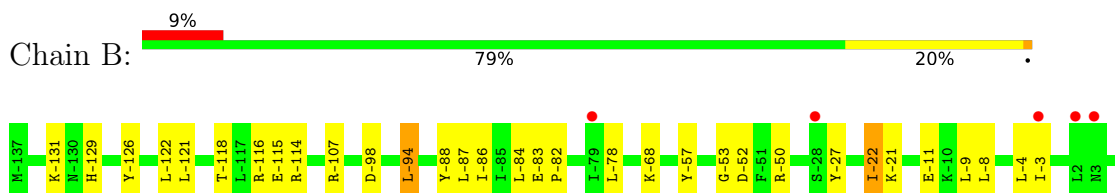
- Molecule 1: AF2299 protein, Phosphatidylinositol synthase

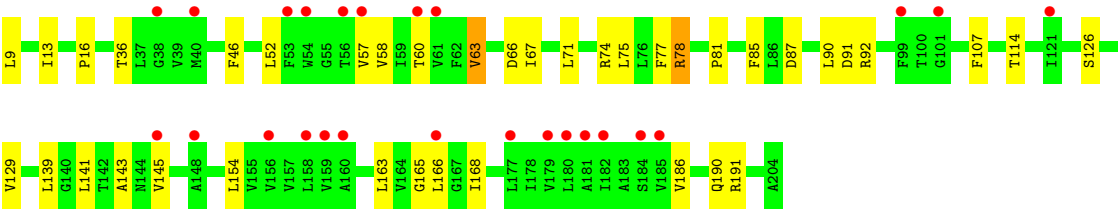


- Molecule 1: AF2299 protein, Phosphatidylinositol synthase

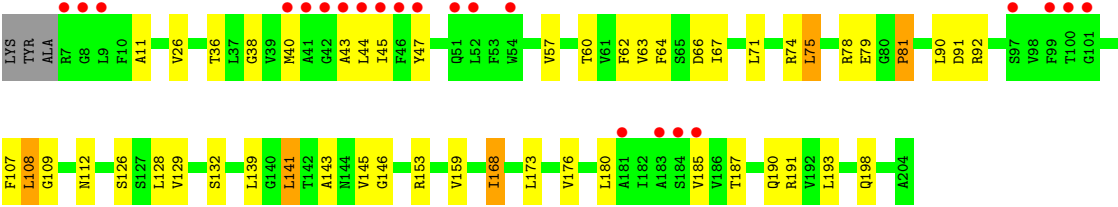
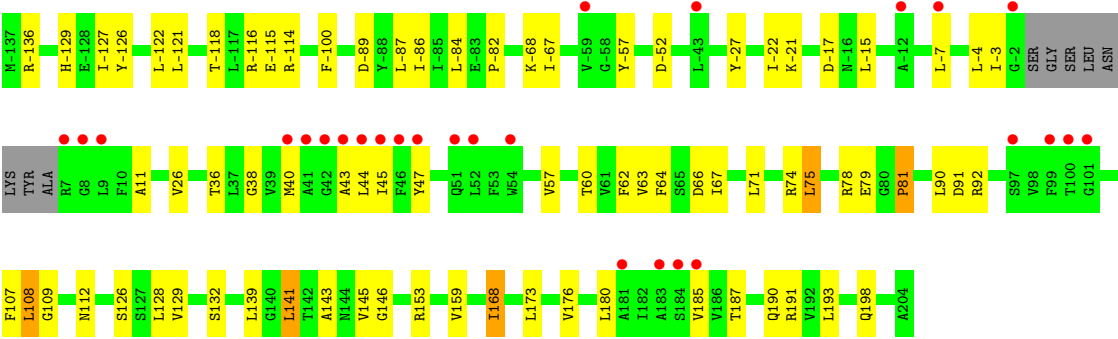
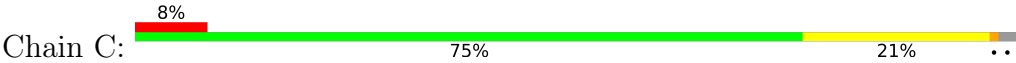


- Molecule 1: AF2299 protein, Phosphatidylinositol synthase





● 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	89.00Å 62.49Å 169.76Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	166.97 – 3.62 166.97 – 3.62	Depositor EDS
% Data completeness (in resolution range)	98.4 (166.97-3.62) 99.1 (166.97-3.62)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.58Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.300 0.279 , 0.298	Depositor DCC
R_{free} test set	1045 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtrriage
Anisotropy	0.626	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10844	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8K6, MG, 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	0.36	0/2641	0.93	9/3596 (0.3%)
1	B	0.35	0/2653	0.94	10/3616 (0.3%)
1	C	0.37	0/2600	0.96	15/3542 (0.4%)
1	D	0.35	0/2656	0.92	4/3620 (0.1%)
All	All	0.36	0/10550	0.94	38/14374 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	80	GLY	CA-C-N	9.94	130.21	119.28
1	D	80	GLY	C-N-CA	9.94	130.21	119.28
1	B	145	VAL	N-CA-C	9.92	123.22	108.54
1	C	145	VAL	N-CA-C	9.88	123.17	108.54
1	D	145	VAL	N-CA-C	9.73	122.94	108.54
1	A	145	VAL	N-CA-C	9.64	122.81	108.54
1	A	80	GLY	N-CA-C	7.54	127.71	112.34
1	B	81	PRO	N-CA-C	-6.97	104.24	113.65
1	C	81	PRO	CA-C-N	6.92	129.55	120.28
1	C	81	PRO	C-N-CA	6.92	129.55	120.28
1	C	81	PRO	N-CA-C	-6.89	104.34	113.65
1	B	78	ARG	CA-C-N	-6.77	112.83	123.12
1	B	78	ARG	C-N-CA	-6.77	112.83	123.12
1	C	-86	ILE	N-CA-C	6.72	117.32	107.37
1	C	78	ARG	CA-C-N	-6.69	113.83	122.79
1	C	78	ARG	C-N-CA	-6.69	113.83	122.79
1	B	81	PRO	CA-C-N	6.33	128.77	120.28
1	B	81	PRO	C-N-CA	6.33	128.77	120.28
1	C	193	LEU	N-CA-C	6.04	117.53	111.07
1	C	81	PRO	CA-C-O	5.88	128.49	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-17	ASP	N-CA-C	5.85	117.74	111.36
1	A	-67	ILE	N-CA-C	5.85	116.35	108.17
1	A	80	GLY	CA-C-N	5.70	125.38	119.05
1	A	80	GLY	C-N-CA	5.70	125.38	119.05
1	C	112	ASN	CA-C-N	5.51	125.17	119.05
1	C	112	ASN	C-N-CA	5.51	125.17	119.05
1	D	-17	ASP	N-CA-C	5.34	117.18	111.36
1	B	145	VAL	CB-CA-C	-5.20	104.99	111.08
1	B	-86	ILE	N-CA-C	5.17	115.02	107.37
1	C	145	VAL	CB-CA-C	-5.17	105.04	111.08
1	B	81	PRO	CA-C-O	5.16	127.39	119.55
1	A	112	ASN	CA-C-N	5.15	124.77	119.05
1	A	112	ASN	C-N-CA	5.15	124.77	119.05
1	C	185	VAL	N-CA-C	5.12	115.34	110.42
1	A	-86	ILE	N-CA-C	5.11	114.94	107.37
1	A	-65	VAL	N-CA-C	5.09	117.16	108.86
1	B	63	VAL	N-CA-C	5.06	115.83	110.72
1	C	-67	ILE	N-CA-C	5.00	115.18	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2591	0	2635	54	0
1	B	2602	0	2646	41	0
1	C	2551	0	2603	42	0
1	D	2605	0	2650	54	0
2	A	56	0	80	2	0
2	B	42	0	60	1	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0
All	All	10844	0	11136	193	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.

All (193) 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:C1'	4:C:310:58A:O4'	1.65	1.29
4:A:311:58A:O4'	4:A:311:58A:C1'	1.65	1.27
4:B:309:58A:C1'	4:B:309:58A:O4'	1.65	1.21
4:D:315:58A:C1'	4:D:315:58A:O4'	1.65	1.15
1:D:66:ASP:OD1	4:D:315:58A:OAW	1.62	1.14
1:C:66:ASP:OD1	4:C:310:58A:OAW	1.69	1.08
1:A:66:ASP:OD2	1:A:91:ASP:OD2	1.77	1.01
1:B:36:THR:HG21	1:B:90:LEU:HB3	1.46	0.95
1:A:36:THR:HG21	1:A:90:LEU:HB3	1.51	0.93
1:C:36:THR:HG21	1:C:90:LEU:HB3	1.54	0.89
1:C:-4:LEU:O	1:C:74:ARG:NH1	2.15	0.79
1:B:66:ASP:OD2	1:B:91:ASP:OD2	2.01	0.78
1:D:66:ASP:CG	4:D:315:58A:OAW	2.26	0.77
1:C:66:ASP:OD2	1:C:91:ASP:OD2	2.03	0.77
1:A:-83:GLU:HB3	1:A:-21:LYS:HE2	1.67	0.76
1:C:66:ASP:CG	4:C:310:58A:OAW	2.29	0.75
1:C:-68:LYS:HD2	1:C:-27:TYR:HB2	1.69	0.74
1:B:-122:LEU:HD11	1:B:-11:GLU:HB2	1.71	0.73
1:D:-126:TYR:HB3	1:D:-116:ARG:HB2	1.70	0.71
1:A:66:ASP:O	4:A:311:58A:OAT	2.09	0.69
1:A:-4:LEU:HD22	1:A:74:ARG:HB3	1.75	0.68
1:D:143:ALA:O	1:D:191:ARG:NH1	2.26	0.68
1:D:-107:ARG:NH2	1:D:77:PHE:O	2.26	0.67
1:B:-83:GLU:HB3	1:B:-21:LYS:HE2	1.76	0.67
1:D:-122:LEU:O	1:D:-114:ARG:NH2	2.29	0.66
1:B:-121:LEU:HB3	1:B:75:LEU:HD21	1.77	0.65
4:A:311:58A:H40	4:A:311:58A:H67	1.77	0.65
1:C:74:ARG:NH2	4:C:310:58A:OAS	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-4:LEU:O	1:D:74:ARG:NH1	2.31	0.64
1:A:-127:ILE:HD11	1:A:-15:LEU:HD21	1.81	0.63
1:D:74:ARG:NH2	4:D:315:58A:OAS	2.32	0.62
1:D:92:ARG:NH2	1:D:130:SER:OG	2.32	0.62
1:A:66:ASP:O	1:A:69:ASP:OD1	2.16	0.62
1:B:-4:LEU:HD22	1:B:74:ARG:HB3	1.81	0.62
1:B:139:LEU:HD21	1:C:81:PRO:O	2.00	0.62
1:D:92:ARG:HH11	1:D:95:ASP:HB2	1.66	0.61
1:C:159:VAL:HA	4:C:310:58A:H70	1.83	0.61
1:A:-114:ARG:NH1	1:A:75:LEU:O	2.34	0.60
1:B:-3:ILE:HG22	1:B:71:LEU:HD11	1.83	0.60
1:A:-126:TYR:HB3	1:A:-116:ARG:HB2	1.83	0.60
1:A:-122:LEU:O	1:A:-114:ARG:NH2	2.34	0.60
2:C:301:8K6:H162	2:C:302:8K6:H162	1.83	0.60
1:B:67:ILE:O	1:B:71:LEU:HD13	2.02	0.59
1:B:16:PRO:HB2	2:B:306:8K6:H141	1.85	0.58
1:D:-122:LEU:HD11	1:D:-11:GLU:HB2	1.86	0.58
1:A:67:ILE:O	1:A:71:LEU:HD13	2.05	0.57
1:A:-88:TYR:HE2	1:A:-53:GLY:HA2	1.69	0.57
1:B:92:ARG:HH22	1:B:126:SER:HB3	1.69	0.57
1:A:-69:ARG:HG3	1:A:-30:LEU:HD21	1.85	0.57
1:D:27:SER:OG	1:D:78:ARG:NH2	2.39	0.56
1:C:143:ALA:O	1:C:191:ARG:NH1	2.38	0.56
1:D:9:LEU:O	1:D:13:ILE:HG13	2.06	0.56
1:A:153:ARG:HD3	1:A:180:LEU:HD11	1.88	0.56
1:C:-136:ARG:NH1	1:C:-89:ASP:OD2	2.39	0.55
1:D:153:ARG:NE	1:D:180:LEU:HD11	2.22	0.55
1:A:-88:TYR:CE2	1:A:-53:GLY:HA2	2.41	0.55
1:D:139:LEU:HD21	1:A:81:PRO:O	2.06	0.55
1:D:-121:LEU:HB3	1:D:75:LEU:HD21	1.86	0.55
1:D:-136:ARG:NE	1:D:-89:ASP:OD2	2.39	0.55
1:D:-118:THR:OG1	1:D:-115:GLU:HG2	2.08	0.54
1:A:-103:ASP:OD1	1:A:-101:ARG:NH1	2.41	0.54
1:B:-118:THR:OG1	1:B:-115:GLU:HG2	2.07	0.54
1:A:118:LEU:O	1:A:121:ILE:HG22	2.06	0.54
1:C:126:SER:O	1:C:129:VAL:HG12	2.08	0.54
1:D:-68:LYS:HD2	1:D:-27:TYR:HB2	1.89	0.53
1:D:139:LEU:HG	1:A:81:PRO:HB3	1.90	0.53
1:A:-69:ARG:HE	1:A:-69:ARG:H	1.56	0.53
1:B:-107:ARG:NH2	1:B:77:PHE:O	2.41	0.53
1:C:-122:LEU:O	1:C:-114:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-118:THR:OG1	1:C:-115:GLU:HG2	2.07	0.53
1:A:-129:HIS:CE1	1:A:-82:PRO:HD3	2.42	0.53
1:D:44:LEU:HD21	1:D:97:SER:HB3	1.91	0.53
1:D:66:ASP:OD2	1:D:91:ASP:OD2	2.27	0.53
1:A:-118:THR:OG1	1:A:-115:GLU:HG2	2.09	0.52
1:C:-129:HIS:CE1	1:C:-82:PRO:HD3	2.43	0.52
1:A:-2:GLY:HA2	1:A:-1:SER:C	2.34	0.52
1:D:-127:ILE:HD11	1:D:-15:LEU:HD21	1.91	0.52
1:D:-69:ARG:HA	1:D:-56:PHE:HD1	1.74	0.52
1:B:9:LEU:O	1:B:13:ILE:HG13	2.10	0.52
1:A:126:SER:O	1:A:129:VAL:HG12	2.10	0.52
1:D:118:LEU:O	1:D:121:ILE:HG22	2.10	0.52
1:B:52:LEU:HB2	1:B:165:GLY:HA3	1.92	0.52
1:C:-126:TYR:HB3	1:C:-116:ARG:HB2	1.91	0.52
1:D:126:SER:O	1:D:129:VAL:HG12	2.11	0.51
1:B:-88:TYR:HE2	1:B:-53:GLY:HA2	1.75	0.51
1:C:128:LEU:O	1:C:132:SER:OG	2.27	0.51
1:A:-2:GLY:HA2	1:A:0:GLY:N	2.26	0.51
1:D:-88:TYR:HE2	1:D:-53:GLY:HA2	1.77	0.50
1:C:146:GLY:HA3	1:C:187:THR:HG23	1.93	0.50
1:D:3:ASN:O	1:D:7:ARG:N	2.35	0.50
1:D:137:GLU:OE1	1:A:135:ARG:NH1	2.45	0.50
1:A:-94:LEU:HD23	1:A:-50:ARG:HA	1.93	0.50
1:B:126:SER:O	1:B:129:VAL:HG12	2.12	0.50
1:C:141:LEU:HB3	1:C:198:GLN:OE1	2.11	0.50
1:A:-69:ARG:HA	1:A:-56:PHE:HD2	1.75	0.49
1:C:64:PHE:O	1:C:67:ILE:HG22	2.11	0.49
1:A:-68:LYS:HD2	1:A:-27:TYR:HB2	1.94	0.49
1:A:-4:LEU:O	1:A:74:ARG:NH1	2.45	0.49
1:D:163:LEU:O	1:D:166:LEU:HG	2.12	0.49
1:D:28:PRO:HG2	1:D:78:ARG:HH21	1.78	0.49
1:B:-126:TYR:HB3	1:B:-116:ARG:HG3	1.95	0.49
1:A:-22:ILE:HD12	1:A:-9:LEU:HD12	1.94	0.49
1:A:92:ARG:HH22	1:A:126:SER:HB3	1.78	0.48
1:A:60:THR:O	1:A:63:VAL:HG12	2.13	0.48
1:C:-3:ILE:HD13	1:C:11:ALA:HB2	1.95	0.48
1:A:64:PHE:O	1:A:67:ILE:HG12	2.14	0.47
1:B:-22:ILE:HD12	1:B:-9:LEU:HD12	1.95	0.47
1:C:43:ALA:O	1:C:47:TYR:HB2	2.13	0.47
1:B:-94:LEU:HD23	1:B:-50:ARG:HA	1.96	0.47
1:B:-88:TYR:CE2	1:B:-53:GLY:HA2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-68:LYS:HD2	1:B:-27:TYR:HB2	1.96	0.47
1:B:143:ALA:O	1:B:191:ARG:NH1	2.48	0.47
1:C:108:LEU:HD12	1:C:109:GLY:H	1.79	0.47
1:D:60:THR:O	1:D:63:VAL:HG12	2.15	0.47
1:A:179:VAL:HG22	2:A:306:8K6:H141	1.97	0.47
1:A:66:ASP:OD2	1:A:91:ASP:CG	2.52	0.46
1:C:38:GLY:HA3	1:C:62:PHE:CG	2.50	0.46
1:C:-114:ARG:NH1	1:C:75:LEU:O	2.48	0.46
1:A:63:VAL:HG21	1:A:154:LEU:HD13	1.98	0.46
1:C:-116:ARG:HG3	1:C:-100:PHE:CZ	2.50	0.46
1:D:-1:SER:HB3	1:D:2:LEU:HD13	1.98	0.46
1:A:146:GLY:HA3	1:A:187:THR:HG23	1.98	0.46
1:A:104:ILE:HD13	2:A:301:8K6:H142	1.98	0.46
1:C:153:ARG:HD3	1:C:180:LEU:HD11	1.98	0.46
1:D:32:THR:HG22	1:D:90:LEU:HD12	1.98	0.45
1:D:-42:GLN:HA	1:D:-39:ILE:HG12	1.97	0.45
1:D:38:GLY:HA3	1:D:62:PHE:CG	2.51	0.45
1:B:-114:ARG:HH12	1:B:75:LEU:HD12	1.81	0.45
1:B:57:VAL:HA	1:B:60:THR:HG22	1.98	0.45
1:C:26:VAL:HG22	2:C:306:8K6:H132	1.97	0.45
1:D:-4:LEU:HD22	1:D:74:ARG:HB3	1.99	0.45
1:A:57:VAL:HA	1:A:60:THR:HG22	1.99	0.45
1:C:173:LEU:O	1:C:176:VAL:HG12	2.16	0.45
4:D:315:58A:H56	4:D:315:58A:H28	1.98	0.45
1:C:-121:LEU:HD13	1:C:75:LEU:HD11	1.98	0.45
1:C:173:LEU:HA	1:C:176:VAL:HG12	1.98	0.45
1:D:155:VAL:HG22	4:D:315:58A:H59	1.98	0.45
1:D:159:VAL:HA	4:D:315:58A:H70	1.98	0.45
1:C:-7:LEU:HD11	1:C:71:LEU:HD21	1.97	0.45
1:D:128:LEU:O	1:D:132:SER:OG	2.35	0.44
4:A:311:58A:OAT	4:A:311:58A:OAW	2.36	0.44
1:C:-129:HIS:NE2	1:C:-84:LEU:O	2.37	0.44
1:A:-133:TYR:HA	1:A:-101:ARG:O	2.18	0.44
1:D:-52:ASP:N	1:D:-52:ASP:OD1	2.50	0.44
1:D:139:LEU:HD23	1:D:141:LEU:HD13	2.00	0.44
1:A:38:GLY:HA3	1:A:62:PHE:CG	2.52	0.44
1:A:43:ALA:O	1:A:47:TYR:HB2	2.17	0.44
1:A:77:PHE:HD1	1:A:77:PHE:HA	1.69	0.44
1:B:85:PHE:HB2	1:C:139:LEU:CD2	2.48	0.44
1:C:45:ILE:HG12	2:C:304:8K6:H151	1.99	0.44
1:B:-131:LYS:NZ	1:B:-98:ASP:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-129:HIS:NE2	1:B:-84:LEU:O	2.44	0.44
1:B:-122:LEU:O	1:B:-114:ARG:NH2	2.49	0.44
1:D:-88:TYR:CE2	1:D:-53:GLY:HA2	2.53	0.44
1:B:-114:ARG:NH1	1:B:75:LEU:O	2.50	0.43
1:B:163:LEU:O	1:B:166:LEU:HG	2.17	0.43
1:D:83:GLY:C	4:D:315:58A:H6	2.43	0.43
1:A:70:GLY:HA3	4:A:311:58A:OAS	2.18	0.43
1:B:-52:ASP:N	1:B:-52:ASP:OD1	2.52	0.43
1:A:-133:TYR:HB3	1:A:-99:PHE:CD2	2.53	0.43
1:B:87:ASP:OD1	1:B:91:ASP:OD2	2.35	0.43
1:D:57:VAL:HA	1:D:60:THR:HG22	2.00	0.43
1:D:43:ALA:O	1:D:47:TYR:HB2	2.19	0.42
1:D:34:VAL:HG11	2:D:307:8K6:H122	2.01	0.42
1:A:143:ALA:O	1:A:191:ARG:NH1	2.52	0.42
1:C:57:VAL:HA	1:C:60:THR:HG22	2.00	0.42
1:B:-129:HIS:CD2	1:B:-82:PRO:HD3	2.53	0.42
1:C:-52:ASP:OD1	1:C:-52:ASP:N	2.52	0.42
1:D:-3:ILE:HG23	1:D:71:LEU:HD13	2.01	0.42
1:D:146:GLY:HA3	1:D:187:THR:HG23	2.01	0.42
1:A:-52:ASP:N	1:A:-52:ASP:OD1	2.50	0.42
1:D:108:LEU:HD12	1:D:109:GLY:H	1.84	0.42
1:D:-116:ARG:HG3	1:D:-100:PHE:CE1	2.55	0.42
1:A:66:ASP:HA	1:A:69:ASP:OD2	2.20	0.42
1:B:186:VAL:O	1:B:190:GLN:HG3	2.20	0.41
1:C:-87:LEU:HD12	1:C:-57:TYR:O	2.19	0.41
1:D:15:LEU:N	1:D:16:PRO:HD2	2.35	0.41
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.81	0.41
1:B:-78:LEU:HD22	1:B:-8:LEU:HA	2.03	0.41
1:C:-127:ILE:HD11	1:C:-15:LEU:HD21	2.02	0.41
1:C:92:ARG:HA	1:C:92:ARG:HD2	1.84	0.41
1:C:168:ILE:HD13	1:C:168:ILE:HA	1.92	0.41
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.88	0.41
1:D:178:ILE:O	1:D:182:ILE:HG13	2.20	0.41
1:A:186:VAL:O	1:A:190:GLN:HG3	2.21	0.41
1:B:46:PHE:HE2	1:B:58:VAL:HG21	1.86	0.41
1:A:163:LEU:HA	1:A:166:LEU:HG	2.02	0.40
1:B:163:LEU:HA	1:B:166:LEU:HG	2.03	0.40
1:C:146:GLY:HA2	1:C:190:GLN:OE1	2.21	0.40
1:A:-121:LEU:HD12	1:A:-8:LEU:HD23	2.03	0.40
1:B:-87:LEU:HD12	1:B:-57:TYR:O	2.21	0.40
1:D:153:ARG:HE	1:D:153:ARG:HB2	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:O	1:B:9:LEU:HG	2.21	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	336/342 (98%)	329 (98%)	7 (2%)	0	100	100
1	B	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
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 [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	268/283 (95%)	261 (97%)	7 (3%)	40	58
1	B	270/283 (95%)	262 (97%)	8 (3%)	36	56
1	C	266/283 (94%)	255 (96%)	11 (4%)	27	50
1	D	271/283 (96%)	261 (96%)	10 (4%)	30	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1075/1132 (95%)	1039 (97%)	36 (3%)	33 54

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	-22	ILE
1	D	2	LEU
1	D	44	LEU
1	D	79	GLU
1	D	107	PHE
1	D	108	LEU
1	D	141	LEU
1	D	168	ILE
1	D	171	TRP
1	D	189	PHE
1	A	-69	ARG
1	A	-22	ILE
1	A	5	TYR
1	A	67	ILE
1	A	107	PHE
1	A	141	LEU
1	A	168	ILE
1	B	-94	LEU
1	B	-22	ILE
1	B	63	VAL
1	B	78	ARG
1	B	107	PHE
1	B	114	THR
1	B	141	LEU
1	B	168	ILE
1	C	-22	ILE
1	C	-21	LYS
1	C	40	MET
1	C	44	LEU
1	C	63	VAL
1	C	75	LEU
1	C	79	GLU
1	C	107	PHE
1	C	108	LEU
1	C	141	LEU
1	C	168	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-130	ASN
1	B	190	GLN

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 oligosaccharides 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	D	304	-	6,6,17	0.31	0	5,5,16	0.71	0
2	8K6	B	303	-	6,6,17	0.31	0	5,5,16	0.70	0
2	8K6	D	306	-	6,6,17	0.32	0	5,5,16	0.68	0
2	8K6	A	302	-	6,6,17	0.31	0	5,5,16	0.69	0
2	8K6	C	305	-	6,6,17	0.32	0	5,5,16	0.70	0
2	8K6	A	306	-	6,6,17	0.32	0	5,5,16	0.69	0
2	8K6	D	307	-	6,6,17	0.31	0	5,5,16	0.67	0
4	58A	C	310	3	65,65,69	2.62	17 (26%)	78,82,86	1.11	7 (8%)
2	8K6	C	304	-	6,6,17	0.32	0	5,5,16	0.69	0
4	58A	A	311	3	65,65,69	2.61	18 (27%)	78,82,86	1.09	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	8K6	A	307	-	6,6,17	0.32	0	5,5,16	0.70	0
2	8K6	B	302	-	6,6,17	0.32	0	5,5,16	0.68	0
2	8K6	B	306	-	6,6,17	0.32	0	5,5,16	0.69	0
2	8K6	D	311	-	6,6,17	0.30	0	5,5,16	0.71	0
2	8K6	C	301	-	6,6,17	0.32	0	5,5,16	0.68	0
4	58A	D	315	3	65,65,69	2.63	18 (27%)	78,82,86	1.10	6 (7%)
2	8K6	D	308	-	6,6,17	0.33	0	5,5,16	0.69	0
4	58A	B	309	3	65,65,69	2.65	18 (27%)	78,82,86	1.10	5 (6%)
2	8K6	D	305	-	6,6,17	0.33	0	5,5,16	0.65	0
2	8K6	D	302	-	6,6,17	0.31	0	5,5,16	0.68	0
2	8K6	C	303	-	6,6,17	0.32	0	5,5,16	0.70	0
2	8K6	D	310	-	6,6,17	0.31	0	5,5,16	0.70	0
2	8K6	D	301	-	6,6,17	0.31	0	5,5,16	0.68	0
2	8K6	A	301	-	6,6,17	0.32	0	5,5,16	0.68	0
2	8K6	A	304	-	6,6,17	0.31	0	5,5,16	0.71	0
2	8K6	B	305	-	6,6,17	0.32	0	5,5,16	0.70	0
2	8K6	C	302	-	6,6,17	0.32	0	5,5,16	0.66	0
2	8K6	D	303	-	6,6,17	0.32	0	5,5,16	0.67	0
2	8K6	C	306	-	6,6,17	0.31	0	5,5,16	0.73	0
2	8K6	A	308	-	6,6,17	0.31	0	5,5,16	0.70	0
2	8K6	C	307	-	6,6,17	0.30	0	5,5,16	0.74	0
2	8K6	D	309	-	6,6,17	0.33	0	5,5,16	0.63	0
2	8K6	B	301	-	6,6,17	0.32	0	5,5,16	0.67	0
2	8K6	B	304	-	6,6,17	0.30	0	5,5,16	0.73	0
2	8K6	A	303	-	6,6,17	0.31	0	5,5,16	0.71	0
2	8K6	A	305	-	6,6,17	0.32	0	5,5,16	0.68	0
2	8K6	D	312	-	6,6,17	0.33	0	5,5,16	0.70	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	8K6	D	304	-	-	1/4/4/15	-
2	8K6	B	303	-	-	0/4/4/15	-
2	8K6	D	306	-	-	0/4/4/15	-
2	8K6	A	302	-	-	0/4/4/15	-
2	8K6	C	305	-	-	0/4/4/15	-
2	8K6	A	306	-	-	0/4/4/15	-
2	8K6	D	307	-	-	0/4/4/15	-
4	58A	C	310	3	-	29/61/77/81	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8K6	C	304	-	-	0/4/4/15	-
4	58A	A	311	3	-	26/61/77/81	0/2/2/2
2	8K6	A	307	-	-	0/4/4/15	-
2	8K6	B	302	-	-	0/4/4/15	-
2	8K6	B	306	-	-	0/4/4/15	-
2	8K6	D	311	-	-	0/4/4/15	-
2	8K6	C	301	-	-	0/4/4/15	-
4	58A	D	315	3	-	37/61/77/81	0/2/2/2
2	8K6	D	308	-	-	0/4/4/15	-
4	58A	B	309	3	-	31/61/77/81	0/2/2/2
2	8K6	D	305	-	-	2/4/4/15	-
2	8K6	D	302	-	-	1/4/4/15	-
2	8K6	C	303	-	-	0/4/4/15	-
2	8K6	D	310	-	-	0/4/4/15	-
2	8K6	D	301	-	-	1/4/4/15	-
2	8K6	A	301	-	-	0/4/4/15	-
2	8K6	A	304	-	-	0/4/4/15	-
2	8K6	B	305	-	-	0/4/4/15	-
2	8K6	C	302	-	-	3/4/4/15	-
2	8K6	D	303	-	-	0/4/4/15	-
2	8K6	C	306	-	-	0/4/4/15	-
2	8K6	A	308	-	-	0/4/4/15	-
2	8K6	C	307	-	-	0/4/4/15	-
2	8K6	D	309	-	-	2/4/4/15	-
2	8K6	B	301	-	-	1/4/4/15	-
2	8K6	B	304	-	-	0/4/4/15	-
2	8K6	A	303	-	-	0/4/4/15	-
2	8K6	A	305	-	-	0/4/4/15	-
2	8K6	D	312	-	-	0/4/4/15	-

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	315	58A	O4'-C1'	10.14	1.65	1.42
4	A	311	58A	O4'-C1'	10.14	1.65	1.42
4	B	309	58A	O4'-C1'	10.14	1.65	1.42
4	C	310	58A	O4'-C1'	10.09	1.65	1.42
4	C	310	58A	O4'-C4'	-6.45	1.30	1.45
4	A	311	58A	O4'-C4'	-6.45	1.30	1.45
4	D	315	58A	O4'-C4'	-6.41	1.30	1.45
4	B	309	58A	O4'-C4'	-6.36	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	309	58A	C2'-C1'	-6.33	1.33	1.53
4	D	315	58A	C2'-C1'	-6.29	1.33	1.53
4	C	310	58A	C2'-C1'	-6.24	1.33	1.53
4	A	311	58A	C2'-C1'	-6.20	1.34	1.53
4	B	309	58A	PAR-OAU	6.13	1.66	1.59
4	B	309	58A	PAV-OAU	6.01	1.66	1.59
4	D	315	58A	PAR-OAU	5.97	1.65	1.59
4	C	310	58A	PAR-OAU	5.93	1.65	1.59
4	A	311	58A	PAR-OAU	5.89	1.65	1.59
4	D	315	58A	PAV-OAU	5.70	1.65	1.59
4	C	310	58A	PAV-OAU	5.68	1.65	1.59
4	A	311	58A	PAV-OAU	5.26	1.65	1.59
4	B	309	58A	CAD-NAE	4.85	1.45	1.33
4	C	310	58A	CAD-NAE	4.78	1.45	1.33
4	D	315	58A	CAD-NAE	4.77	1.45	1.33
4	A	311	58A	CAD-NAE	4.74	1.45	1.33
4	B	309	58A	CCD-CCC	4.33	1.56	1.31
4	D	315	58A	CCD-CCC	4.32	1.56	1.31
4	C	310	58A	CCD-CCC	4.32	1.56	1.31
4	A	311	58A	CCD-CCC	4.31	1.56	1.31
4	C	310	58A	CBN-CBM	4.19	1.55	1.31
4	B	309	58A	CBN-CBM	4.18	1.55	1.31
4	D	315	58A	CBN-CBM	4.17	1.55	1.31
4	A	311	58A	CBN-CBM	4.17	1.55	1.31
4	C	310	58A	O3'-C3'	-3.77	1.33	1.43
4	D	315	58A	O3'-C3'	-3.77	1.33	1.43
4	A	311	58A	O3'-C3'	-3.77	1.33	1.43
4	B	309	58A	O3'-C3'	-3.75	1.33	1.43
4	D	315	58A	CAB-NAH	-3.65	1.32	1.40
4	B	309	58A	CAB-NAH	-3.64	1.32	1.40
4	C	310	58A	CAB-NAH	-3.49	1.32	1.40
4	A	311	58A	CAB-NAH	-3.47	1.32	1.40
4	A	311	58A	OBD-CBE	3.34	1.43	1.33
4	D	315	58A	OBD-CBE	3.33	1.43	1.33
4	C	310	58A	OBD-CBE	3.31	1.43	1.33
4	B	309	58A	OBD-CBE	3.25	1.42	1.33
4	A	311	58A	OBB-CBU	2.93	1.42	1.34
4	C	310	58A	OBB-CBU	2.86	1.42	1.34
4	B	309	58A	OBB-CBU	2.83	1.42	1.34
4	C	310	58A	OBB-CBA	-2.82	1.40	1.46
4	D	315	58A	OBB-CBU	2.82	1.42	1.34
4	D	315	58A	OBB-CBA	-2.82	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	309	58A	OBB-CBA	-2.80	1.40	1.46
4	B	309	58A	OAA-CAB	-2.69	1.18	1.23
4	A	311	58A	OBB-CBA	-2.68	1.40	1.46
4	D	315	58A	OAA-CAB	-2.67	1.18	1.23
4	C	310	58A	OAA-CAB	-2.58	1.18	1.23
4	A	311	58A	OAA-CAB	-2.58	1.18	1.23
4	B	309	58A	O2'-C2'	2.46	1.49	1.43
4	C	310	58A	O2'-C2'	2.46	1.49	1.43
4	D	315	58A	O2'-C2'	2.45	1.49	1.43
4	A	311	58A	O2'-C2'	2.44	1.49	1.43
4	B	309	58A	C3'-C4'	2.42	1.59	1.53
4	A	311	58A	C3'-C4'	2.37	1.59	1.53
4	C	310	58A	C3'-C4'	2.32	1.58	1.53
4	D	315	58A	C3'-C4'	2.29	1.58	1.53
4	B	309	58A	CAG-NAH	-2.15	1.33	1.38
4	A	311	58A	CAG-NAH	-2.13	1.33	1.38
4	D	315	58A	CAG-NAH	-2.10	1.33	1.38
4	A	311	58A	PAV-OAY	2.08	1.67	1.59
4	C	310	58A	CAG-NAH	-2.06	1.33	1.38
4	D	315	58A	C1'-NAH	-2.04	1.41	1.47
4	B	309	58A	C1'-NAH	-2.03	1.41	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	58A	OBB-CBU-CBV	4.09	120.32	111.48
4	B	309	58A	OBB-CBU-CBV	4.02	120.18	111.48
4	D	315	58A	OBB-CBU-CBV	4.00	120.14	111.48
4	C	310	58A	OBB-CBU-CBV	3.94	120.00	111.48
4	C	310	58A	OBD-CBE-CBF	2.88	120.60	111.83
4	B	309	58A	OBD-CBE-CBF	2.84	120.50	111.83
4	C	310	58A	OAA-CAB-NAC	-2.80	117.92	122.33
4	A	311	58A	OAA-CAB-NAC	-2.78	117.95	122.33
4	A	311	58A	C4'-O4'-C1'	-2.69	103.53	109.47
4	D	315	58A	OBD-CBE-CBF	2.64	119.87	111.83
4	C	310	58A	C4'-O4'-C1'	-2.57	103.78	109.47
4	D	315	58A	OAA-CAB-NAC	-2.55	118.32	122.33
4	B	309	58A	OAA-CAB-NAC	-2.53	118.35	122.33
4	D	315	58A	NAH-CAB-NAC	2.50	123.15	118.80
4	A	311	58A	OBD-CBE-CBF	2.49	119.43	111.83
4	A	311	58A	NAH-CAB-NAC	2.47	123.09	118.80
4	D	315	58A	C3'-C2'-C1'	2.39	105.98	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	309	58A	NAH-CAB-NAC	2.38	122.94	118.80
4	C	310	58A	NAH-CAB-NAC	2.38	122.92	118.80
4	B	309	58A	C3'-C2'-C1'	2.30	105.81	101.46
4	A	311	58A	C3'-C2'-C1'	2.24	105.71	101.46
4	C	310	58A	C3'-C2'-C1'	2.22	105.66	101.46
4	D	315	58A	C4'-O4'-C1'	-2.13	104.77	109.47
4	C	310	58A	CAF-CAD-NAC	-2.01	117.94	121.32

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	315	58A	O4'-C4'-C5'-O5'
4	D	315	58A	C3'-C4'-C5'-O5'
4	D	315	58A	CAZ-OAY-PAV-OAU
4	D	315	58A	CAZ-OAY-PAV-OAX
4	D	315	58A	CAZ-OAY-PAV-OAW
4	D	315	58A	OBB-CBA-CBC-OB
4	D	315	58A	CBV-CBU-OBB-CBA
4	A	311	58A	O4'-C4'-C5'-O5'
4	A	311	58A	CAZ-OAY-PAV-OAU
4	A	311	58A	CAZ-OAY-PAV-OAX
4	B	309	58A	O4'-C4'-C5'-O5'
4	B	309	58A	C3'-C4'-C5'-O5'
4	B	309	58A	CAZ-OAY-PAV-OAU
4	B	309	58A	CAZ-OAY-PAV-OAX
4	B	309	58A	CAZ-OAY-PAV-OAW
4	B	309	58A	OBB-CBA-CBC-OB
4	C	310	58A	O4'-C4'-C5'-O5'
4	C	310	58A	C3'-C4'-C5'-O5'
4	C	310	58A	CAZ-OAY-PAV-OAU
4	C	310	58A	CAZ-OAY-PAV-OAX
4	C	310	58A	CAZ-OAY-PAV-OAW
4	D	315	58A	OCC-CBU-OBB-CBA
4	B	309	58A	OCC-CBU-OBB-CBA
4	B	309	58A	CBV-CBU-OBB-CBA
4	A	311	58A	CBV-CBU-OBB-CBA
4	A	311	58A	OCC-CBU-OBB-CBA
4	C	310	58A	CBV-CBU-OBB-CBA
4	C	310	58A	OCC-CBU-OBB-CBA
4	A	311	58A	CCB-CCC-CCD-CCE
4	B	309	58A	CCB-CCC-CCD-CCE

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Mol	Chain	Res	Type	Atoms
4	C	310	58A	CCB-CCC-CCD-CCE
4	D	315	58A	CBF-CBE-OBDBBC
4	B	309	58A	CBF-CBE-OBDBBC
4	A	311	58A	C3'-C4'-C5'-O5'
4	B	309	58A	CBU-CBV-CBW-CBX
4	A	311	58A	CBH-CBI-CBJ-CBK
4	B	309	58A	CBP-CBQ-CBR-CBS
4	B	309	58A	CBH-CBI-CBJ-CBK
4	C	310	58A	CBF-CBG-CBH-CBI
4	A	311	58A	CBV-CBW-CBX-CBY
4	D	315	58A	OCL-CBE-OBDBBC
4	B	309	58A	OCL-CBE-OBDBBC
2	B	301	8K6	C13-C14-C15-C16
4	D	315	58A	CBF-CBG-CBH-CBI
4	D	315	58A	CBV-CBW-CBX-CBY
4	A	311	58A	CBO-CBP-CBQ-CBR
4	C	310	58A	CBH-CBI-CBJ-CBK
4	C	310	58A	CBW-CBX-CBY-CBZ
4	D	315	58A	CCF-CCG-CCH-CCI
4	C	310	58A	CBO-CBP-CBQ-CBR
4	C	310	58A	CBP-CBQ-CBR-CBS
4	D	315	58A	CBO-CBP-CBQ-CBR
4	C	310	58A	CCF-CCG-CCH-CCI
4	A	311	58A	CBF-CBG-CBH-CBI
4	C	310	58A	CBV-CBW-CBX-CBY
4	B	309	58A	CBF-CBG-CBH-CBI
4	A	311	58A	CBX-CBY-CBZ-CCA
4	D	315	58A	OAY-CAZ-CBA-CBC
4	B	309	58A	CCF-CCG-CCH-CCI
4	B	309	58A	CAZ-CBA-CBC-OBDBBC
4	D	315	58A	CBP-CBQ-CBR-CBS
4	A	311	58A	CBP-CBQ-CBR-CBS
2	D	302	8K6	C13-C14-C15-C16
4	D	315	58A	CCG-CCH-CCI-CCJ
4	B	309	58A	CBW-CBX-CBY-CBZ
4	A	311	58A	CBQ-CBR-CBS-CBT
2	D	301	8K6	C11-C12-C13-C14
2	C	302	8K6	C12-C13-C14-C15
4	D	315	58A	CBH-CBI-CBJ-CBK
4	B	309	58A	CBV-CBW-CBX-CBY
4	D	315	58A	OAY-CAZ-CBA-OBDBBC
4	C	310	58A	OAY-CAZ-CBA-CBC

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Mol	Chain	Res	Type	Atoms
4	D	315	58A	CCB-CCC-CCD-CCE
4	C	310	58A	OBB-CBA-CBC-OB
4	C	310	58A	CBJ-CBK-CBL-CBM
4	A	311	58A	CBI-CBJ-CBK-CBL
4	B	309	58A	PAR-OAU-PAV-OAW
4	C	310	58A	PAR-OAU-PAV-OAW
4	A	311	58A	CCF-CCG-CCH-CCI
4	B	309	58A	OAY-CAZ-CBA-CBC
4	D	315	58A	CBU-CBV-CBW-CBX
4	B	309	58A	OAY-CAZ-CBA-OB
4	C	310	58A	OAY-CAZ-CBA-OB
4	D	315	58A	CAZ-CBA-CBC-OB
4	C	310	58A	CAZ-CBA-CBC-OB
4	A	311	58A	CAZ-OAY-PAV-OAW
2	D	304	8K6	C12-C13-C14-C15
4	C	310	58A	CBG-CBH-CBI-CBJ
4	A	311	58A	CBM-CBN-CBO-CBP
4	B	309	58A	CCA-CCB-CCC-CCD
4	A	311	58A	CBN-CBO-CBP-CBQ
4	D	315	58A	PAR-OAU-PAV-OAW
4	A	311	58A	PAR-OAU-PAV-OAW
4	D	315	58A	CBN-CBO-CBP-CBQ
4	D	315	58A	CCD-CCE-CCF-CCG
4	B	309	58A	CBJ-CBK-CBL-CBM
4	C	310	58A	CBN-CBO-CBP-CBQ
4	C	310	58A	CBU-CBV-CBW-CBX
2	D	309	8K6	C14-C15-C16-C17
4	B	309	58A	CBX-CBY-CBZ-CCA
4	C	310	58A	CBQ-CBR-CBS-CBT
2	C	302	8K6	C11-C12-C13-C14
2	D	309	8K6	C12-C13-C14-C15
4	D	315	58A	CCE-CCF-CCG-CCH
2	D	305	8K6	C12-C13-C14-C15
4	D	315	58A	CBW-CBX-CBY-CBZ
4	A	311	58A	CCD-CCE-CCF-CCG
4	A	311	58A	CCG-CCH-CCI-CCJ
2	D	305	8K6	C13-C14-C15-C16
4	D	315	58A	CBQ-CBR-CBS-CBT
4	C	310	58A	CCA-CCB-CCC-CCD
4	B	309	58A	CBG-CBH-CBI-CBJ
4	D	315	58A	CCC-CCD-CCE-CCF
4	A	311	58A	CBK-CBL-CBM-CBN

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Mol	Chain	Res	Type	Atoms
4	A	311	58A	CCC-CCD-CCE-CCF
4	B	309	58A	CCC-CCD-CCE-CCF
4	D	315	58A	OBB-CBU-CBV-CBW
4	D	315	58A	CCA-CCB-CCC-CCD
4	D	315	58A	CBK-CBL-CBM-CBN
4	C	310	58A	CCC-CCD-CCE-CCF
2	C	302	8K6	C14-C15-C16-C17
4	D	315	58A	PAR-OAU-PAV-OAX
4	A	311	58A	PAR-OAU-PAV-OAX
4	C	310	58A	OBD-CBE-CBF-CBG
4	B	309	58A	OBD-CBE-CBF-CBG
4	D	315	58A	OBD-CBE-CBF-CBG
4	D	315	58A	CBX-CBY-CBZ-CCA
4	B	309	58A	OBB-CBU-CBV-CBW
4	B	309	58A	OCL-CBE-CBF-CBG
4	D	315	58A	OCL-CBE-CBF-CBG
4	D	315	58A	OCL-CBE-CBF-CBG
4	A	311	58A	PAV-OAU-PAR-OAS
4	C	310	58A	OCL-CBE-CBF-CBG
4	B	309	58A	OCL-CBE-CBF-CBG

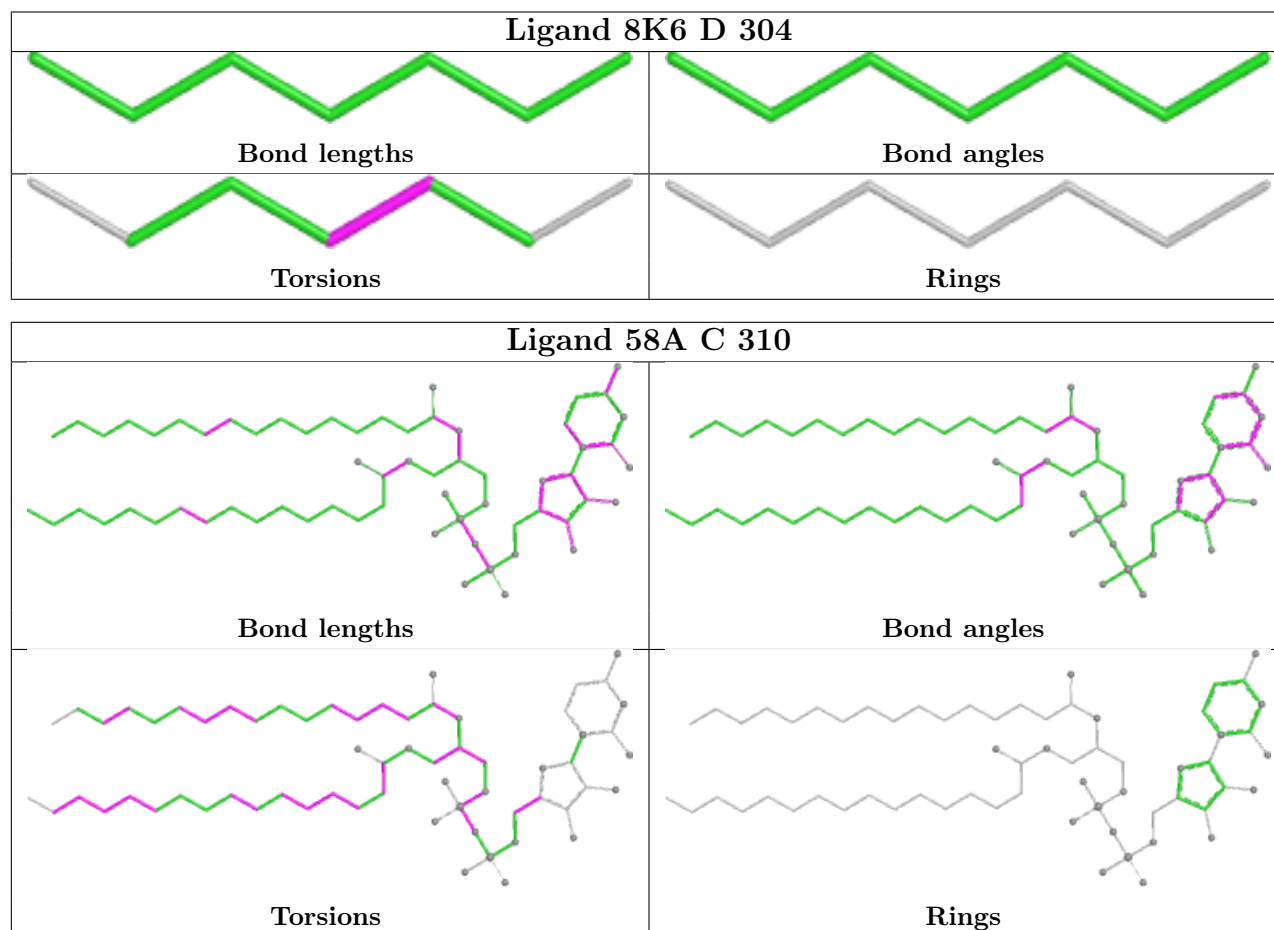
There are no ring outliers.

12 monomers are involved in 26 short contacts:

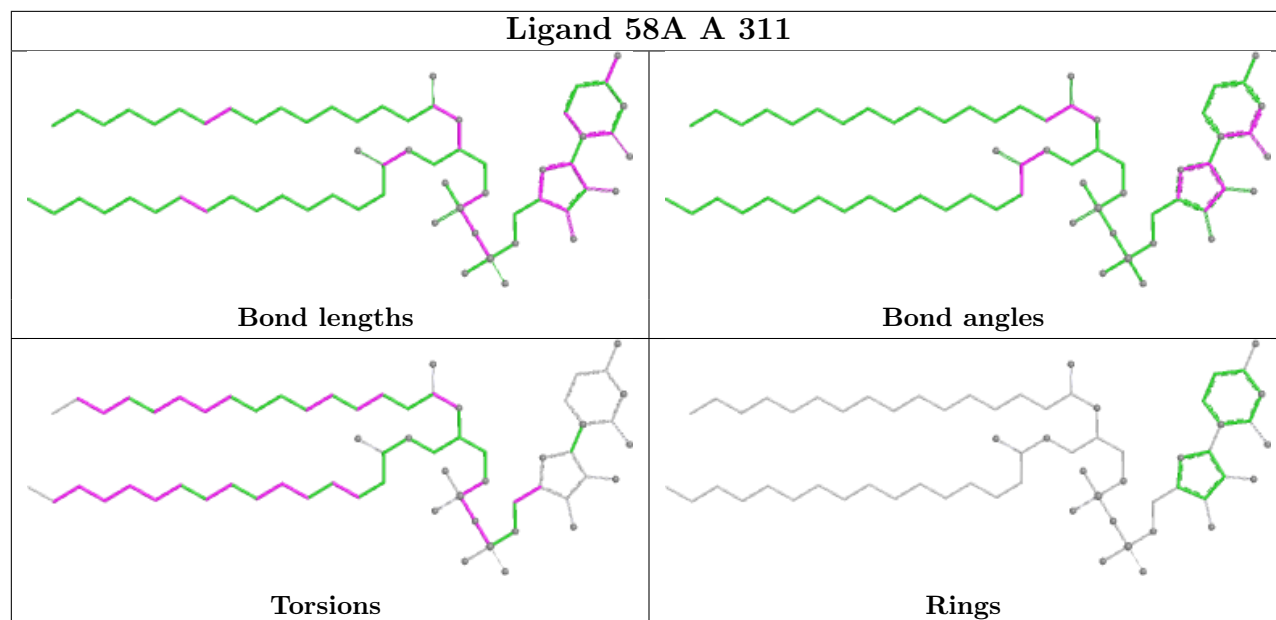
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	306	8K6	1	0
2	D	307	8K6	1	0
4	C	310	58A	5	0
2	C	304	8K6	1	0
4	A	311	58A	5	0
2	B	306	8K6	1	0
2	C	301	8K6	1	0
4	D	315	58A	8	0
4	B	309	58A	1	0
2	A	301	8K6	1	0
2	C	302	8K6	1	0
2	C	306	8K6	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

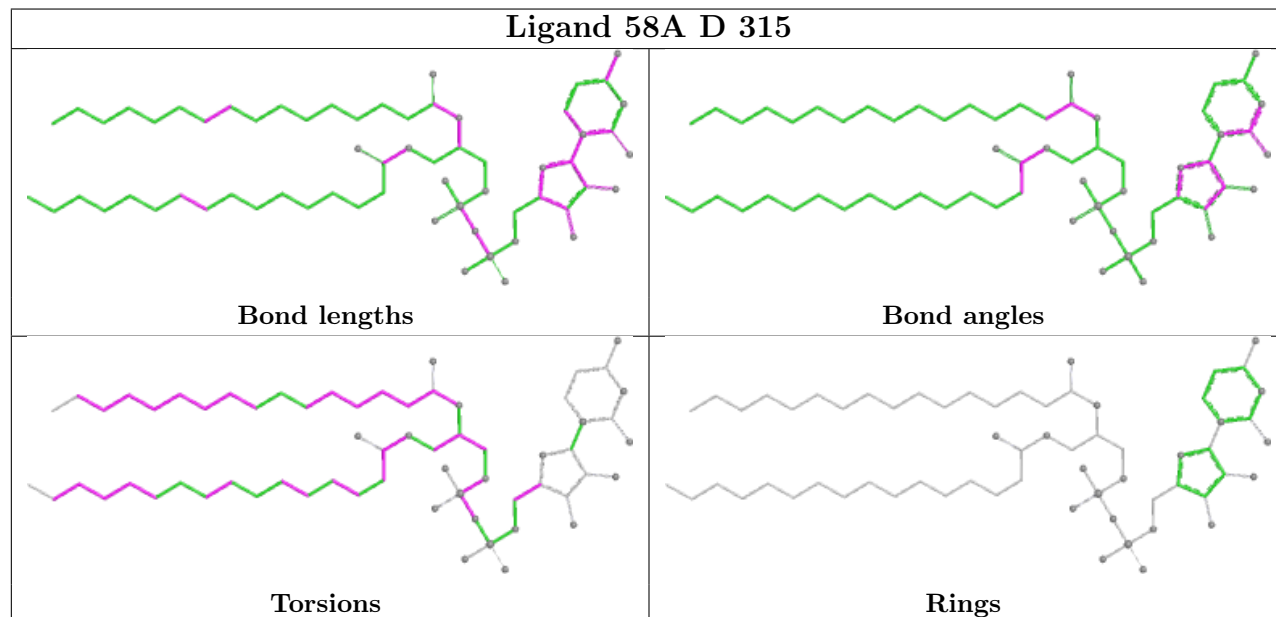
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

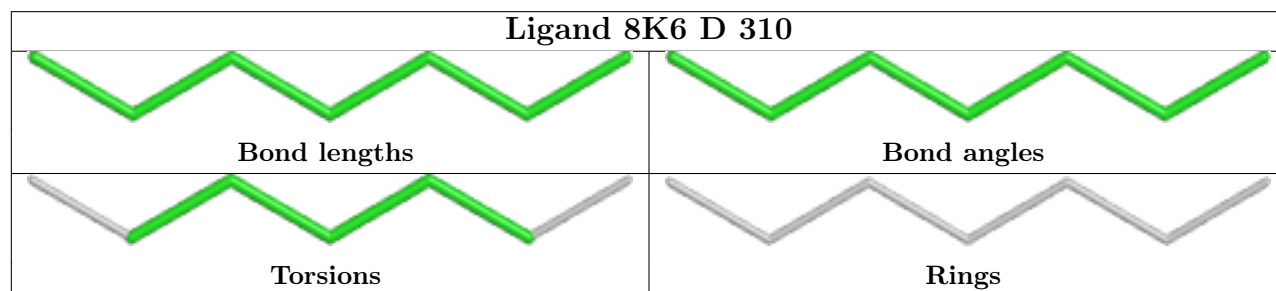
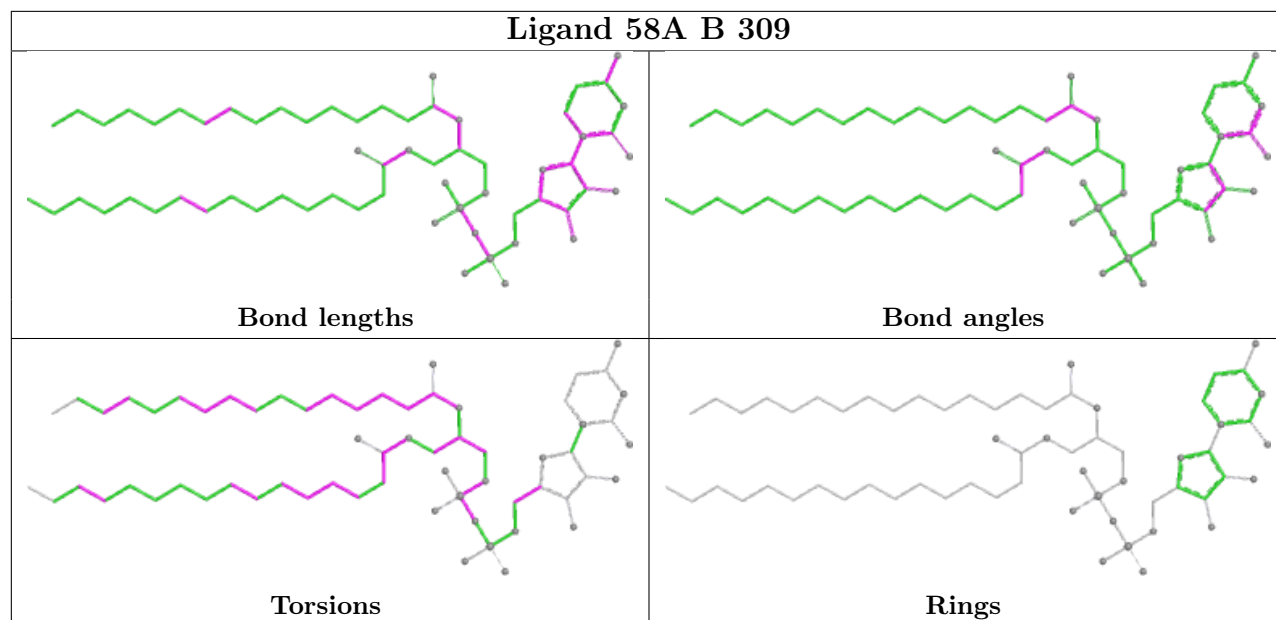


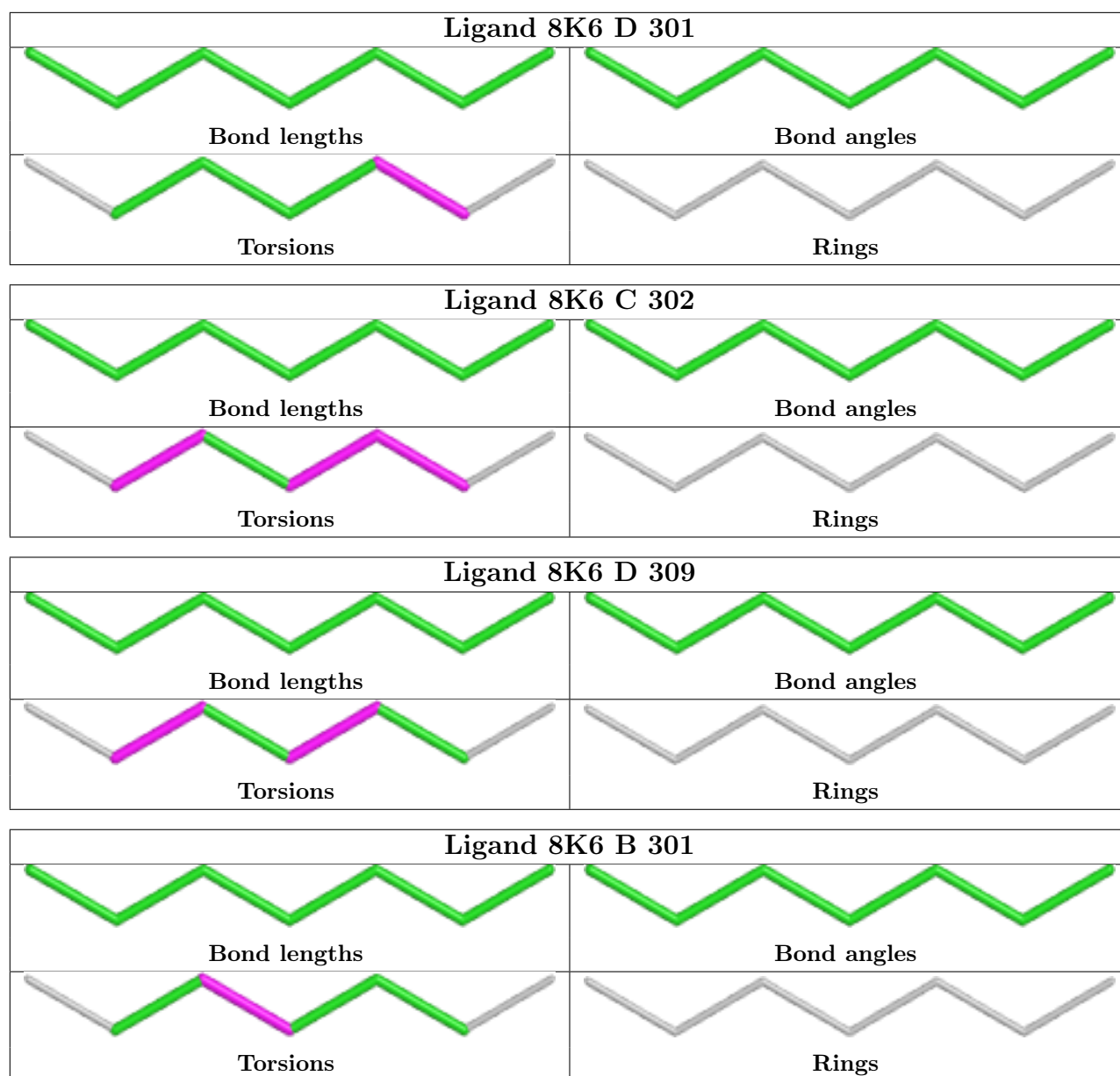
Ligand 58A A 311



Ligand 58A D 315







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	340/342 (99%)	0.64	12 (3%) 47 28	38, 68, 106, 154	0
1	B	342/342 (100%)	0.71	30 (8%) 15 12	37, 69, 119, 151	0
1	C	334/342 (97%)	0.82	27 (8%) 18 13	44, 87, 149, 176	0
1	D	342/342 (100%)	0.63	10 (2%) 53 32	35, 66, 127, 152	0
All	All	1358/1368 (99%)	0.70	79 (5%) 29 18	35, 70, 134, 176	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	VAL	4.3
1	A	156	VAL	4.2
1	C	43	ALA	3.8
1	B	156	VAL	3.5
1	D	179	VAL	3.5
1	B	180	LEU	3.5
1	C	44	LEU	3.5
1	C	101	GLY	3.5
1	A	148	ALA	3.4
1	D	182	ILE	3.3
1	C	40	MET	3.2
1	D	159	VAL	3.0
1	B	121	ILE	3.0
1	B	166	LEU	3.0
1	B	159	VAL	3.0
1	B	184	SER	2.9
1	C	51	GLN	2.9
1	C	-43	LEU	2.8
1	A	121	ILE	2.8
1	B	57	VAL	2.8
1	B	54	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	185	VAL	2.8
1	C	-2	GLY	2.8
1	C	7	ARG	2.7
1	C	-59	VAL	2.7
1	C	52	LEU	2.7
1	B	40	MET	2.7
1	B	101	GLY	2.6
1	B	56	THR	2.6
1	B	-3	ILE	2.6
1	C	45	ILE	2.6
1	D	49	MET	2.6
1	C	-12	ALA	2.5
1	B	61	VAL	2.5
1	A	120	LEU	2.4
1	C	42	GLY	2.4
1	C	100	THR	2.4
1	B	181	ALA	2.4
1	C	99	PHE	2.4
1	C	46	PHE	2.4
1	D	54	TRP	2.4
1	C	181	ALA	2.4
1	B	3	ASN	2.4
1	D	166	LEU	2.4
1	D	79	GLU	2.4
1	C	41	ALA	2.4
1	A	16	PRO	2.3
1	A	46	PHE	2.3
1	A	17	ILE	2.3
1	B	182	ILE	2.3
1	B	158	LEU	2.3
1	B	179	VAL	2.3
1	A	6	ALA	2.3
1	B	185	VAL	2.3
1	A	24	TRP	2.2
1	B	148	ALA	2.2
1	D	162	GLY	2.2
1	C	47	TYR	2.2
1	B	160	ALA	2.2
1	C	8	GLY	2.2
1	B	-79	ILE	2.2
1	B	53	PHE	2.2
1	D	100	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	-7	LEU	2.2
1	B	145	VAL	2.1
1	A	11	ALA	2.1
1	C	183	ALA	2.1
1	C	54	TRP	2.1
1	C	9	LEU	2.1
1	A	180	LEU	2.1
1	B	60	THR	2.1
1	B	38	GLY	2.1
1	C	97	SER	2.1
1	A	1	SER	2.0
1	B	-28	SER	2.0
1	B	99	PHE	2.0
1	B	2	LEU	2.0
1	B	177	LEU	2.0
1	C	184	SER	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 oligosaccharides 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
2	8K6	C	301	7/18	0.43	0.34	61,69,83,92	0
2	8K6	D	304	7/18	0.57	0.33	60,74,85,91	0
2	8K6	B	303	7/18	0.64	0.33	50,51,57,64	0
2	8K6	D	312	7/18	0.67	0.27	51,52,54,61	0
2	8K6	C	306	7/18	0.68	0.38	63,65,70,79	0
2	8K6	D	307	7/18	0.72	0.24	38,40,44,44	0
2	8K6	C	302	7/18	0.73	0.28	44,51,58,60	0

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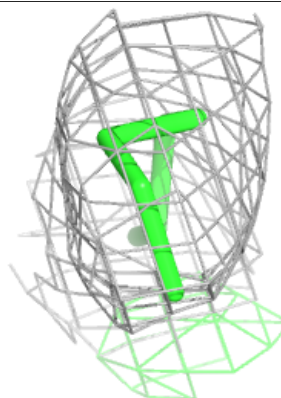
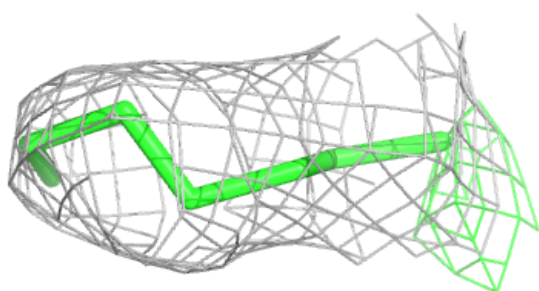
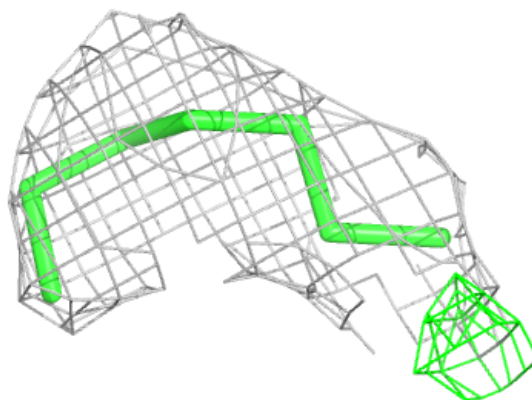
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8K6	B	305	7/18	0.73	0.32	57,68,77,90	0
2	8K6	D	306	7/18	0.74	0.24	40,41,46,47	0
2	8K6	D	310	7/18	0.74	0.40	63,73,75,90	0
2	8K6	B	306	7/18	0.75	0.28	47,51,52,53	0
2	8K6	D	308	7/18	0.76	0.24	32,33,41,44	0
2	8K6	D	301	7/18	0.77	0.28	36,36,40,43	0
2	8K6	B	301	7/18	0.78	0.27	37,39,41,42	0
2	8K6	A	301	7/18	0.79	0.22	40,40,44,46	0
2	8K6	A	302	7/18	0.80	0.20	46,49,54,65	0
2	8K6	D	309	7/18	0.80	0.28	55,57,64,76	0
2	8K6	C	307	7/18	0.80	0.26	46,50,56,60	0
2	8K6	D	305	7/18	0.81	0.24	26,28,31,34	0
2	8K6	B	302	7/18	0.81	0.23	27,28,29,29	0
2	8K6	A	306	7/18	0.81	0.31	44,48,54,63	0
2	8K6	C	303	7/18	0.82	0.24	44,47,54,56	0
2	8K6	C	304	7/18	0.82	0.29	51,53,55,57	0
2	8K6	D	311	7/18	0.82	0.27	61,62,69,84	0
2	8K6	D	303	7/18	0.82	0.20	37,38,40,40	0
2	8K6	A	305	7/18	0.83	0.27	45,48,50,56	0
2	8K6	A	307	7/18	0.84	0.18	33,35,39,39	0
2	8K6	A	303	7/18	0.84	0.23	35,37,40,41	0
2	8K6	D	302	7/18	0.85	0.23	40,45,48,48	0
2	8K6	A	304	7/18	0.85	0.41	36,38,41,44	0
4	58A	C	310	64/68	0.86	0.19	59,73,101,139	0
2	8K6	B	304	7/18	0.87	0.17	36,37,39,42	0
2	8K6	A	308	7/18	0.87	0.19	35,36,37,37	0
2	8K6	C	305	7/18	0.88	0.31	63,66,71,71	0
4	58A	B	309	64/68	0.89	0.20	55,75,116,127	0
4	58A	D	315	64/68	0.89	0.17	56,67,84,126	0
3	MG	A	309	1/1	0.90	0.12	59,59,59,59	0
4	58A	A	311	64/68	0.90	0.16	48,63,91,113	0
3	MG	D	313	1/1	0.93	0.14	64,64,64,64	0
3	MG	C	308	1/1	0.93	0.11	70,70,70,70	0
3	MG	B	307	1/1	0.95	0.15	63,63,63,63	0
3	MG	B	308	1/1	0.96	0.06	63,63,63,63	0
3	MG	D	314	1/1	0.96	0.05	63,63,63,63	0
3	MG	C	309	1/1	0.97	0.04	69,69,69,69	0
3	MG	A	310	1/1	0.99	0.08	61,61,61,61	0

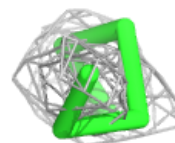
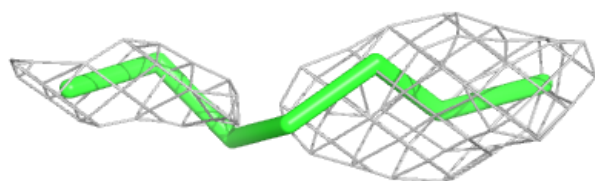
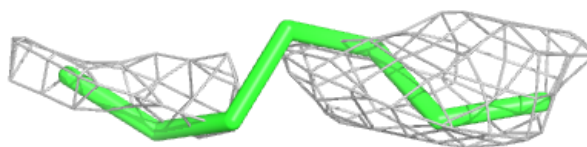
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 8K6 D 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 8K6 C 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

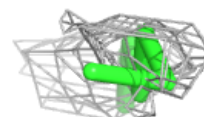
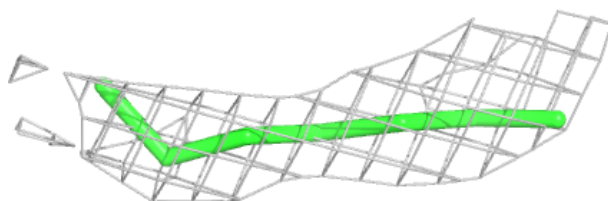
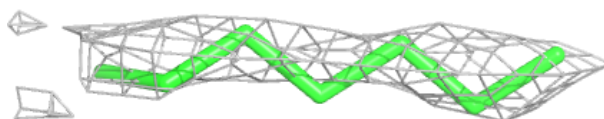


Electron density around 8K6 D 310:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

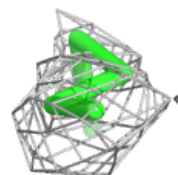
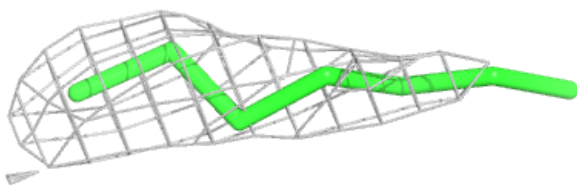
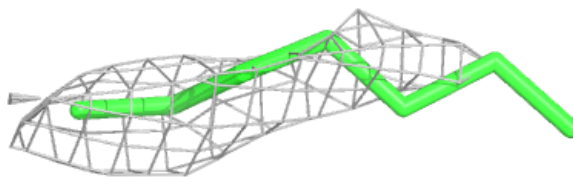
**Electron density around 8K6 D 301:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

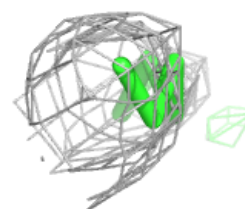
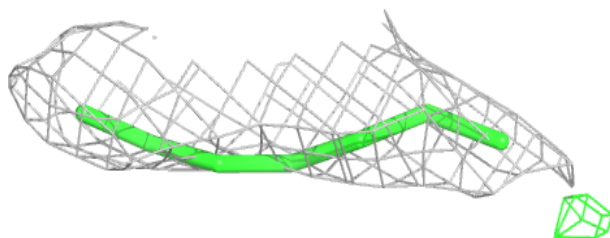
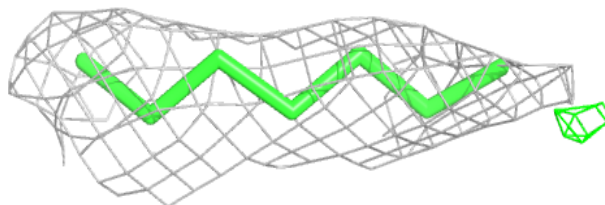


Electron density around 8K6 B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

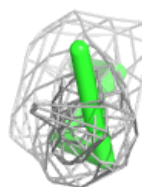
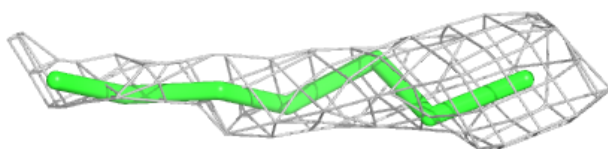
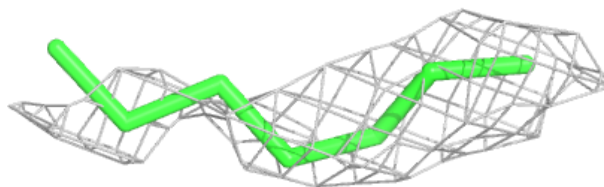
**Electron density around 8K6 D 309:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

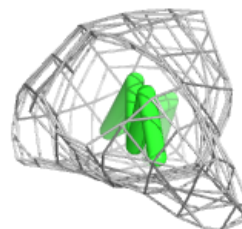
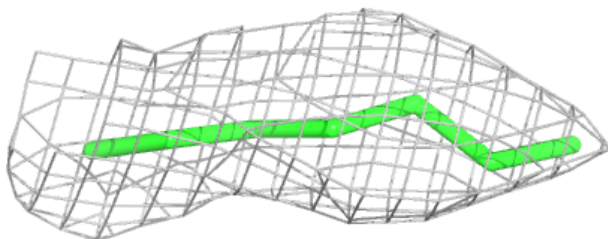
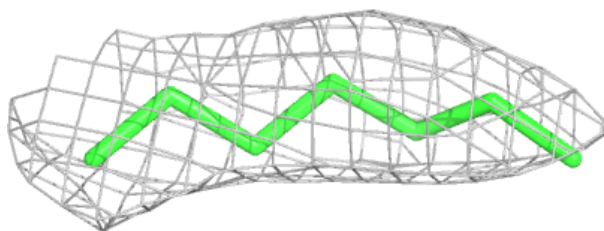


Electron density around 8K6 D 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

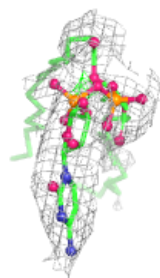
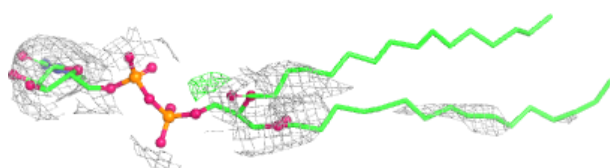
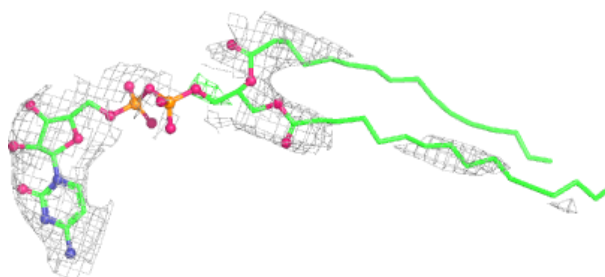
**Electron density around 8K6 D 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

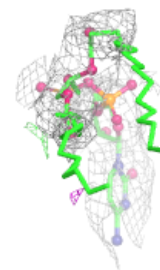
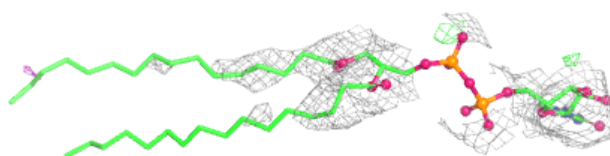
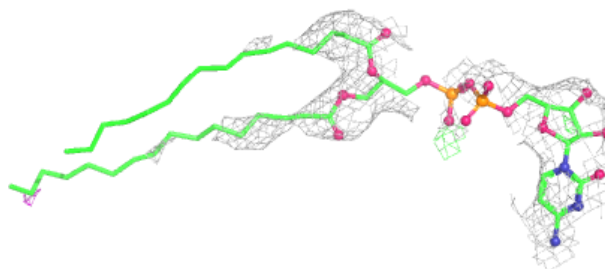


Electron density around 58A C 310:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

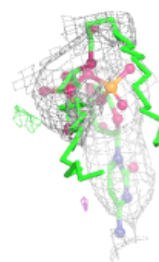
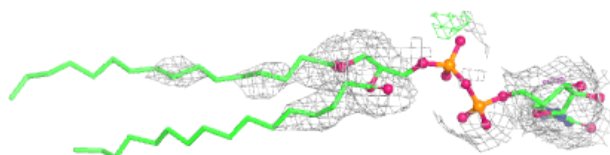
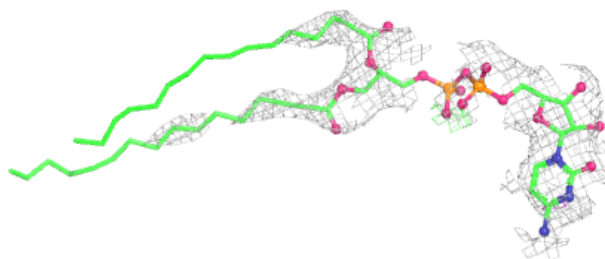
**Electron density around 58A B 309:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

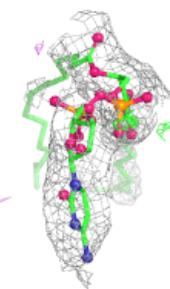
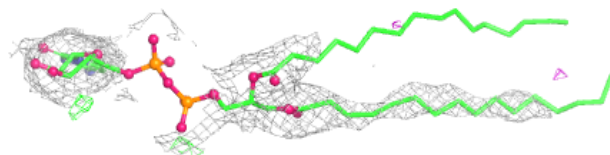
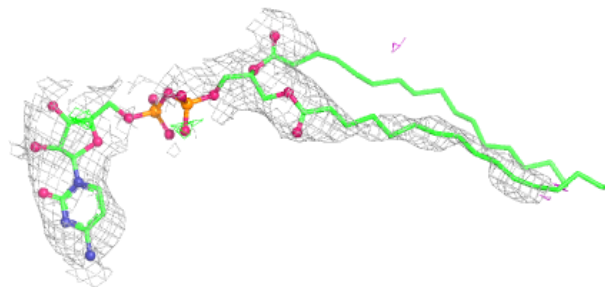


Electron density around 58A D 315:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 58A A 311:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.