



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:08 PM UTC

PDB ID : 5ERL / pdb_00005erl
Title : Crystal structure of the epimerase SnoN in complex with Ni²⁺, succinate and nogalamycin RO
Authors : Selvaraj, B.; Lindqvist, Y.; Siitonen, V.; Metsa-Ketela, M.; Schneider, G.
Deposited on : 2015-11-14
Resolution : 2.85 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

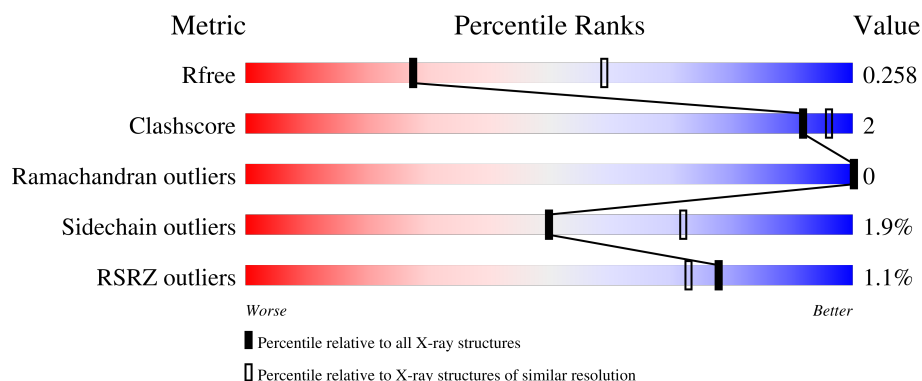
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	305	
1	B	305	
1	C	305	
1	D	305	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SIN	A	301	-	X	-	-
3	SIN	C	301	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8080 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 SnoN,SnoN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1957	1233	352	365	7			
1	B	256	Total	C	N	O	S	0	1	0
			1949	1229	348	365	7			
1	C	257	Total	C	N	O	S	0	1	0
			1960	1235	352	366	7			
1	D	258	Total	C	N	O	S	0	0	0
			1963	1236	353	367	7			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9RN67
A	-10	ALA	-	expression tag	UNP Q9RN67
A	-9	HIS	-	expression tag	UNP Q9RN67
A	-8	HIS	-	expression tag	UNP Q9RN67
A	-7	HIS	-	expression tag	UNP Q9RN67
A	-6	HIS	-	expression tag	UNP Q9RN67
A	-5	HIS	-	expression tag	UNP Q9RN67
A	-4	HIS	-	expression tag	UNP Q9RN67
A	-3	HIS	-	expression tag	UNP Q9RN67
A	-2	ARG	-	expression tag	UNP Q9RN67
A	-1	SER	-	expression tag	UNP Q9RN67
A	0	ALA	-	expression tag	UNP Q9RN67
A	1	ASP	-	expression tag	UNP Q9RN67
B	-11	MET	-	initiating methionine	UNP Q9RN67
B	-10	ALA	-	expression tag	UNP Q9RN67
B	-9	HIS	-	expression tag	UNP Q9RN67
B	-8	HIS	-	expression tag	UNP Q9RN67
B	-7	HIS	-	expression tag	UNP Q9RN67
B	-6	HIS	-	expression tag	UNP Q9RN67
B	-5	HIS	-	expression tag	UNP Q9RN67
B	-4	HIS	-	expression tag	UNP Q9RN67

Continued on next page...

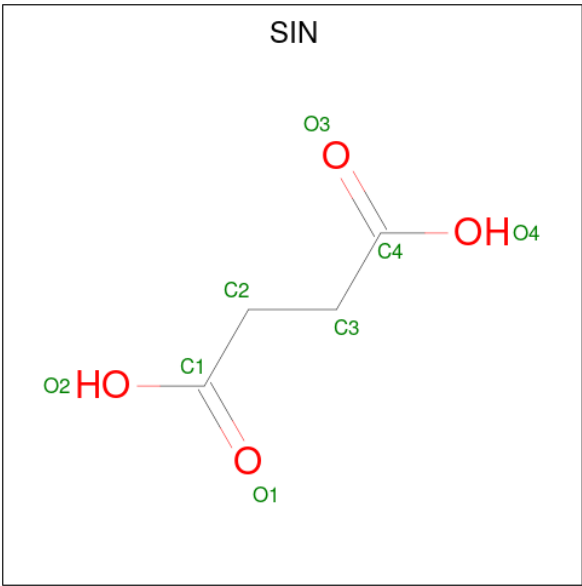
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9RN67
B	-2	ARG	-	expression tag	UNP Q9RN67
B	-1	SER	-	expression tag	UNP Q9RN67
B	0	ALA	-	expression tag	UNP Q9RN67
B	1	ASP	-	expression tag	UNP Q9RN67
C	-11	MET	-	initiating methionine	UNP Q9RN67
C	-10	ALA	-	expression tag	UNP Q9RN67
C	-9	HIS	-	expression tag	UNP Q9RN67
C	-8	HIS	-	expression tag	UNP Q9RN67
C	-7	HIS	-	expression tag	UNP Q9RN67
C	-6	HIS	-	expression tag	UNP Q9RN67
C	-5	HIS	-	expression tag	UNP Q9RN67
C	-4	HIS	-	expression tag	UNP Q9RN67
C	-3	HIS	-	expression tag	UNP Q9RN67
C	-2	ARG	-	expression tag	UNP Q9RN67
C	-1	SER	-	expression tag	UNP Q9RN67
C	0	ALA	-	expression tag	UNP Q9RN67
C	1	ASP	-	expression tag	UNP Q9RN67
D	-11	MET	-	initiating methionine	UNP Q9RN67
D	-10	ALA	-	expression tag	UNP Q9RN67
D	-9	HIS	-	expression tag	UNP Q9RN67
D	-8	HIS	-	expression tag	UNP Q9RN67
D	-7	HIS	-	expression tag	UNP Q9RN67
D	-6	HIS	-	expression tag	UNP Q9RN67
D	-5	HIS	-	expression tag	UNP Q9RN67
D	-4	HIS	-	expression tag	UNP Q9RN67
D	-3	HIS	-	expression tag	UNP Q9RN67
D	-2	ARG	-	expression tag	UNP Q9RN67
D	-1	SER	-	expression tag	UNP Q9RN67
D	0	ALA	-	expression tag	UNP Q9RN67
D	1	ASP	-	expression tag	UNP Q9RN67

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

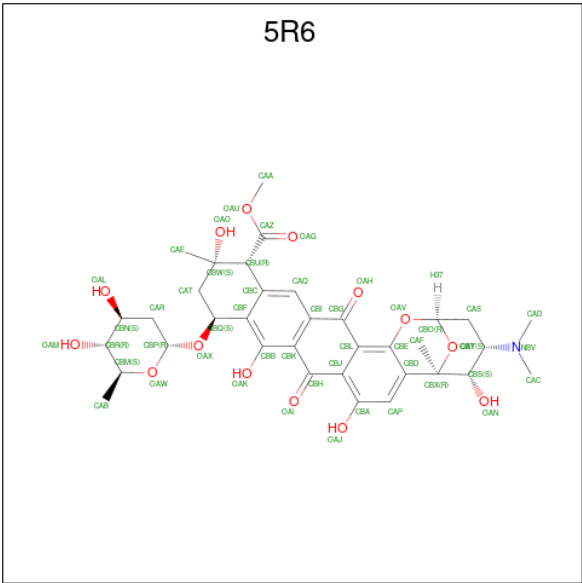
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0
2	B	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0

- Molecule 3 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



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

- Molecule 4 is Nogalamycin RO (CCD ID: 5R6) (formula: C₃₅H₄₁NO₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			50	35	1	14		
4	B	1	Total	C	N	O	0	0
			50	35	1	14		
4	C	1	Total	C	N	O	0	0
			50	35	1	14		
4	D	1	Total	C	N	O	0	0
			50	35	1	14		

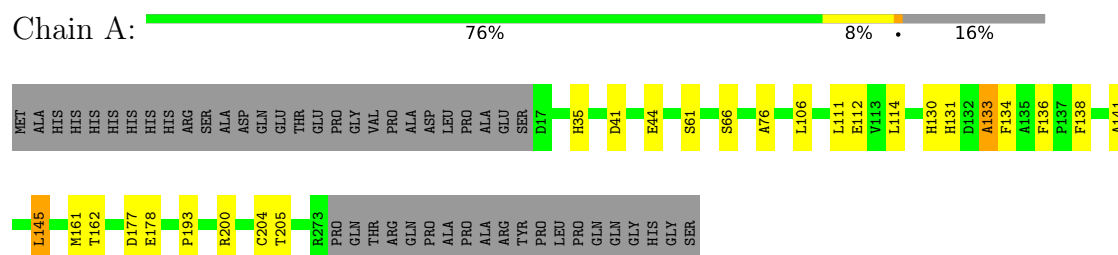
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	2	Total	O	0	0
			2	2		
5	C	1	Total	O	0	0
			1	1		
5	D	4	Total	O	0	0
			4	4		

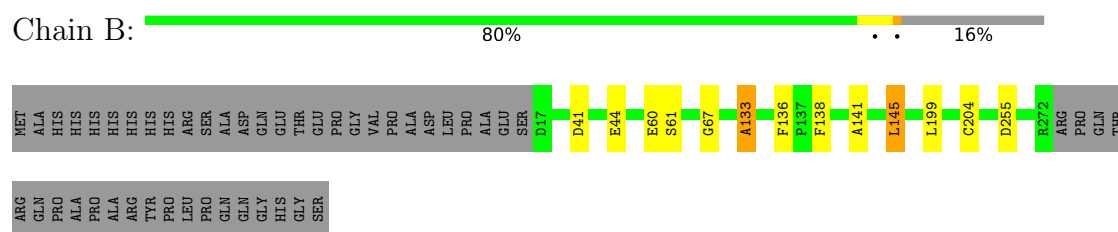
3 Residue-property plots

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.

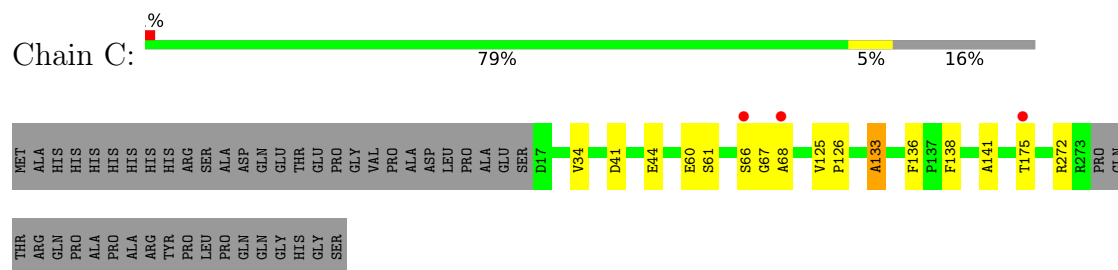
• Molecule 1: SnoN,SnoN



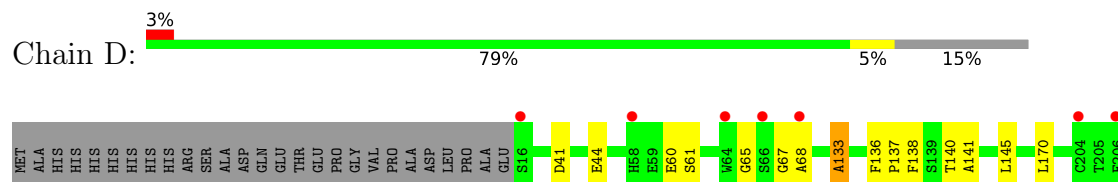
• Molecule 1: SnoN,SnoN



• Molecule 1: SnoN,SnoN



• Molecule 1: SnoN,SnoN



Y231	PRO
D255	GLN
E273	THR
	ARG
	GLN
	PRO
	ALA
	PRO
	ALA
	ARG
	TYR
	PRO
	LEU
	PRO
	GLN
	GLY
	HIS
	GLY
	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.32Å 117.78Å 160.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.85 48.80 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.80-2.85) 99.2 (48.80-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.200 , 0.224 0.236 , 0.258	Depositor DCC
R_{free} test set	1628 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 5R6, SIN

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	1.45	9/2010 (0.4%)	1.25	4/2746 (0.1%)
1	B	1.18	2/2005 (0.1%)	1.14	3/2740 (0.1%)
1	C	1.15	1/2016 (0.0%)	1.14	4/2754 (0.1%)
1	D	1.16	4/2016 (0.2%)	1.15	4/2754 (0.1%)
All	All	1.24	16/8047 (0.2%)	1.17	15/10994 (0.1%)

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	D	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	HIS	CA-C	-5.89	1.45	1.52
1	A	200	ARG	N-CA	5.85	1.53	1.46
1	D	170	LEU	CA-C	-5.76	1.46	1.53
1	A	193	PRO	CA-C	-5.75	1.45	1.52
1	D	137	PRO	CA-CB	-5.67	1.50	1.53
1	A	134	PHE	N-CA	5.63	1.53	1.46
1	A	76	ALA	C-O	-5.58	1.17	1.23
1	B	199	LEU	CA-C	-5.53	1.45	1.52
1	D	68	ALA	N-CA	5.48	1.52	1.46
1	D	255	ASP	CA-C	5.46	1.58	1.53
1	B	255	ASP	CA-C	5.42	1.58	1.53
1	A	162	THR	C-O	-5.34	1.17	1.24
1	A	131	HIS	CA-CB	5.30	1.61	1.52
1	A	205	THR	N-CA	5.25	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	THR	CA-CB	5.10	1.59	1.52
1	A	130	HIS	C-O	-5.03	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ALA	N-CA-C	8.48	121.37	111.02
1	B	133	ALA	N-CA-C	8.43	120.09	111.07
1	A	177	ASP	N-CA-C	7.87	124.04	113.97
1	C	133	ALA	N-CA-C	7.35	118.99	110.97
1	D	133	ALA	N-CA-C	6.28	117.82	110.97
1	C	67	GLY	CA-C-N	5.97	128.27	120.28
1	C	67	GLY	C-N-CA	5.97	128.27	120.28
1	D	67	GLY	CA-C-N	5.84	128.10	120.28
1	D	67	GLY	C-N-CA	5.84	128.10	120.28
1	A	114	LEU	N-CA-C	5.58	118.57	109.59
1	A	106	LEU	N-CA-C	5.29	117.90	109.81
1	B	67	GLY	CA-C-N	5.19	127.24	120.28
1	B	67	GLY	C-N-CA	5.19	127.24	120.28
1	D	140	THR	N-CA-C	5.10	118.54	112.72
1	C	67	GLY	N-CA-C	-5.01	108.76	115.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	65	GLY	Peptide

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	1957	0	1905	7	0
1	B	1949	0	1897	4	0
1	C	1960	0	1910	6	0
1	D	1963	0	1910	3	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	4	1	0
3	B	8	0	4	0	0
3	C	8	0	4	0	0
3	D	8	0	4	0	0
4	A	50	0	0	1	0
4	B	50	0	0	3	0
4	C	50	0	0	0	0
4	D	50	0	0	1	0
5	A	8	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	4	0	0	0	0
All	All	8080	0	7638	25	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 2.

All (25) 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:136:PHE:HB3	1:A:138:PHE:CE2	2.39	0.57
4:A:302:5R6:OAK	4:A:302:5R6:OAI	2.21	0.54
1:A:41:ASP:OD1	1:A:44:GLU:HG3	2.10	0.51
1:D:136:PHE:HB3	1:D:138:PHE:CE2	2.45	0.51
1:C:133:ALA:O	1:C:141:ALA:HB1	2.10	0.51
1:A:133:ALA:O	1:A:141:ALA:HB1	2.12	0.50
1:B:133:ALA:O	1:B:141:ALA:HB1	2.12	0.49
4:D:302:5R6:OAJ	4:D:302:5R6:OAI	2.29	0.49
4:B:302:5R6:OAU	4:B:302:5R6:OAO	2.31	0.48
1:B:136:PHE:HB3	1:B:138:PHE:CE2	2.49	0.48
4:B:302:5R6:OAH	4:B:302:5R6:OAV	2.27	0.48
1:D:41:ASP:OD1	1:D:44:GLU:HG3	2.14	0.48
1:A:145:LEU:HD12	1:A:145:LEU:C	2.39	0.47
1:B:41:ASP:OD1	1:B:44:GLU:HG3	2.15	0.47
1:C:41:ASP:OD1	1:C:44:GLU:HG3	2.14	0.47
1:B:145:LEU:C	1:B:145:LEU:HD12	2.39	0.47
1:D:133:ALA:O	1:D:141:ALA:HB1	2.18	0.44
1:C:272:ARG:HA	1:C:272:ARG:HD2	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:SD	3:A:301:SIN:H22	2.58	0.43
4:B:302:5R6:OAI	4:B:302:5R6:OAJ	2.34	0.42
1:A:111:LEU:C	1:A:111:LEU:HD23	2.45	0.42
1:C:136:PHE:HB3	1:C:138:PHE:CE2	2.54	0.42
1:C:66[B]:SER:HB2	1:C:68:ALA:HB3	2.02	0.41
1:A:111:LEU:HD23	1:A:112:GLU:N	2.35	0.41
1:C:125:VAL:HB	1:C:126:PRO:CD	2.52	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	255/305 (84%)	249 (98%)	6 (2%)	0	100	100
1	B	255/305 (84%)	251 (98%)	4 (2%)	0	100	100
1	C	256/305 (84%)	252 (98%)	4 (2%)	0	100	100
1	D	256/305 (84%)	252 (98%)	4 (2%)	0	100	100
All	All	1022/1220 (84%)	1004 (98%)	18 (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	198/237 (84%)	193 (98%)	5 (2%)	42	66
1	B	198/237 (84%)	194 (98%)	4 (2%)	48	71
1	C	199/237 (84%)	196 (98%)	3 (2%)	57	77
1	D	199/237 (84%)	196 (98%)	3 (2%)	57	77
All	All	794/948 (84%)	779 (98%)	15 (2%)	50	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	66	SER
1	A	145	LEU
1	A	178	GLU
1	A	204	CYS
1	B	60	GLU
1	B	61	SER
1	B	145	LEU
1	B	204	CYS
1	C	34	VAL
1	C	60	GLU
1	C	61	SER
1	D	60	GLU
1	D	61	SER
1	D	145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	HIS
1	B	207	HIS
1	C	58	HIS
1	C	207	HIS
1	D	58	HIS
1	D	207	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
4	5R6	A	302	-	53,56,56	3.32	26 (49%)	70,91,91	2.12	21 (30%)
3	SIN	B	301	2	7,7,7	1.81	2 (28%)	8,8,8	2.48	4 (50%)
4	5R6	D	302	-	53,56,56	2.44	19 (35%)	70,91,91	1.45	12 (17%)
4	5R6	C	302	-	53,56,56	2.27	19 (35%)	70,91,91	1.46	14 (20%)
3	SIN	D	301	2	7,7,7	1.76	2 (28%)	8,8,8	1.96	2 (25%)
3	SIN	A	301	2	7,7,7	3.88	6 (85%)	8,8,8	1.98	2 (25%)
3	SIN	C	301	2	7,7,7	2.77	5 (71%)	8,8,8	2.09	3 (37%)
4	5R6	B	302	-	53,56,56	2.61	17 (32%)	70,91,91	1.71	13 (18%)

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
4	5R6	A	302	-	-	5/14/94/94	0/1/7/7
3	SIN	B	301	2	-	0/5/5/5	-
4	5R6	D	302	-	-	4/14/94/94	0/1/7/7
4	5R6	C	302	-	-	8/14/94/94	0/1/7/7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIN	D	301	2	-	2/5/5/5	-
3	SIN	A	301	2	-	3/5/5/5	-
3	SIN	C	301	2	-	2/5/5/5	-
4	5R6	B	302	-	-	8/14/94/94	0/1/7/7

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	5R6	CBN-CBR	11.55	1.70	1.52
4	A	302	5R6	OAW-CBP	7.81	1.62	1.42
4	B	302	5R6	CBF-CBQ	-6.82	1.39	1.51
4	D	302	5R6	CBU-CAZ	-6.77	1.44	1.52
4	B	302	5R6	OAW-CBM	6.74	1.60	1.44
4	C	302	5R6	CBC-CBU	-6.43	1.43	1.52
4	D	302	5R6	CBF-CBQ	-6.18	1.41	1.51
4	A	302	5R6	OAQ-CBW	-6.14	1.34	1.44
4	A	302	5R6	CBF-CBQ	-5.99	1.41	1.51
4	D	302	5R6	CBN-CBR	5.86	1.61	1.52
3	A	301	SIN	O1-C1	5.76	1.40	1.22
4	B	302	5R6	CBC-CBU	-5.76	1.44	1.52
3	A	301	SIN	O3-C4	5.72	1.40	1.22
4	A	302	5R6	OAY-CBO	-5.64	1.33	1.42
4	B	302	5R6	CBN-CBR	5.48	1.60	1.52
4	B	302	5R6	OAW-CBP	5.41	1.56	1.42
3	C	301	SIN	C3-C4	5.10	1.62	1.50
4	C	302	5R6	CBX-CBD	-5.10	1.43	1.52
4	B	302	5R6	CBX-CBD	-5.00	1.43	1.52
4	A	302	5R6	OAU-CAZ	4.95	1.45	1.33
4	A	302	5R6	OAV-CBO	4.91	1.51	1.42
4	C	302	5R6	CBF-CBQ	-4.79	1.43	1.51
4	A	302	5R6	CAT-CBQ	4.78	1.61	1.52
4	C	302	5R6	CBU-CAZ	-4.72	1.47	1.52
4	C	302	5R6	CBN-CBR	4.70	1.59	1.52
4	D	302	5R6	OAN-CBS	4.49	1.51	1.42
4	A	302	5R6	CBR-CBM	4.48	1.62	1.52
4	A	302	5R6	CAS-CBO	-4.45	1.39	1.50
4	A	302	5R6	CBU-CAZ	-4.44	1.47	1.52
4	D	302	5R6	OAW-CBP	4.38	1.53	1.42
4	B	302	5R6	CBL-CBG	-4.10	1.38	1.47
4	B	302	5R6	CAT-CBW	-4.10	1.46	1.53
4	D	302	5R6	CAT-CBQ	3.90	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	5R6	CBX-CBS	-3.89	1.41	1.53
3	A	301	SIN	C2-C1	3.88	1.59	1.50
4	A	302	5R6	OAM-CBR	3.86	1.52	1.43
4	C	302	5R6	CBI-CBG	-3.86	1.40	1.48
4	D	302	5R6	CBI-CBG	-3.74	1.40	1.48
4	D	302	5R6	OAU-CAZ	3.70	1.42	1.33
4	D	302	5R6	CBK-CBH	-3.62	1.39	1.47
4	A	302	5R6	CBC-CBU	-3.62	1.47	1.52
4	B	302	5R6	CAE-CBW	3.58	1.58	1.52
4	B	302	5R6	CBU-CAZ	-3.52	1.48	1.52
4	B	302	5R6	OAU-CAZ	3.42	1.41	1.33
4	A	302	5R6	CBK-CBH	-3.36	1.39	1.47
4	B	302	5R6	CBI-CBG	-3.32	1.41	1.48
4	C	302	5R6	CAT-CBQ	3.27	1.58	1.52
3	B	301	SIN	C3-C4	3.25	1.58	1.50
4	B	302	5R6	CBK-CBH	-3.18	1.40	1.47
3	A	301	SIN	C3-C2	3.13	1.62	1.51
4	C	302	5R6	CBK-CBH	-3.12	1.40	1.47
4	D	302	5R6	CBX-CBD	-3.05	1.46	1.52
4	D	302	5R6	CBC-CBU	-3.05	1.48	1.52
4	D	302	5R6	CBL-CBG	-3.03	1.40	1.47
3	A	301	SIN	C3-C4	2.98	1.57	1.50
4	A	302	5R6	CAB-CBM	2.98	1.58	1.51
4	C	302	5R6	OAW-CBP	2.98	1.50	1.42
4	A	302	5R6	CBK-CBB	-2.91	1.36	1.41
4	A	302	5R6	CBL-CBG	-2.90	1.40	1.47
4	A	302	5R6	OAL-CBN	2.89	1.49	1.43
4	D	302	5R6	CBJ-CBH	-2.84	1.41	1.47
4	C	302	5R6	OAU-CAZ	2.83	1.40	1.33
4	C	302	5R6	CBL-CBG	-2.81	1.41	1.47
3	C	301	SIN	O3-C4	2.79	1.31	1.22
4	B	302	5R6	OAX-CBP	2.79	1.49	1.41
3	D	301	SIN	C2-C1	2.73	1.56	1.50
4	D	302	5R6	CAE-CBW	2.73	1.57	1.52
4	C	302	5R6	OAN-CBS	2.71	1.48	1.42
4	B	302	5R6	CAR-CBP	2.69	1.57	1.50
4	A	302	5R6	CAF-CBX	2.67	1.56	1.52
3	C	301	SIN	O1-C1	2.55	1.30	1.22
4	B	302	5R6	CBJ-CBH	-2.54	1.41	1.47
4	C	302	5R6	CAE-CBW	2.51	1.56	1.52
4	D	302	5R6	OAW-CBM	2.50	1.50	1.44
4	A	302	5R6	CBI-CBG	-2.43	1.43	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	302	5R6	CAB-CBM	2.40	1.57	1.51
4	D	302	5R6	CBR-CBM	2.39	1.58	1.52
4	C	302	5R6	CBJ-CBH	-2.39	1.42	1.47
3	C	301	SIN	C2-C1	2.37	1.56	1.50
4	D	302	5R6	OAQ-CBW	2.32	1.48	1.44
3	A	301	SIN	O2-C1	2.32	1.38	1.30
4	A	302	5R6	CAR-CBP	2.31	1.56	1.50
4	C	302	5R6	OAY-CBO	-2.31	1.38	1.42
4	B	302	5R6	CAB-CBM	2.28	1.57	1.51
3	B	301	SIN	O4-C4	-2.26	1.23	1.30
4	D	302	5R6	CAP-CBD	2.26	1.42	1.39
4	A	302	5R6	CAQ-CBI	2.22	1.43	1.39
3	D	301	SIN	C3-C4	2.21	1.55	1.50
4	A	302	5R6	CBJ-CBA	-2.18	1.38	1.41
4	C	302	5R6	OAV-CBE	-2.14	1.34	1.37
4	C	302	5R6	OAV-CBO	-2.10	1.39	1.42
4	C	302	5R6	CBE-CBD	-2.09	1.37	1.41
3	C	301	SIN	C3-C2	2.09	1.59	1.51
4	C	302	5R6	CBR-CBM	2.08	1.57	1.52
4	A	302	5R6	CBE-CBD	-2.06	1.37	1.41
4	A	302	5R6	OAW-CBM	2.00	1.49	1.44

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	5R6	OAW-CBM-CAB	6.00	120.04	106.74
4	A	302	5R6	OAW-CBP-CAR	5.82	119.86	110.84
4	A	302	5R6	CAR-CBN-CBR	-5.35	102.96	110.67
4	A	302	5R6	OAY-CBX-CBD	4.57	119.46	109.51
4	A	302	5R6	OAL-CBN-CBR	4.51	119.50	110.15
4	B	302	5R6	OAX-CBP-OAW	4.45	124.32	109.97
3	A	301	SIN	O2-C1-O1	4.20	134.13	123.33
3	B	301	SIN	O4-C4-O3	-4.09	112.81	123.33
4	A	302	5R6	OAK-CBB-CBK	-4.05	112.07	120.95
4	B	302	5R6	OAU-CAZ-CBU	4.02	118.48	110.74
4	A	302	5R6	OAQ-CBW-CAT	-3.92	99.32	108.05
3	B	301	SIN	O1-C1-C2	-3.89	110.74	123.09
3	D	301	SIN	O2-C1-C2	3.88	126.25	114.00
4	A	302	5R6	OAW-CBM-CAB	3.75	115.07	106.74
4	A	302	5R6	CAQ-CBC-CBF	-3.70	114.36	119.70
4	B	302	5R6	OAG-CAZ-CBU	-3.70	118.97	125.22
4	D	302	5R6	OAW-CBM-CAB	3.63	114.78	106.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	5R6	CBW-CAT-CBQ	-3.57	105.30	114.23
4	D	302	5R6	OAJ-CBA-CBJ	-3.53	114.61	121.14
4	A	302	5R6	CBF-CBC-CBU	3.49	126.44	115.52
4	D	302	5R6	OAG-CAZ-CBU	-3.46	119.37	125.22
4	C	302	5R6	OAW-CBM-CBR	3.44	115.75	109.55
3	A	301	SIN	O2-C1-C2	-3.31	103.53	114.00
4	A	302	5R6	OAV-CBE-CBD	-3.22	115.18	122.69
3	C	301	SIN	O4-C4-O3	-3.21	115.07	123.33
3	C	301	SIN	O4-C4-C3	3.05	123.65	114.00
4	B	302	5R6	OAJ-CBA-CBJ	-3.05	115.49	121.14
4	A	302	5R6	CAE-CBW-CAT	3.04	116.28	110.67
4	A	302	5R6	CBA-CAP-CBD	3.02	124.23	120.16
4	B	302	5R6	CAC-NBV-CAD	-2.97	101.76	110.49
4	A	302	5R6	OAX-CBP-CAR	-2.92	102.67	108.28
4	C	302	5R6	CAB-CBM-CBR	-2.91	107.76	113.08
3	D	301	SIN	O1-C1-C2	-2.90	113.89	123.09
4	B	302	5R6	CAB-CBM-CBR	-2.90	107.78	113.08
4	C	302	5R6	CBF-CBC-CBU	2.76	124.17	115.52
4	C	302	5R6	OAM-CBR-CBM	-2.74	103.69	109.74
4	D	302	5R6	CAA-OAU-CAZ	2.71	122.06	115.92
3	B	301	SIN	O4-C4-C3	2.71	122.55	114.00
4	D	302	5R6	CBF-CBC-CBU	2.69	123.94	115.52
3	C	301	SIN	O2-C1-C2	-2.64	105.67	114.00
4	C	302	5R6	CBN-CBR-CBM	2.63	117.77	110.00
4	D	302	5R6	CBI-CBG-CBL	2.60	122.17	117.97
4	D	302	5R6	CBN-CBR-CBM	2.55	117.53	110.00
4	A	302	5R6	CBB-CBF-CBQ	2.52	124.50	119.01
4	D	302	5R6	CBJ-CBL-CBG	-2.51	116.60	120.00
4	B	302	5R6	CBE-CBL-CBG	-2.51	118.80	122.55
4	C	302	5R6	OAJ-CBA-CBJ	-2.50	116.52	121.14
4	D	302	5R6	OAL-CBN-CBR	2.41	115.15	110.15
4	A	302	5R6	OAU-CAZ-OAG	-2.38	119.21	123.85
4	B	302	5R6	CBF-CBC-CBU	2.36	122.89	115.52
4	C	302	5R6	OAV-CBE-CBD	-2.33	117.25	122.69
4	C	302	5R6	OAU-CAZ-CBU	2.29	115.14	110.74
4	B	302	5R6	CAQ-CBI-CBK	-2.28	117.41	120.33
4	A	302	5R6	CBK-CBB-CBF	2.27	125.45	121.28
4	A	302	5R6	OAJ-CBA-CBJ	-2.27	116.94	121.14
4	C	302	5R6	CAP-CBD-CBX	2.26	125.19	120.67
3	B	301	SIN	O2-C1-C2	2.25	121.11	114.00
4	A	302	5R6	CBI-CAQ-CBC	2.20	125.69	118.84
4	B	302	5R6	CBN-CBR-CBM	2.20	116.50	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	5R6	OAM-CBR-CBM	-2.18	104.92	109.74
4	C	302	5R6	CAR-CBN-CBR	2.14	113.76	110.67
4	D	302	5R6	OAU-CAZ-CBU	2.13	114.83	110.74
4	C	302	5R6	CBW-CAT-CBQ	-2.12	108.94	114.23
4	C	302	5R6	OAG-CAZ-CBU	-2.11	121.66	125.22
4	D	302	5R6	OAV-CBE-CBD	-2.10	117.79	122.69
4	C	302	5R6	OAO-CBW-CAT	-2.10	103.37	108.05
4	C	302	5R6	CAQ-CBC-CBU	-2.06	116.60	121.16
4	D	302	5R6	CAP-CBD-CBX	2.05	124.77	120.67
4	A	302	5R6	CBO-CAS-CBT	2.04	116.13	110.48
4	A	302	5R6	CAP-CBD-CBE	-2.03	114.31	117.15
4	B	302	5R6	CBL-CBJ-CBH	2.02	122.73	120.00

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	5R6	CAT-CBQ-OAX-CBP
4	B	302	5R6	OAG-CAZ-CBU-CBW
4	B	302	5R6	OAU-CAZ-CBU-CBW
4	C	302	5R6	OAW-CBP-OAX-CBQ
4	D	302	5R6	CAR-CBP-OAX-CBQ
4	B	302	5R6	CBU-CAZ-OAU-CAA
4	B	302	5R6	OAG-CAZ-OAU-CAA
4	C	302	5R6	CBU-CAZ-OAU-CAA
4	C	302	5R6	CAR-CBP-OAX-CBQ
4	B	302	5R6	OAW-CBP-OAX-CBQ
4	C	302	5R6	OAG-CAZ-OAU-CAA
4	D	302	5R6	OAW-CBP-OAX-CBQ
4	B	302	5R6	CAR-CBP-OAX-CBQ
4	A	302	5R6	CAS-CBT-NBV-CAC
4	D	302	5R6	CAS-CBT-NBV-CAC
4	A	302	5R6	OAG-CAZ-OAU-CAA
4	B	302	5R6	CAS-CBT-NBV-CAD
4	C	302	5R6	OAU-CAZ-CBU-CBW
4	B	302	5R6	CBF-CBQ-OAX-CBP
4	C	302	5R6	CBF-CBQ-OAX-CBP
4	D	302	5R6	CBF-CBQ-OAX-CBP
4	C	302	5R6	CAS-CBT-NBV-CAC
3	C	301	SIN	O2-C1-C2-C3
3	C	301	SIN	O1-C1-C2-C3
3	A	301	SIN	C2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	301	SIN	O1-C1-C2-C3
4	A	302	5R6	OAG-CAZ-CBU-CBC
3	A	301	SIN	O2-C1-C2-C3
4	C	302	5R6	OAG-CAZ-CBU-CBW
4	A	302	5R6	CBS-CBT-NBV-CAD
3	D	301	SIN	C2-C3-C4-O3
3	D	301	SIN	C2-C3-C4-O4

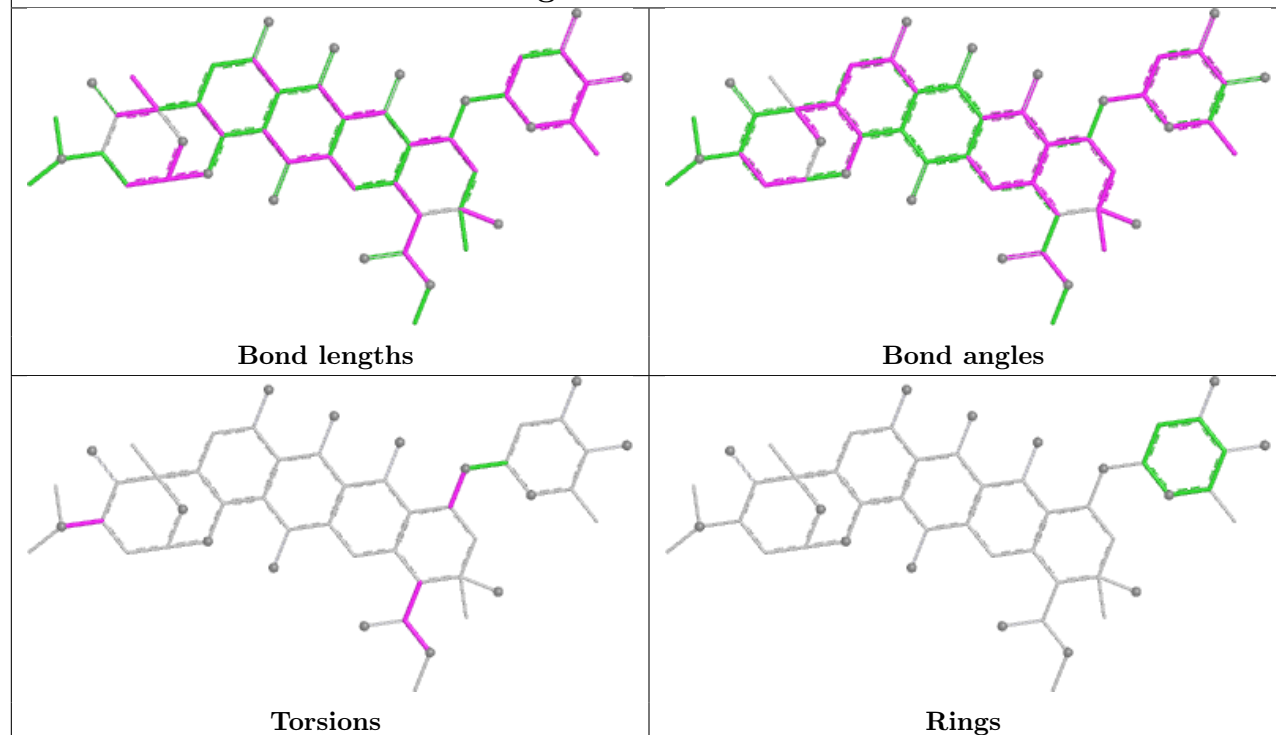
There are no ring outliers.

4 monomers are involved in 6 short contacts:

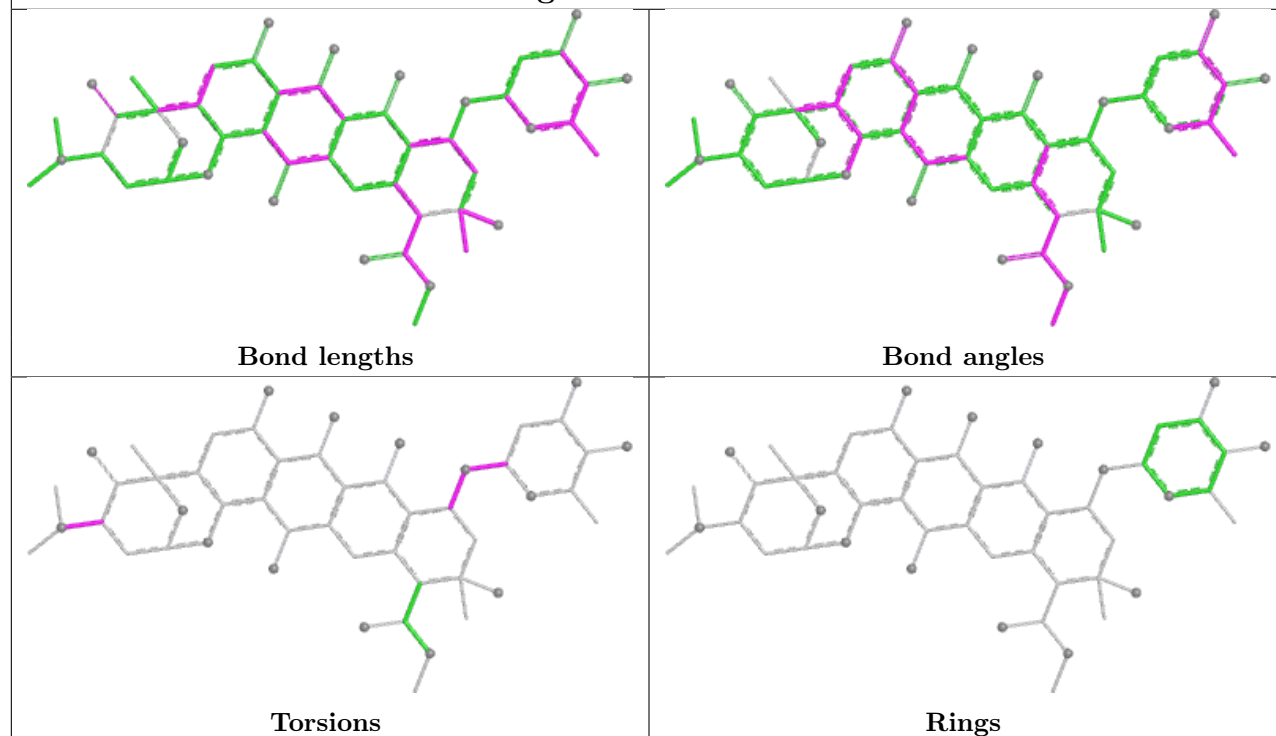
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	5R6	1	0
4	D	302	5R6	1	0
3	A	301	SIN	1	0
4	B	302	5R6	3	0

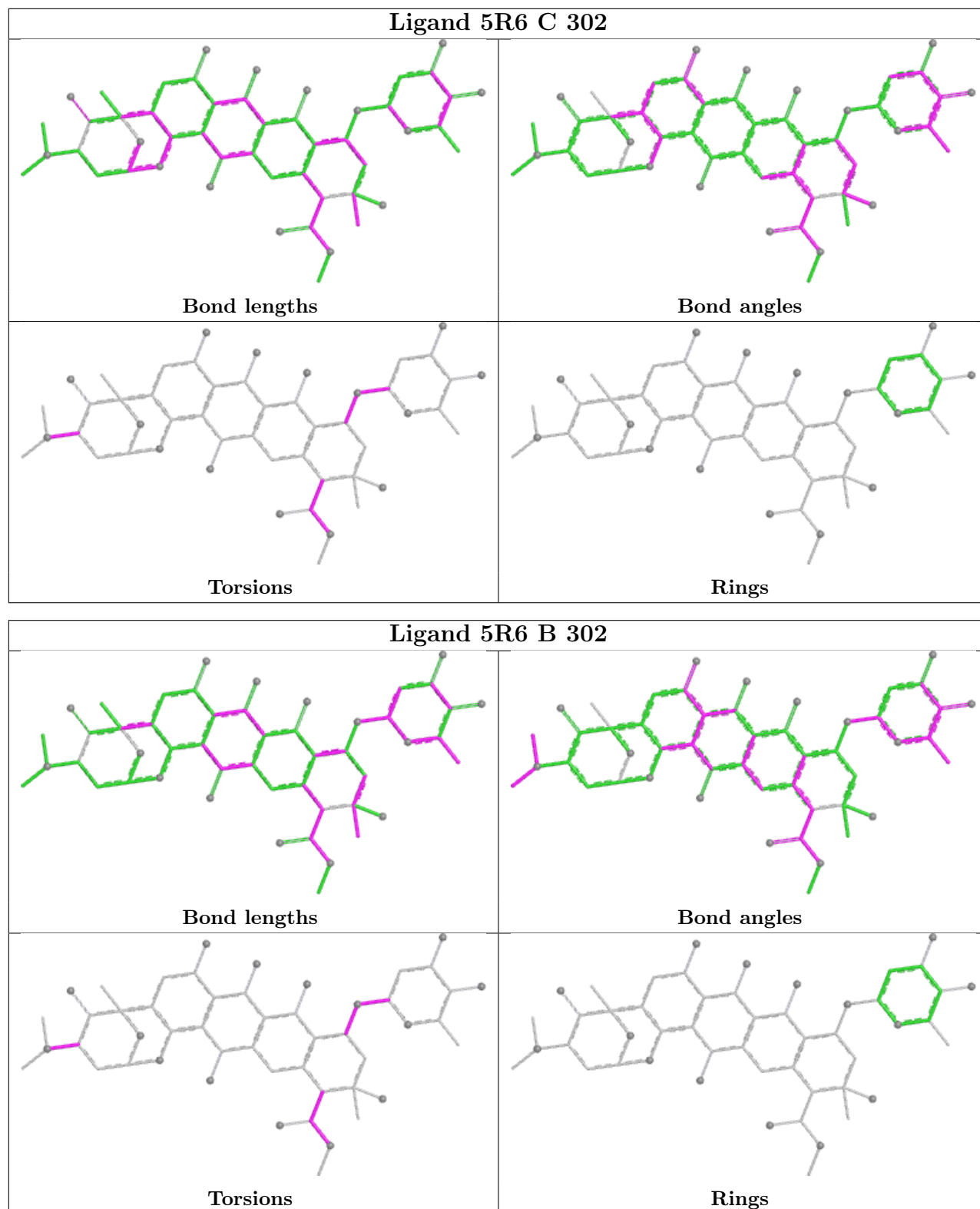
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 5R6 A 302



Ligand 5R6 D 302





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	257/305 (84%)	-0.28	0 100 100	41, 59, 99, 121	0
1	B	256/305 (83%)	0.11	0 100 100	52, 88, 128, 153	1 (0%)
1	C	257/305 (84%)	0.12	3 (1%) 76 71	60, 89, 136, 170	1 (0%)
1	D	258/305 (84%)	0.42	8 (3%) 51 43	60, 105, 159, 206	0
All	All	1028/1220 (84%)	0.09	11 (1%) 78 73	41, 84, 144, 206	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	CYS	2.9
1	D	16	SER	2.6
1	D	66	SER	2.5
1	C	66[A]	SER	2.4
1	D	58	HIS	2.4
1	D	64	TRP	2.3
1	D	231	TYR	2.3
1	D	68	ALA	2.2
1	D	206	PHE	2.2
1	C	68	ALA	2.2
1	C	175	THR	2.2

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

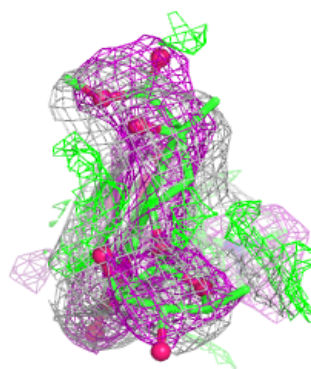
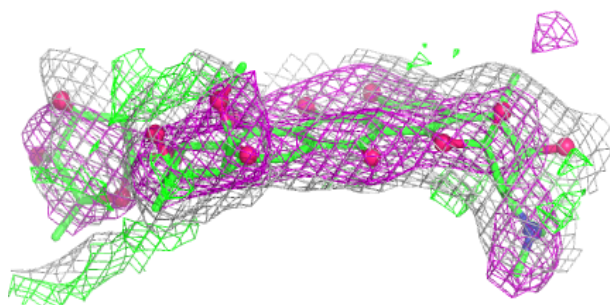
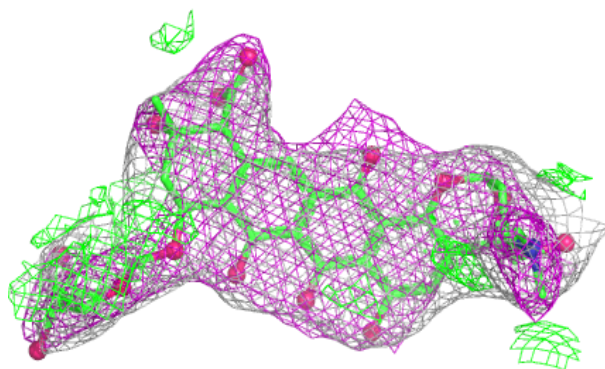
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5R6	C	302	50/50	0.70	0.15	20,33,62,63	0
4	5R6	D	302	50/50	0.70	0.14	22,25,31,31	0
4	5R6	B	302	50/50	0.75	0.13	18,26,41,44	0
3	SIN	C	301	8/8	0.82	0.23	11,13,13,14	0
3	SIN	D	301	8/8	0.85	0.24	11,12,13,14	0
4	5R6	A	302	50/50	0.87	0.11	8,12,33,34	0
3	SIN	B	301	8/8	0.89	0.19	12,13,13,14	0
3	SIN	A	301	8/8	0.92	0.13	11,13,14,14	0
2	NI	A	300	1/1	0.98	0.12	12,12,12,12	0
2	NI	B	300	1/1	0.98	0.17	18,18,18,18	0
2	NI	C	300	1/1	0.98	0.19	16,16,16,16	0
2	NI	D	300	1/1	0.98	0.23	17,17,17,17	0

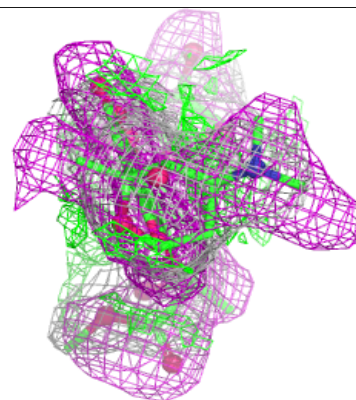
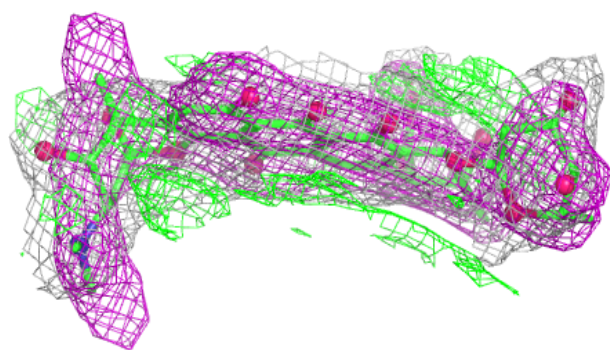
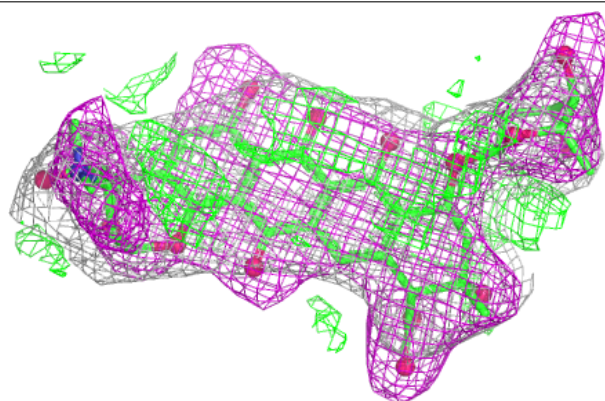
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5R6 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)

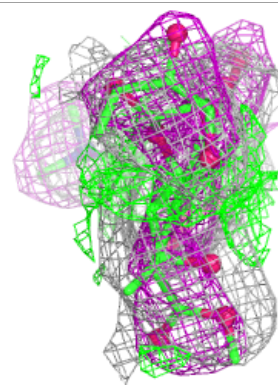
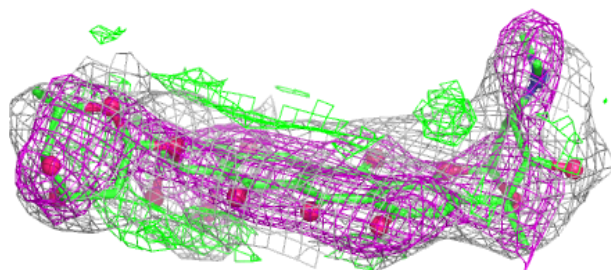
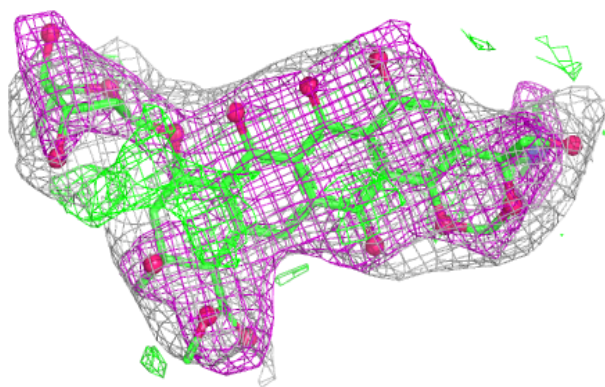
**Electron density around 5R6 D 302:**

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

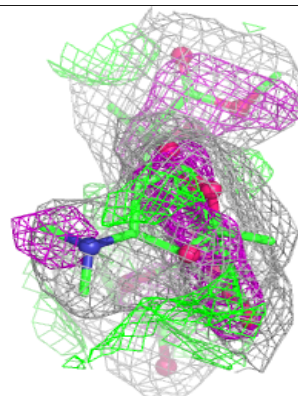
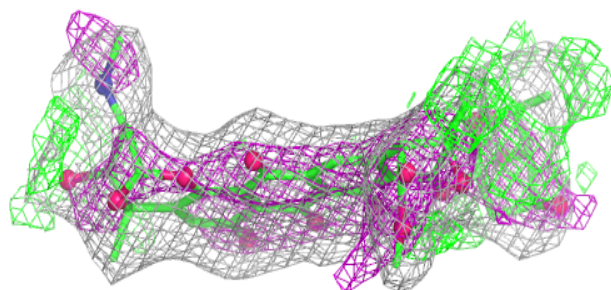
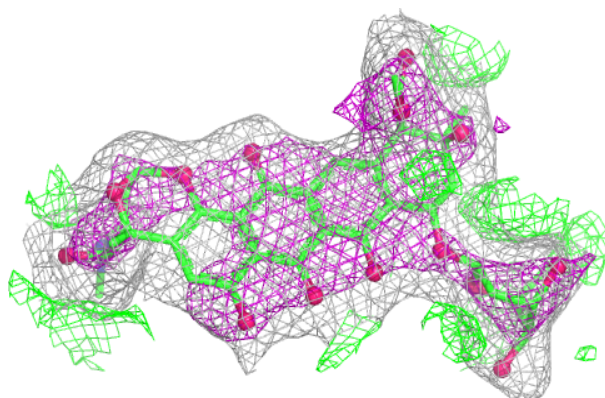


Electron density around 5R6 B 302:

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

**Electron density around 5R6 A 302:**

$2mF_o-DF_c$ (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.