



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:58 AM UTC

PDB ID : 1U1F / pdb_00001u1f
Title : Structure of e. coli uridine phosphorylase complexed to 5-(m-(benzyloxy)benzyl)acyclouridine (BBAU)
Authors : Bu, W.; Settembre, E.C.; Ealick, S.E.
Deposited on : 2004-07-15
Resolution : 2.30 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:

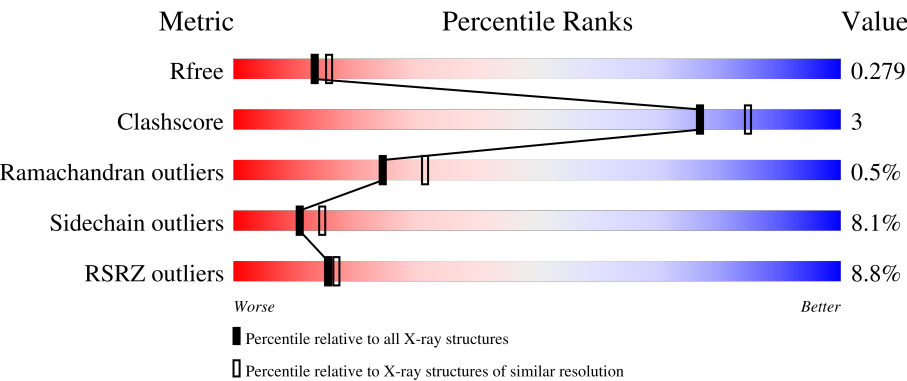
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	256	6% 82%12%5%
1	B	256	4% 86%12%..
1	C	256	% 88%9%..
1	D	256	2% 87%11%.
1	E	256	15% 79%17%..

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Mol	Chain	Length	Quality of chain
1	F	256	23% 83% 13%

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	K	A	1002	-	-	-	X
4	183	E	7300	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11915 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1817	1139	317	350	11			
1	B	251	Total	C	N	O	S	0	0	0
			1885	1181	329	364	11			
1	C	250	Total	C	N	O	S	0	0	0
			1876	1175	327	363	11			
1	D	250	Total	C	N	O	S	0	0	0
			1876	1175	327	363	11			
1	E	247	Total	C	N	O	S	0	0	0
			1848	1157	323	357	11			
1	F	250	Total	C	N	O	S	0	0	0
			1876	1175	327	363	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P12758
A	-1	SER	-	cloning artifact	UNP P12758
A	0	HIS	-	cloning artifact	UNP P12758
A	1	MET	-	cloning artifact	UNP P12758
B	-2	GLY	-	cloning artifact	UNP P12758
B	-1	SER	-	cloning artifact	UNP P12758
B	0	HIS	-	cloning artifact	UNP P12758
B	1	MET	-	cloning artifact	UNP P12758
C	-2	GLY	-	cloning artifact	UNP P12758
C	-1	SER	-	cloning artifact	UNP P12758
C	0	HIS	-	cloning artifact	UNP P12758
C	1	MET	-	cloning artifact	UNP P12758
D	-2	GLY	-	cloning artifact	UNP P12758
D	-1	SER	-	cloning artifact	UNP P12758
D	0	HIS	-	cloning artifact	UNP P12758
D	1	MET	-	cloning artifact	UNP P12758
E	-2	GLY	-	cloning artifact	UNP P12758

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	cloning artifact	UNP P12758
E	0	HIS	-	cloning artifact	UNP P12758
E	1	MET	-	cloning artifact	UNP P12758
F	-2	GLY	-	cloning artifact	UNP P12758
F	-1	SER	-	cloning artifact	UNP P12758
F	0	HIS	-	cloning artifact	UNP P12758
F	1	MET	-	cloning artifact	UNP P12758

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

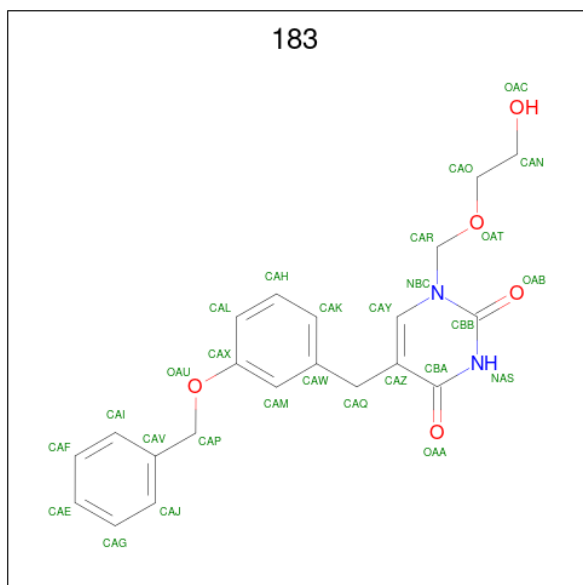


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0

- Molecule 4 is 1-((2-HYDROXYETHOXY)METHYL)-5-(3-(BENZYLOXY)BENZYL)PYRIMIDINE-2,4(1H,3H)-DIONE (CCD ID: 183) (formula: C₂₁H₂₂N₂O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 28 21 2 5	0	0
4	B	1	Total C N O 28 21 2 5	0	0
4	C	1	Total C N O 28 21 2 5	0	0
4	D	1	Total C N O 28 21 2 5	0	0
4	E	1	Total C N O 28 21 2 5	0	0
4	F	1	Total C N O 28 21 2 5	0	0

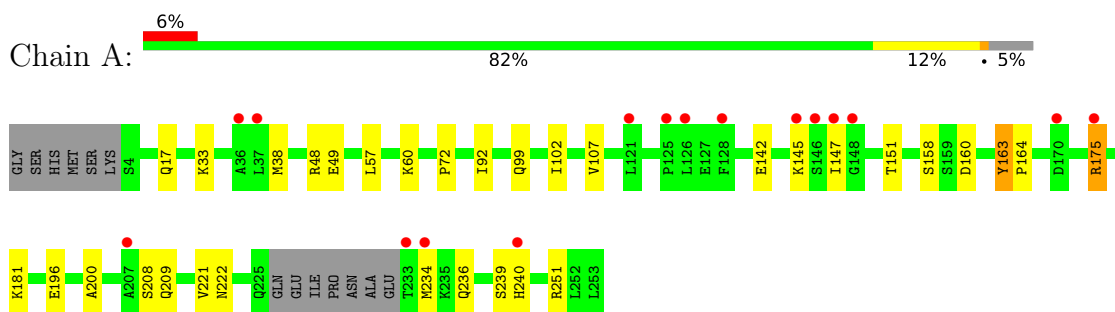
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total 103	O 103	0	0
5	B	81	Total 81	O 81	0	0
5	C	121	Total 121	O 121	0	0
5	D	108	Total 108	O 108	0	0
5	E	69	Total 69	O 69	0	0
5	F	54	Total 54	O 54	0	0

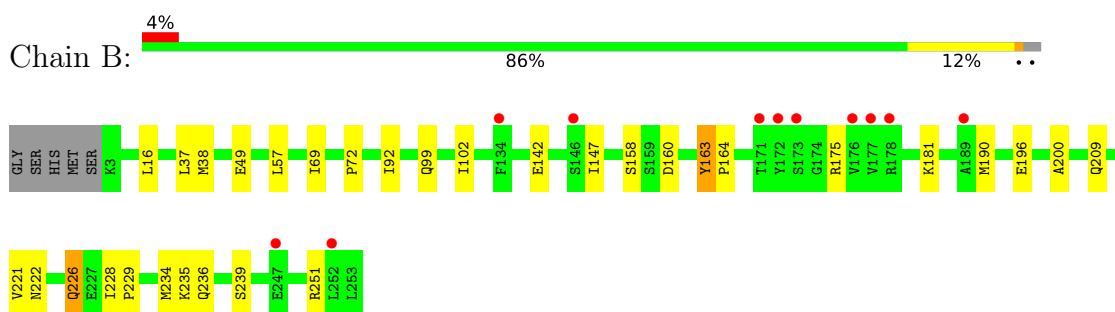
3 Residue-property plots [i](#)

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.

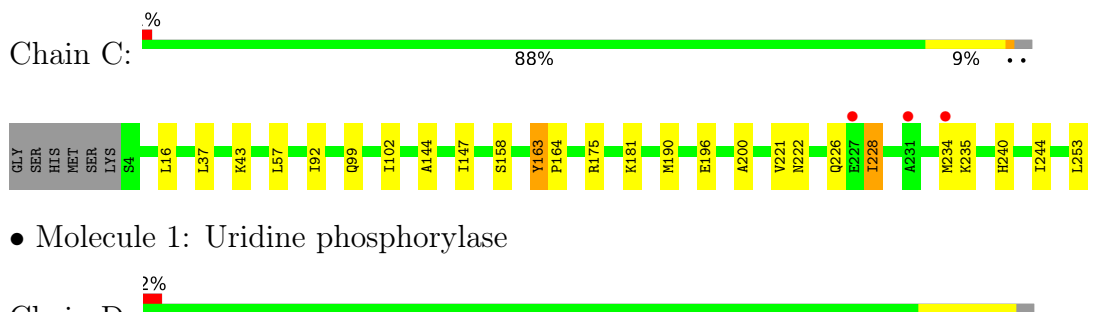
- Molecule 1: Uridine phosphorylase



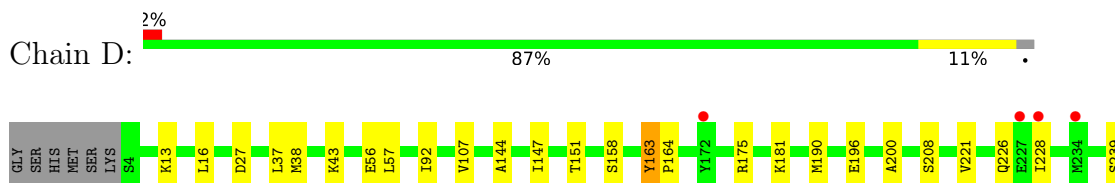
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

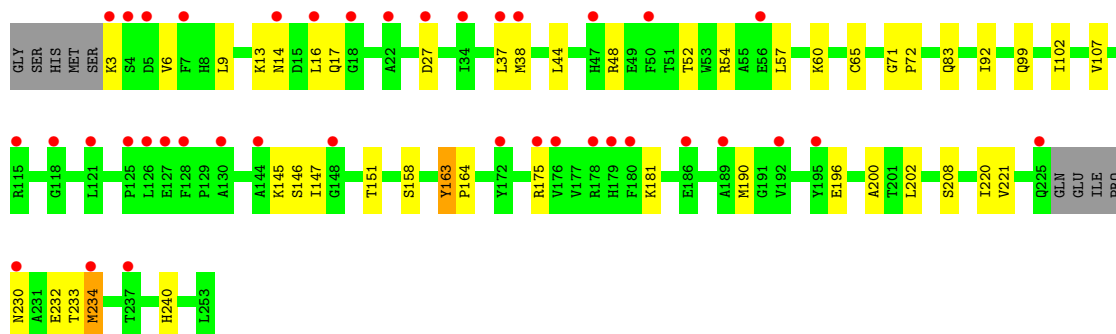
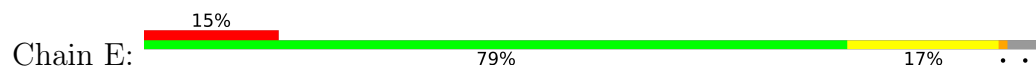


- Molecule 1: Uridine phosphorylase

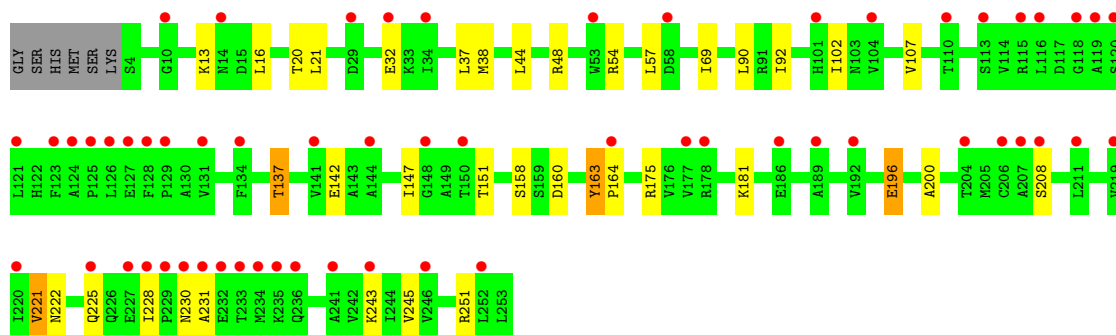
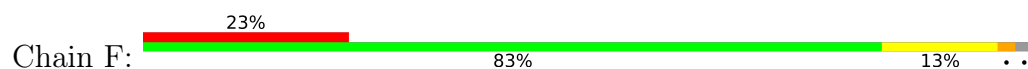




- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.56Å 125.81Å 141.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.30 48.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.80-2.30) 98.3 (48.80-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.199 , 0.228 (Not available) , 0.279	Depositor DCC
R_{free} test set	5195 reflections (7.13%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	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	0.90	EDS
Total number of atoms	11915	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: 183, PO4, K

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	0.41	0/1847	0.84	0/2507
1	B	0.40	0/1917	0.84	0/2602
1	C	0.42	0/1908	0.85	0/2591
1	D	0.41	0/1908	0.85	0/2591
1	E	0.40	0/1878	0.83	1/2548 (0.0%)
1	F	0.39	0/1908	0.83	0/2591
All	All	0.41	0/11366	0.84	1/15430 (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	E	71	GLY	O-C-N	5.07	122.89	121.07

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	1817	0	1813	14	0
1	B	1885	0	1886	15	0
1	C	1876	0	1873	9	0
1	D	1876	0	1873	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1848	0	1843	16	0
1	F	1876	0	1873	16	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	28	0	22	0	0
4	B	28	0	22	1	0
4	C	28	0	22	0	0
4	D	28	0	22	0	0
4	E	28	0	22	0	0
4	F	28	0	22	1	0
5	A	103	0	0	0	0
5	B	81	0	0	0	0
5	C	121	0	0	0	0
5	D	108	0	0	1	0
5	E	69	0	0	0	0
5	F	54	0	0	2	0
All	All	11915	0	11293	66	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 3.

All (66) 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:38:MET:HG2	1:A:57:LEU:HD13	1.80	0.64
1:D:38:MET:HG2	1:D:57:LEU:HD13	1.84	0.59
1:B:38:MET:HG2	1:B:57:LEU:HD13	1.85	0.59
1:F:38:MET:HG2	1:F:57:LEU:HD13	1.87	0.57
1:F:44:LEU:HD11	1:F:54:ARG:HB2	1.86	0.56
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.88	0.56
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.88	0.56
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.87	0.55
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.89	0.54
1:B:99:GLN:HB2	1:B:102:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:THR:HG23	1:E:65:CYS:HB2	1.90	0.53
1:F:102:ILE:O	1:F:222:ASN:ND2	2.42	0.53
1:F:163:TYR:HB2	1:F:164:PRO:HD3	1.90	0.53
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.90	0.53
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.90	0.53
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.89	0.53
1:E:99:GLN:HB2	1:E:102:ILE:HD12	1.91	0.53
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.91	0.52
1:A:99:GLN:HB2	1:A:102:ILE:HD12	1.91	0.52
1:A:163:TYR:HB2	1:A:164:PRO:HD3	1.92	0.51
1:C:163:TYR:HB2	1:C:164:PRO:CD	2.41	0.51
1:D:163:TYR:HB2	1:D:164:PRO:HD3	1.93	0.51
1:F:163:TYR:HB2	1:F:164:PRO:CD	2.41	0.50
1:F:137:THR:HG22	5:F:8333:HOH:O	2.10	0.50
1:D:27:ASP:HB2	5:D:6335:HOH:O	2.11	0.49
1:A:107:VAL:HG23	1:A:151:THR:HG23	1.94	0.49
1:F:222:ASN:HB3	1:F:225:GLN:HB2	1.94	0.49
1:B:163:TYR:HB2	1:B:164:PRO:CD	2.44	0.48
1:D:163:TYR:HB2	1:D:164:PRO:CD	2.43	0.48
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.43	0.48
1:B:222:ASN:H	1:B:226:GLN:HE21	1.61	0.48
1:E:48:ARG:HD3	1:F:69:ILE:HD11	1.95	0.48
1:A:163:TYR:HB2	1:A:164:PRO:CD	2.44	0.48
1:C:57:LEU:HB3	1:C:253:LEU:HD11	1.96	0.47
1:E:220:ILE:HD12	1:E:234:MET:HE2	1.98	0.46
1:A:102:ILE:O	1:A:222:ASN:ND2	2.46	0.46
1:D:144:ALA:HA	1:D:244:ILE:HG12	1.98	0.46
1:E:230:ASN:HD22	1:E:233:THR:H	1.64	0.46
1:B:190:MET:HG2	1:F:208:SER:HB2	1.97	0.45
1:C:99:GLN:HB2	1:C:102:ILE:HD12	1.98	0.45
1:A:48:ARG:HD3	1:B:69:ILE:HD11	1.98	0.45
1:E:38:MET:HG2	1:E:57:LEU:HD13	1.98	0.45
1:E:44:LEU:HD11	1:E:54:ARG:HB2	1.99	0.44
1:E:6:VAL:HG21	1:E:9:LEU:HB2	2.00	0.44
1:F:196:GLU:HB2	5:F:8347:HOH:O	2.16	0.44
1:E:27:ASP:OD1	1:F:48:ARG:HG2	2.18	0.44
1:C:163:TYR:HB2	1:C:164:PRO:HD3	1.99	0.43
1:A:160:ASP:O	1:B:72:PRO:HA	2.18	0.43
1:D:107:VAL:HG23	1:D:151:THR:HG23	1.99	0.43
1:F:107:VAL:HG23	1:F:151:THR:HG23	2.00	0.43
1:F:221:VAL:HG11	4:F:8300:183:HAK	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:HB2	1:C:190:MET:HG2	2.01	0.43
1:C:102:ILE:O	1:C:222:ASN:ND2	2.47	0.43
1:D:190:MET:HG2	1:E:208:SER:HB2	2.00	0.42
1:A:72:PRO:HA	1:B:160:ASP:O	2.20	0.42
1:D:208:SER:HB2	1:E:190:MET:HG2	2.01	0.42
1:E:107:VAL:HG23	1:E:151:THR:HG23	2.02	0.42
1:A:209:GLN:HA	1:B:175:ARG:HH22	1.84	0.42
1:C:228:ILE:H	1:C:228:ILE:HG13	1.58	0.41
1:B:234:MET:HG3	4:B:4300:183:HAG	2.01	0.41
1:A:49:GLU:HB3	1:B:49:GLU:HB3	2.02	0.41
1:B:228:ILE:HA	1:B:229:PRO:HD3	1.87	0.41
1:F:21:LEU:HD21	1:F:90:LEU:HD12	2.03	0.41
1:A:175:ARG:HH22	1:B:209:GLN:HA	1.86	0.41
1:E:72:PRO:HA	1:F:160:ASP:O	2.21	0.40
1:C:144:ALA:HA	1:C:244:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/256 (93%)	237 (99%)	1 (0%)	1 (0%)	30	38
1	B	249/256 (97%)	248 (100%)	0	1 (0%)	30	38
1	C	248/256 (97%)	244 (98%)	3 (1%)	1 (0%)	30	38
1	D	248/256 (97%)	246 (99%)	1 (0%)	1 (0%)	30	38
1	E	243/256 (95%)	240 (99%)	2 (1%)	1 (0%)	30	38
1	F	248/256 (97%)	243 (98%)	3 (1%)	2 (1%)	16	20
All	All	1475/1536 (96%)	1458 (99%)	10 (1%)	7 (0%)	24	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	231	ALA
1	A	163	TYR
1	B	163	TYR
1	C	163	TYR
1	D	163	TYR
1	E	163	TYR
1	F	163	TYR

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	193/206 (94%)	177 (92%)	16 (8%)	10	14
1	B	201/206 (98%)	188 (94%)	13 (6%)	15	22
1	C	200/206 (97%)	186 (93%)	14 (7%)	14	19
1	D	200/206 (97%)	185 (92%)	15 (8%)	12	17
1	E	196/206 (95%)	176 (90%)	20 (10%)	7	8
1	F	200/206 (97%)	182 (91%)	18 (9%)	9	12
All	All	1190/1236 (96%)	1094 (92%)	96 (8%)	11	14

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	33	LYS
1	A	60	LYS
1	A	92	ILE
1	A	142	GLU
1	A	145	LYS
1	A	147	ILE
1	A	175	ARG
1	A	181	LYS
1	A	196	GLU
1	A	221	VAL
1	A	234	MET

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Mol	Chain	Res	Type
1	A	236	GLN
1	A	239	SER
1	A	240	HIS
1	A	251	ARG
1	B	16	LEU
1	B	37	LEU
1	B	92	ILE
1	B	142	GLU
1	B	147	ILE
1	B	181	LYS
1	B	196	GLU
1	B	221	VAL
1	B	226	GLN
1	B	235	LYS
1	B	236	GLN
1	B	239	SER
1	B	251	ARG
1	C	16	LEU
1	C	37	LEU
1	C	43	LYS
1	C	92	ILE
1	C	147	ILE
1	C	175	ARG
1	C	181	LYS
1	C	196	GLU
1	C	221	VAL
1	C	226	GLN
1	C	228	ILE
1	C	234	MET
1	C	235	LYS
1	C	240	HIS
1	D	13	LYS
1	D	16	LEU
1	D	37	LEU
1	D	43	LYS
1	D	56	GLU
1	D	92	ILE
1	D	147	ILE
1	D	175	ARG
1	D	181	LYS
1	D	196	GLU
1	D	221	VAL

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Mol	Chain	Res	Type
1	D	226	GLN
1	D	228	ILE
1	D	239	SER
1	D	240	HIS
1	E	3	LYS
1	E	13	LYS
1	E	14	ASN
1	E	16	LEU
1	E	17	GLN
1	E	37	LEU
1	E	60	LYS
1	E	83	GLN
1	E	92	ILE
1	E	145	LYS
1	E	146	SER
1	E	147	ILE
1	E	175	ARG
1	E	181	LYS
1	E	196	GLU
1	E	202	LEU
1	E	221	VAL
1	E	232	GLU
1	E	234	MET
1	E	240	HIS
1	F	13	LYS
1	F	16	LEU
1	F	20	THR
1	F	32	GLU
1	F	37	LEU
1	F	92	ILE
1	F	137	THR
1	F	142	GLU
1	F	147	ILE
1	F	175	ARG
1	F	181	LYS
1	F	196	GLU
1	F	221	VAL
1	F	228	ILE
1	F	230	ASN
1	F	243	LYS
1	F	245	VAL
1	F	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	101	HIS
1	B	47	HIS
1	B	101	HIS
1	B	226	GLN
1	C	17	GLN
1	C	47	HIS
1	C	101	HIS
1	C	226	GLN
1	D	17	GLN
1	D	103	ASN
1	D	226	GLN
1	D	230	ASN
1	E	230	ASN
1	F	47	HIS
1	F	101	HIS
1	F	152	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	183	F	8300	-	30,30,30	3.55	22 (73%)	37,39,39	2.74	9 (24%)
4	183	C	5300	-	30,30,30	3.47	22 (73%)	37,39,39	2.69	8 (21%)
2	PO4	F	7301	-	4,4,4	0.95	0	6,6,6	0.45	0
4	183	D	6300	-	30,30,30	3.49	22 (73%)	37,39,39	2.67	8 (21%)
4	183	E	7300	-	30,30,30	3.53	22 (73%)	37,39,39	2.75	9 (24%)
2	PO4	A	4301	-	4,4,4	0.89	0	6,6,6	0.50	0
2	PO4	D	5301	-	4,4,4	0.92	0	6,6,6	0.49	0
2	PO4	E	8301	-	4,4,4	0.95	0	6,6,6	0.39	0
4	183	A	3300	-	30,30,30	3.54	22 (73%)	37,39,39	2.72	8 (21%)
2	PO4	C	6301	-	4,4,4	0.88	0	6,6,6	0.50	0
4	183	B	4300	-	30,30,30	3.52	22 (73%)	37,39,39	2.71	8 (21%)
2	PO4	B	3301	-	4,4,4	0.95	0	6,6,6	0.48	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
4	183	F	8300	-	-	3/14/14/14	0/3/3/3
4	183	C	5300	-	-	3/14/14/14	0/3/3/3
4	183	D	6300	-	-	3/14/14/14	0/3/3/3
4	183	E	7300	-	-	4/14/14/14	0/3/3/3
4	183	A	3300	-	-	3/14/14/14	0/3/3/3
4	183	B	4300	-	-	3/14/14/14	0/3/3/3

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	8300	183	CBB-NBC	5.32	1.45	1.37
4	E	7300	183	CBB-NBC	5.31	1.45	1.37
4	E	7300	183	CAM-CAX	5.21	1.47	1.39
4	A	3300	183	CAM-CAX	5.18	1.47	1.39
4	F	8300	183	CAM-CAX	5.14	1.47	1.39
4	D	6300	183	CAM-CAX	5.14	1.47	1.39
4	B	4300	183	CBB-NBC	5.14	1.44	1.37
4	A	3300	183	CBB-NBC	5.10	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5300	183	CBB-NBC	5.10	1.44	1.37
4	C	5300	183	CAM-CAX	4.99	1.47	1.39
4	D	6300	183	CBB-NBC	4.97	1.44	1.37
4	B	4300	183	CAM-CAX	4.93	1.47	1.39
4	F	8300	183	CAI-CAV	4.83	1.48	1.38
4	A	3300	183	CAH-CAK	4.80	1.47	1.38
4	E	7300	183	CAI-CAV	4.78	1.48	1.38
4	A	3300	183	CAF-CAI	4.77	1.47	1.38
4	B	4300	183	CAH-CAK	4.77	1.47	1.38
4	C	5300	183	CAH-CAK	4.76	1.47	1.38
4	F	8300	183	CAF-CAI	4.74	1.47	1.38
4	E	7300	183	CAF-CAI	4.70	1.47	1.38
4	C	5300	183	CAF-CAI	4.70	1.46	1.38
4	A	3300	183	CAI-CAV	4.69	1.48	1.38
4	D	6300	183	CAH-CAK	4.69	1.46	1.38
4	B	4300	183	CAF-CAI	4.69	1.46	1.38
4	D	6300	183	CAF-CAI	4.67	1.46	1.38
4	C	5300	183	CAI-CAV	4.67	1.48	1.38
4	F	8300	183	CAH-CAK	4.65	1.46	1.38
4	B	4300	183	CAI-CAV	4.65	1.48	1.38
4	E	7300	183	CAH-CAK	4.64	1.46	1.38
4	D	6300	183	CAI-CAV	4.63	1.48	1.38
4	E	7300	183	CAG-CAJ	4.58	1.46	1.38
4	A	3300	183	CAG-CAJ	4.57	1.46	1.38
4	F	8300	183	CAG-CAJ	4.54	1.46	1.38
4	D	6300	183	CAG-CAJ	4.50	1.46	1.38
4	A	3300	183	CAL-CAX	4.49	1.47	1.38
4	B	4300	183	CAG-CAJ	4.48	1.46	1.38
4	B	4300	183	CAY-NBC	4.44	1.45	1.37
4	B	4300	183	CAL-CAX	4.44	1.47	1.38
4	E	7300	183	CAL-CAX	4.41	1.47	1.38
4	C	5300	183	CAG-CAJ	4.41	1.46	1.38
4	D	6300	183	CAE-CAG	4.40	1.47	1.38
4	F	8300	183	CAE-CAG	4.39	1.47	1.38
4	D	6300	183	CAL-CAX	4.38	1.46	1.38
4	C	5300	183	CAE-CAG	4.37	1.47	1.38
4	F	8300	183	CAL-CAX	4.36	1.46	1.38
4	E	7300	183	CAE-CAG	4.36	1.47	1.38
4	F	8300	183	CAY-NBC	4.36	1.45	1.37
4	C	5300	183	CAL-CAX	4.36	1.46	1.38
4	B	4300	183	CAE-CAG	4.35	1.47	1.38
4	A	3300	183	CAE-CAG	4.35	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3300	183	CAY-NBC	4.35	1.45	1.37
4	E	7300	183	CAY-NBC	4.32	1.45	1.37
4	A	3300	183	CAH-CAL	4.32	1.46	1.38
4	C	5300	183	CAY-NBC	4.30	1.45	1.37
4	E	7300	183	CAM-CAW	4.25	1.46	1.39
4	D	6300	183	CAY-NBC	4.22	1.45	1.37
4	E	7300	183	CAH-CAL	4.21	1.46	1.38
4	D	6300	183	CAH-CAL	4.20	1.46	1.38
4	F	8300	183	CAH-CAL	4.19	1.46	1.38
4	A	3300	183	CAK-CAW	4.17	1.47	1.38
4	B	4300	183	CAH-CAL	4.17	1.46	1.38
4	E	7300	183	CAK-CAW	4.16	1.47	1.38
4	A	3300	183	CAM-CAW	4.16	1.46	1.39
4	C	5300	183	CAH-CAL	4.15	1.46	1.38
4	D	6300	183	CAJ-CAV	4.14	1.47	1.38
4	E	7300	183	CAJ-CAV	4.14	1.47	1.38
4	B	4300	183	CAK-CAW	4.13	1.47	1.38
4	B	4300	183	CAJ-CAV	4.13	1.47	1.38
4	A	3300	183	CAJ-CAV	4.11	1.47	1.38
4	F	8300	183	CAM-CAW	4.11	1.46	1.39
4	C	5300	183	CAJ-CAV	4.11	1.47	1.38
4	F	8300	183	CAJ-CAV	4.10	1.47	1.38
4	F	8300	183	CAK-CAW	4.10	1.47	1.38
4	D	6300	183	CAK-CAW	4.08	1.47	1.38
4	C	5300	183	CAK-CAW	4.08	1.47	1.38
4	D	6300	183	CAR-NBC	-4.07	1.41	1.47
4	B	4300	183	CAM-CAW	4.04	1.46	1.39
4	D	6300	183	CAF-CAE	4.03	1.47	1.38
4	D	6300	183	CAM-CAW	4.02	1.46	1.39
4	B	4300	183	CAQ-CAZ	4.01	1.58	1.51
4	F	8300	183	CAQ-CAZ	4.01	1.58	1.51
4	B	4300	183	CAF-CAE	4.01	1.47	1.38
4	F	8300	183	CAF-CAE	3.99	1.47	1.38
4	A	3300	183	CAF-CAE	3.98	1.47	1.38
4	C	5300	183	CAM-CAW	3.96	1.46	1.39
4	B	4300	183	CAR-NBC	-3.95	1.41	1.47
4	C	5300	183	CAF-CAE	3.94	1.46	1.38
4	E	7300	183	CAR-NBC	-3.93	1.41	1.47
4	E	7300	183	CAF-CAE	3.93	1.46	1.38
4	B	4300	183	CAP-CAV	-3.90	1.41	1.50
4	C	5300	183	CAR-NBC	-3.88	1.41	1.47
4	A	3300	183	CAQ-CAZ	3.86	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	8300	183	CAR-NBC	-3.85	1.41	1.47
4	D	6300	183	CAQ-CAZ	3.85	1.58	1.51
4	E	7300	183	CAQ-CAZ	3.85	1.58	1.51
4	D	6300	183	CAP-CAV	-3.83	1.41	1.50
4	C	5300	183	CAP-CAV	-3.82	1.41	1.50
4	A	3300	183	CAR-NBC	-3.77	1.41	1.47
4	C	5300	183	CAQ-CAZ	3.76	1.57	1.51
4	F	8300	183	CAP-CAV	-3.69	1.42	1.50
4	A	3300	183	CAP-CAV	-3.66	1.42	1.50
4	E	7300	183	CAP-CAV	-3.52	1.42	1.50
4	A	3300	183	CAQ-CAW	3.33	1.57	1.51
4	E	7300	183	CAQ-CAW	3.30	1.56	1.51
4	F	8300	183	CAQ-CAW	3.22	1.56	1.51
4	B	4300	183	CAQ-CAW	3.16	1.56	1.51
4	D	6300	183	CAQ-CAW	3.15	1.56	1.51
4	C	5300	183	CAQ-CAW	3.08	1.56	1.51
4	A	3300	183	OAU-CAP	3.06	1.53	1.43
4	E	7300	183	OAU-CAP	3.02	1.53	1.43
4	F	8300	183	CAY-CAZ	3.02	1.43	1.35
4	F	8300	183	OAU-CAP	3.01	1.52	1.43
4	B	4300	183	CAY-CAZ	2.97	1.43	1.35
4	B	4300	183	OAU-CAP	2.91	1.52	1.43
4	E	7300	183	CAY-CAZ	2.91	1.43	1.35
4	A	3300	183	CAY-CAZ	2.90	1.43	1.35
4	C	5300	183	CAY-CAZ	2.90	1.43	1.35
4	F	8300	183	CBB-NAS	2.89	1.43	1.38
4	B	4300	183	CBB-NAS	2.86	1.43	1.38
4	D	6300	183	CAY-CAZ	2.86	1.43	1.35
4	D	6300	183	OAU-CAP	2.84	1.52	1.43
4	C	5300	183	OAU-CAP	2.84	1.52	1.43
4	F	8300	183	CBA-NAS	2.74	1.44	1.38
4	A	3300	183	CBA-NAS	2.73	1.44	1.38
4	A	3300	183	CBB-NAS	2.67	1.42	1.38
4	B	4300	183	CBA-NAS	2.66	1.43	1.38
4	C	5300	183	CBB-NAS	2.65	1.42	1.38
4	D	6300	183	CBB-NAS	2.63	1.42	1.38
4	E	7300	183	CBB-NAS	2.63	1.42	1.38
4	D	6300	183	CBA-NAS	2.60	1.43	1.38
4	E	7300	183	CBA-NAS	2.59	1.43	1.38
4	C	5300	183	CBA-NAS	2.50	1.43	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	8300	183	CAP-OAU-CAX	12.66	147.78	117.62
4	E	7300	183	CAP-OAU-CAX	12.60	147.64	117.62
4	B	4300	183	CAP-OAU-CAX	12.47	147.32	117.62
4	A	3300	183	CAP-OAU-CAX	12.37	147.08	117.62
4	D	6300	183	CAP-OAU-CAX	12.23	146.74	117.62
4	C	5300	183	CAP-OAU-CAX	11.97	146.13	117.62
4	D	6300	183	CBA-NAS-CBB	-4.43	121.53	127.34
4	C	5300	183	CBA-NAS-CBB	-4.43	121.54	127.34
4	E	7300	183	CBA-NAS-CBB	-4.39	121.58	127.34
4	A	3300	183	CBA-NAS-CBB	-4.35	121.64	127.34
4	E	7300	183	CAZ-CBA-NAS	4.33	121.82	115.21
4	D	6300	183	CAZ-CBA-NAS	4.30	121.77	115.21
4	A	3300	183	CAZ-CBA-NAS	4.28	121.75	115.21
4	B	4300	183	CAZ-CBA-NAS	4.27	121.73	115.21
4	B	4300	183	CBA-NAS-CBB	-4.26	121.76	127.34
4	F	8300	183	CBA-NAS-CBB	-4.20	121.83	127.34
4	F	8300	183	CAR-NBC-CBB	4.15	121.96	117.20
4	C	5300	183	CAZ-CBA-NAS	4.13	121.52	115.21
4	F	8300	183	CAZ-CBA-NAS	4.12	121.50	115.21
4	C	5300	183	NAS-CBB-NBC	4.07	118.35	114.86
4	A	3300	183	OAT-CAR-NBC	4.04	119.67	111.58
4	C	5300	183	CAR-NBC-CBB	4.01	121.80	117.20
4	E	7300	183	CAR-NBC-CBB	3.91	121.69	117.20
4	A	3300	183	CAR-NBC-CBB	3.90	121.68	117.20
4	C	5300	183	OAT-CAR-NBC	3.90	119.39	111.58
4	B	4300	183	OAT-CAR-NBC	3.83	119.26	111.58
4	E	7300	183	OAT-CAR-NBC	3.83	119.25	111.58
4	F	8300	183	NAS-CBB-NBC	3.81	118.13	114.86
4	D	6300	183	NAS-CBB-NBC	3.79	118.11	114.86
4	B	4300	183	CAR-NBC-CBB	3.78	121.54	117.20
4	D	6300	183	CAR-NBC-CBB	3.77	121.53	117.20
4	E	7300	183	NAS-CBB-NBC	3.72	118.05	114.86
4	A	3300	183	NAS-CBB-NBC	3.70	118.03	114.86
4	F	8300	183	OAT-CAR-NBC	3.66	118.92	111.58
4	B	4300	183	NAS-CBB-NBC	3.60	117.95	114.86
4	D	6300	183	OAT-CAR-NBC	3.34	118.27	111.58
4	E	7300	183	OAB-CBB-NAS	-2.26	117.33	121.49
4	C	5300	183	OAB-CBB-NAS	-2.23	117.37	121.49
4	F	8300	183	OAB-CBB-NAS	-2.22	117.39	121.49
4	E	7300	183	OAU-CAP-CAV	2.21	115.65	109.16
4	D	6300	183	OAA-CBA-NAS	-2.20	115.98	120.11
4	A	3300	183	OAA-CBA-NAS	-2.20	115.98	120.11
4	E	7300	183	OAA-CBA-NAS	-2.18	116.02	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3300	183	OAB-CBB-NAS	-2.15	117.53	121.49
4	B	4300	183	OAA-CBA-NAS	-2.15	116.08	120.11
4	F	8300	183	CAY-NBC-CBB	-2.13	119.19	121.29
4	B	4300	183	OAB-CBB-NAS	-2.10	117.61	121.49
4	F	8300	183	OAA-CBA-NAS	-2.07	116.23	120.11
4	D	6300	183	OAB-CBB-NAS	-2.02	117.76	121.49
4	C	5300	183	OAA-CBA-NAS	-2.00	116.34	120.11

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4300	183	CAV-CAP-OAU-CAX
4	A	3300	183	CAV-CAP-OAU-CAX
4	F	8300	183	CAV-CAP-OAU-CAX
4	C	5300	183	CAV-CAP-OAU-CAX
4	A	3300	183	CAM-CAX-OAU-CAP
4	D	6300	183	CAV-CAP-OAU-CAX
4	F	8300	183	CAL-CAX-OAU-CAP
4	F	8300	183	CAM-CAX-OAU-CAP
4	A	3300	183	CAL-CAX-OAU-CAP
4	B	4300	183	CAM-CAX-OAU-CAP
4	B	4300	183	CAL-CAX-OAU-CAP
4	D	6300	183	CAL-CAX-OAU-CAP
4	D	6300	183	CAM-CAX-OAU-CAP
4	E	7300	183	CAL-CAX-OAU-CAP
4	C	5300	183	CAL-CAX-OAU-CAP
4	C	5300	183	CAM-CAX-OAU-CAP
4	E	7300	183	CAM-CAX-OAU-CAP
4	E	7300	183	CAV-CAP-OAU-CAX
4	E	7300	183	OAC-CAN-CAO-OAT

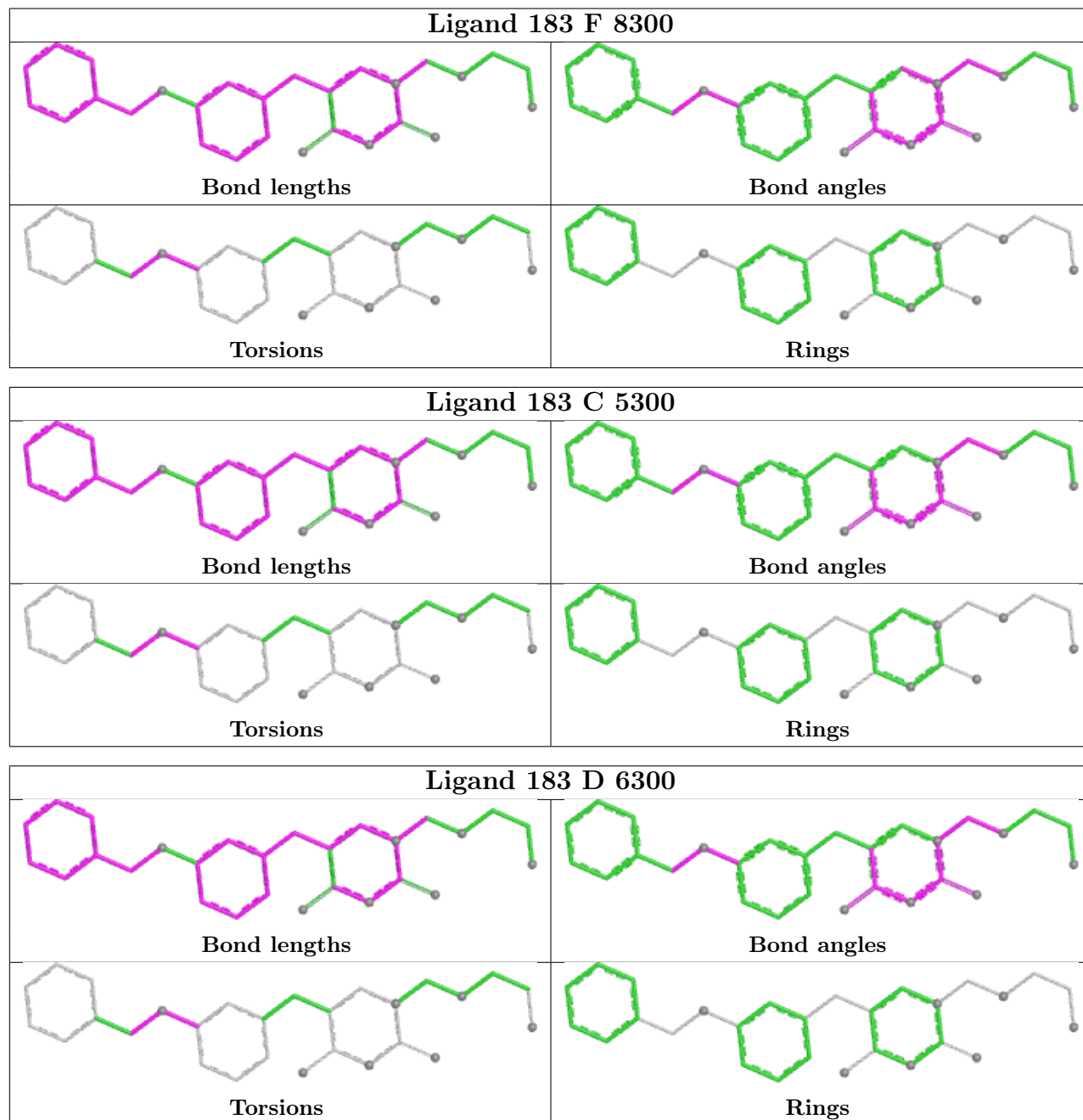
There are no ring outliers.

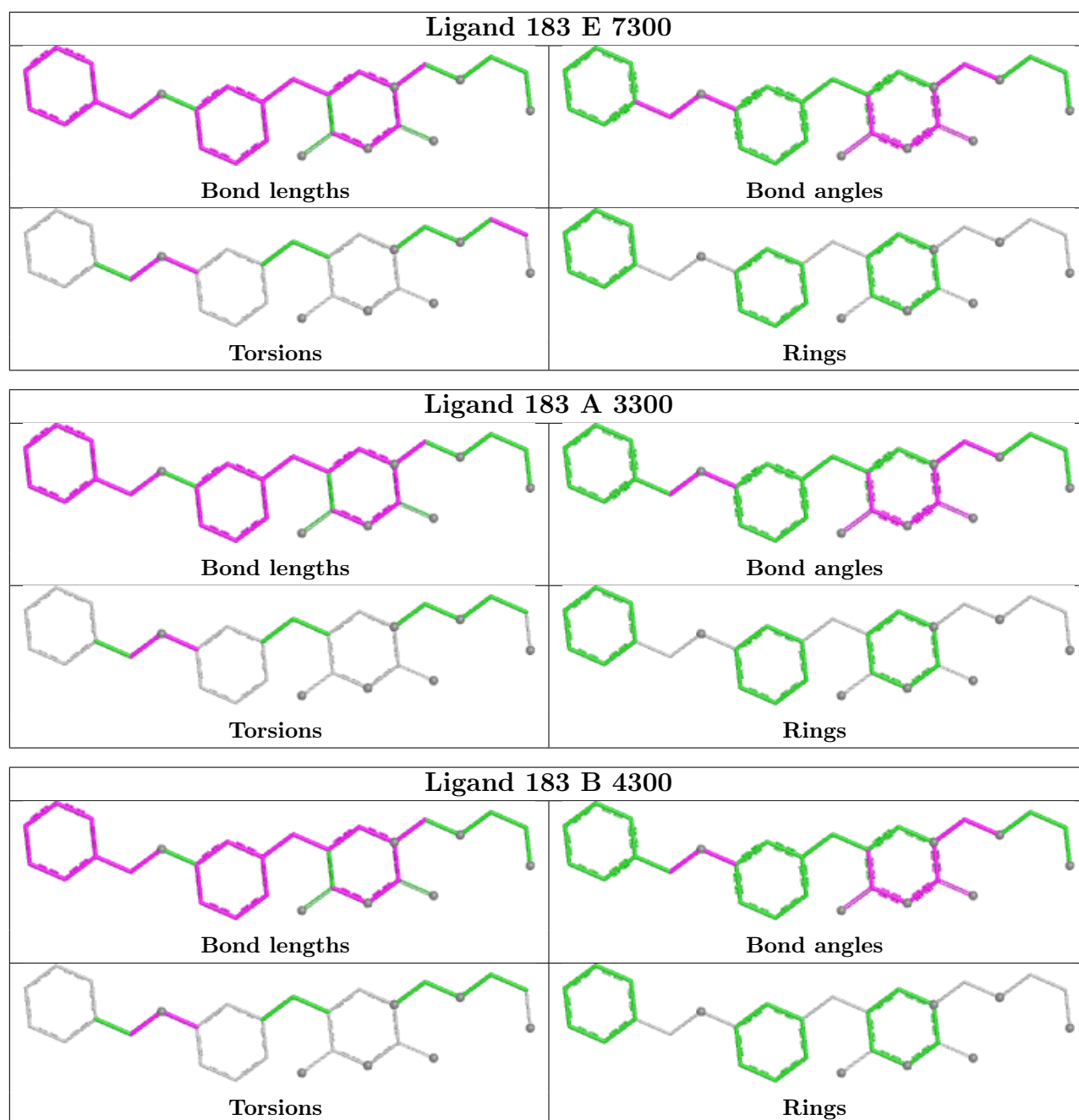
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	8300	183	1	0
4	B	4300	183	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.





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	243/256 (94%)	0.53	16 (6%)	24 26	12, 14, 17, 21	0
1	B	251/256 (98%)	0.59	11 (4%)	39 41	12, 14, 16, 19	0
1	C	250/256 (97%)	-0.05	3 (1%)	76 77	11, 14, 20, 23	0
1	D	250/256 (97%)	0.24	4 (1%)	70 72	11, 14, 19, 24	0
1	E	247/256 (96%)	1.09	39 (15%)	5 5	13, 14, 16, 19	0
1	F	250/256 (97%)	1.46	58 (23%)	2 2	13, 14, 16, 18	0
All	All	1491/1536 (97%)	0.64	131 (8%)	15 17	11, 14, 17, 24	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	GLU	5.4
1	F	252	LEU	5.0
1	F	234	MET	4.8
1	E	4	SER	4.8
1	F	241	ALA	4.7
1	F	126	LEU	4.6
1	F	125	PRO	4.5
1	E	126	LEU	4.3
1	F	227	GLU	3.9
1	F	121	LEU	3.8
1	A	146	SER	3.7
1	E	234	MET	3.7
1	F	230	ASN	3.7
1	F	220	ILE	3.6
1	F	228	ILE	3.6
1	E	18	GLY	3.6
1	E	121	LEU	3.5
1	E	38	MET	3.4
1	E	118	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	234	MET	3.4
1	E	128	PHE	3.4
1	F	207	ALA	3.3
1	D	234	MET	3.3
1	F	144	ALA	3.3
1	F	246	VAL	3.3
1	F	118	GLY	3.3
1	D	228	ILE	3.3
1	E	237	THR	3.2
1	A	125	PRO	3.2
1	A	233	THR	3.2
1	F	236	GLN	3.1
1	E	125	PRO	3.1
1	B	172	TYR	3.0
1	E	180	PHE	3.0
1	A	36	ALA	2.9
1	A	170	ASP	2.9
1	E	176	VAL	2.9
1	E	179	HIS	2.9
1	F	243	LYS	2.8
1	B	173	SER	2.8
1	E	148	GLY	2.8
1	F	115	ARG	2.8
1	F	178	ARG	2.8
1	D	172	TYR	2.8
1	E	189	ALA	2.8
1	E	27	ASP	2.8
1	C	231	ALA	2.8
1	F	229	PRO	2.8
1	E	16	LEU	2.8
1	F	150	THR	2.7
1	F	233	THR	2.7
1	D	227	GLU	2.7
1	E	175	ARG	2.7
1	E	34	ILE	2.7
1	F	116	LEU	2.7
1	B	176	VAL	2.6
1	F	119	ALA	2.6
1	B	171	THR	2.6
1	F	10	GLY	2.6
1	E	192	VAL	2.6
1	A	147	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	121	LEU	2.5
1	E	127	GLU	2.5
1	A	240	HIS	2.5
1	F	211	LEU	2.5
1	F	177	VAL	2.5
1	B	146	SER	2.4
1	B	177	VAL	2.4
1	A	126	LEU	2.4
1	A	175	ARG	2.4
1	F	192	VAL	2.4
1	F	186	GLU	2.4
1	A	207	ALA	2.4
1	F	53	TRP	2.4
1	A	145	LYS	2.4
1	F	235	LYS	2.4
1	F	58	ASP	2.3
1	F	231	ALA	2.3
1	E	47	HIS	2.3
1	C	234	MET	2.3
1	E	5	ASP	2.3
1	F	113	SER	2.3
1	E	186	GLU	2.3
1	F	127	GLU	2.3
1	E	37	LEU	2.3
1	F	148	GLY	2.3
1	F	110	THR	2.3
1	F	34	ILE	2.3
1	A	148	GLY	2.2
1	B	252	LEU	2.2
1	F	123	PHE	2.2
1	F	128	PHE	2.2
1	E	230	ASN	2.2
1	F	29	ASP	2.2
1	C	227	GLU	2.2
1	E	130	ALA	2.2
1	E	144	ALA	2.2
1	F	120	SER	2.2
1	F	164	PRO	2.2
1	B	247	GLU	2.2
1	E	225	GLN	2.2
1	E	195	TYR	2.2
1	B	178	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	115	ARG	2.2
1	F	14	ASN	2.1
1	F	32	GLU	2.1
1	F	131	VAL	2.1
1	F	141	VAL	2.1
1	E	7	PHE	2.1
1	F	134	PHE	2.1
1	F	189	ALA	2.1
1	E	14	ASN	2.1
1	F	129	PRO	2.1
1	B	134	PHE	2.1
1	E	178	ARG	2.1
1	F	206	CYS	2.1
1	F	124	ALA	2.1
1	F	225	GLN	2.1
1	A	128	PHE	2.1
1	F	204	THR	2.0
1	B	189	ALA	2.0
1	E	56	GLU	2.0
1	F	101	HIS	2.0
1	A	37	LEU	2.0
1	E	172	TYR	2.0
1	F	104	VAL	2.0
1	F	219	VAL	2.0
1	E	50	PHE	2.0
1	E	3	LYS	2.0
1	F	208	SER	2.0
1	E	22	ALA	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,

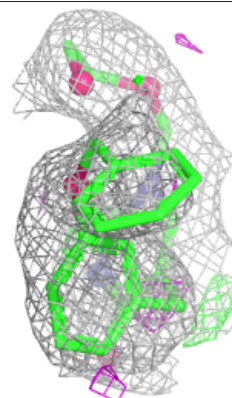
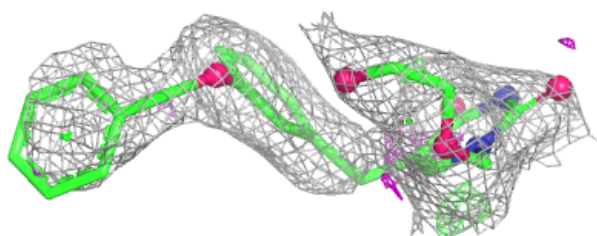
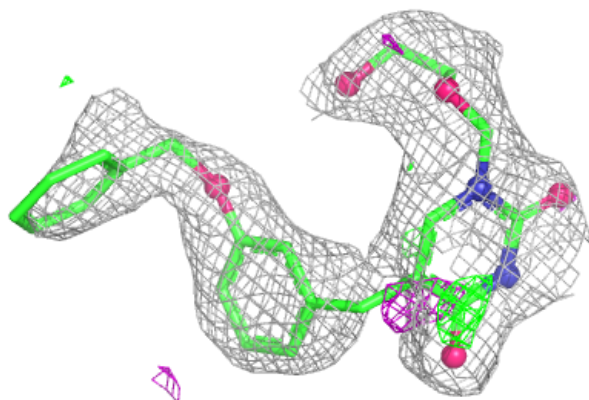
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	A	1002	1/1	0.63	0.50	69,69,69,69	0
3	K	E	1003	1/1	0.78	0.31	75,75,75,75	0
4	183	F	8300	28/28	0.78	0.16	48,49,51,51	0
2	PO4	F	7301	5/5	0.82	0.15	53,53,53,53	0
4	183	E	7300	28/28	0.83	0.12	42,44,49,50	0
4	183	B	4300	28/28	0.83	0.14	40,42,45,45	0
4	183	A	3300	28/28	0.85	0.13	38,42,49,49	0
4	183	D	6300	28/28	0.88	0.12	31,34,42,42	0
2	PO4	A	4301	5/5	0.89	0.16	48,48,48,48	0
2	PO4	B	3301	5/5	0.90	0.12	40,41,41,42	0
3	K	C	1001	1/1	0.92	0.37	49,49,49,49	0
2	PO4	E	8301	5/5	0.92	0.13	48,48,48,48	0
4	183	C	5300	28/28	0.92	0.10	31,33,41,41	0
2	PO4	D	5301	5/5	0.94	0.13	42,42,43,43	0
2	PO4	C	6301	5/5	0.96	0.09	35,35,36,36	0

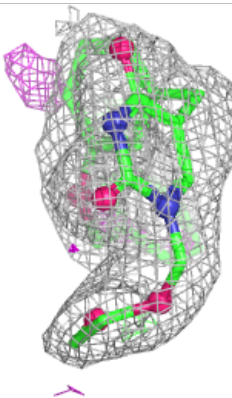
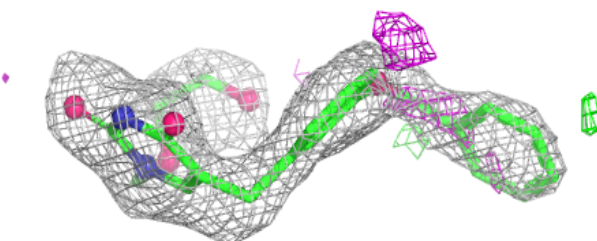
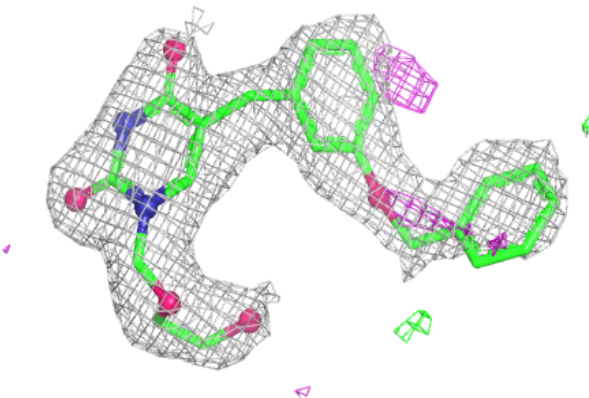
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 183 F 8300:

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

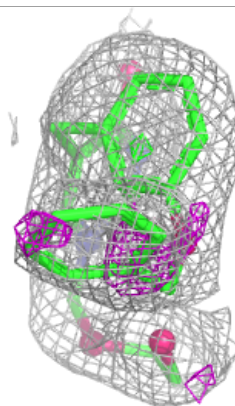
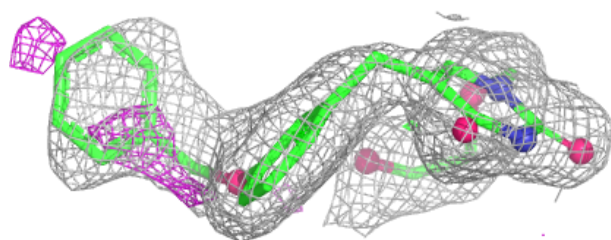
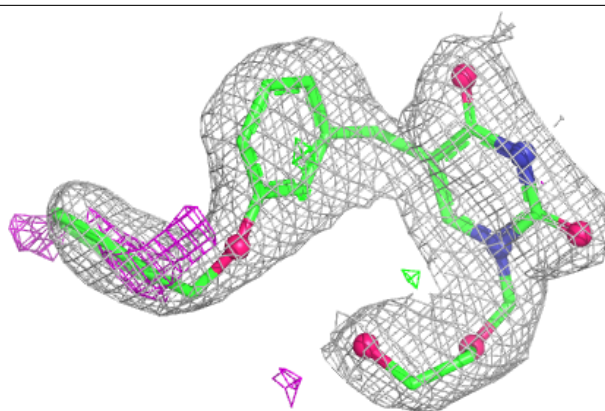
**Electron density around 183 E 7300:**

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

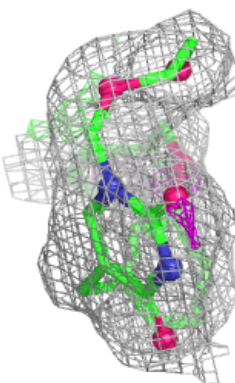
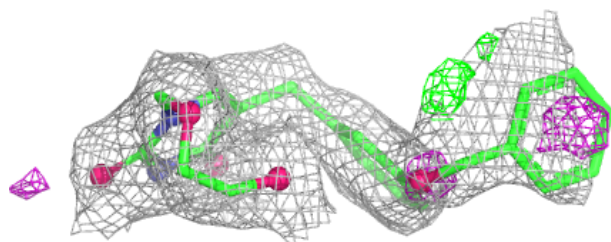
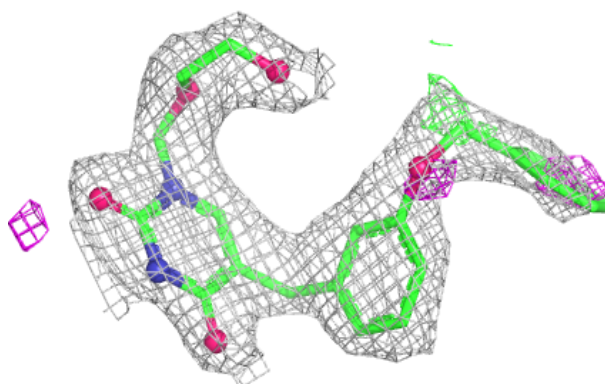


Electron density around 183 B 4300:

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

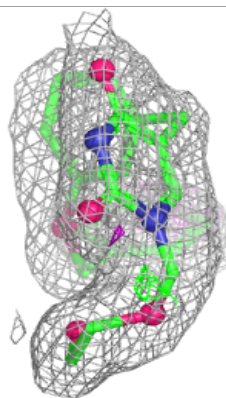
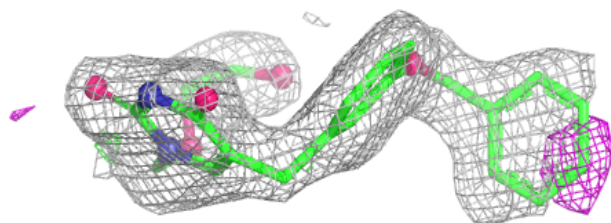
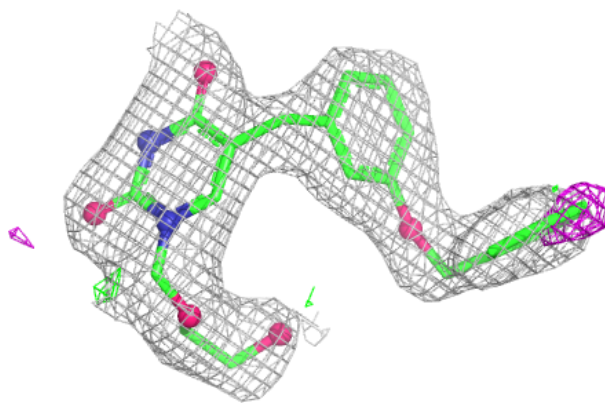
**Electron density around 183 A 3300:**

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

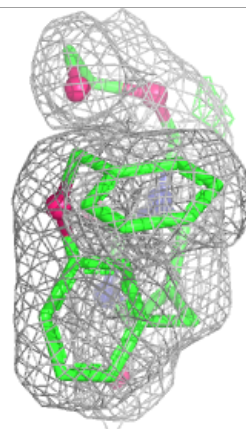
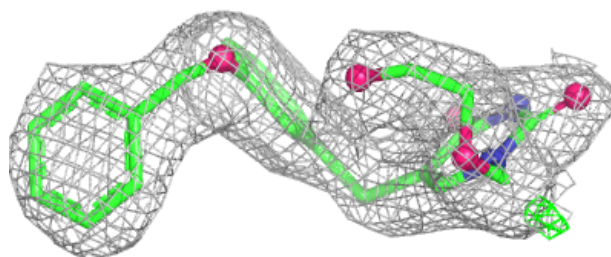
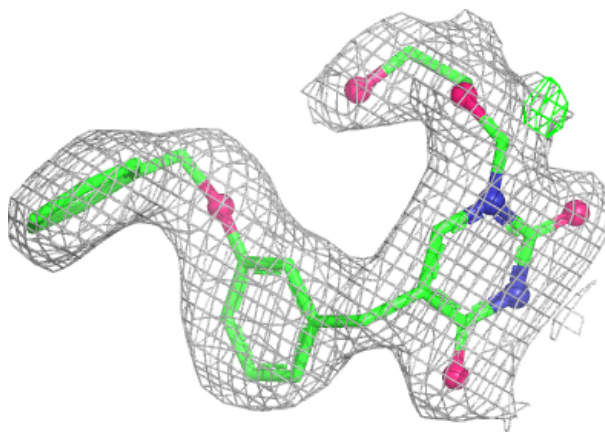


Electron density around 183 D 6300:

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

**Electron density around 183 C 5300:**

$2mF_o-DF_c$ (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.