Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 09:57 am GMT

PDB ID	:	2Y5L
Title	:	orally active aminopyridines as inhibitors of tetrameric fructose 1,6- bisphosphatase
Authors	:	ruf, a.; hebeisen, p.; haap, w.; kuhn, b.; mohr, p.; wessel, h.p.; zutter, u.; kirchner, s.; benz, j.; joseph, c.; alvarez-sanchez, r.; gubler, m.; schott, b.; benardeau, a.; tozzo, e.; kitas, e.
Deposited on	:	2011-01-14
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

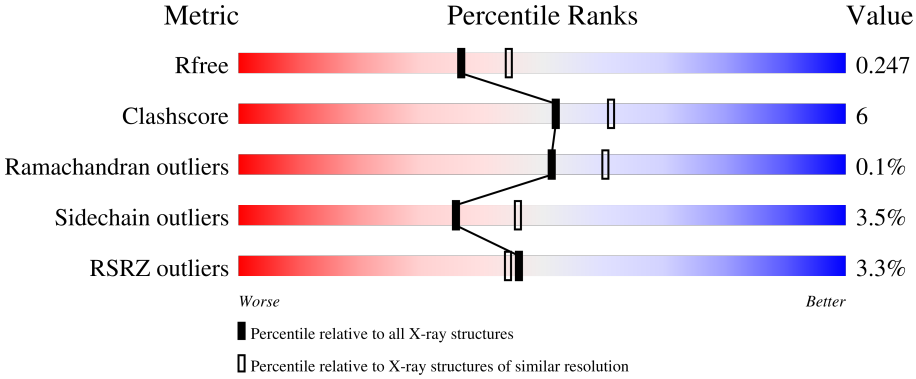
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	338	3% 82% 12% • 5%
1	B	338	3% 79% 14% 6%
1	C	338	2% 81% 12% • 6%
1	D	338	% 82% 12% 6%
1	E	338	5% 81% 13% • 5%

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Mol	Chain	Length	Quality of chain
1	F	338	5% 77% 16% 6%
1	G	338	2% 81% 12% 6%
1	H	338	2% 79% 14% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20167 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.

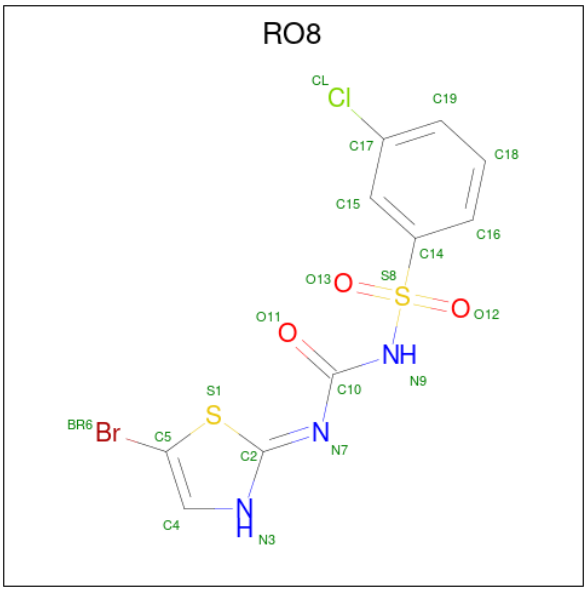
- Molecule 1 is a protein called FRUCTOSE-1,6-BISPHOSPHATASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2447	1558	413	459	17	0	1	1
1	B	318	2432	1548	410	457	17	0	1	1
1	C	318	2426	1545	407	457	17	0	0	1
1	D	318	2432	1548	410	457	17	0	1	1
1	E	320	2448	1559	413	459	17	0	1	1
1	F	318	2431	1547	410	457	17	0	1	1
1	G	318	2431	1547	410	457	17	0	1	1
1	H	318	2426	1545	407	457	17	0	0	1

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	ARG	variant	UNP P09467
B	217	LYS	ARG	variant	UNP P09467
C	217	LYS	ARG	variant	UNP P09467
D	217	LYS	ARG	variant	UNP P09467
E	217	LYS	ARG	variant	UNP P09467
F	217	LYS	ARG	variant	UNP P09467
G	217	LYS	ARG	variant	UNP P09467
H	217	LYS	ARG	variant	UNP P09467

- Molecule 2 is N-{[(2Z)-5-bromo-1,3-thiazol-2(3H)-ylidene]carbamoyl}-3-chlorobenzenesulfonamide (three-letter code: RO8) (formula: $C_{10}H_7BrClN_3O_3S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	Cl	N	O	S		
2	A	1	20	1	10	1	3	3	2	0	0
2	B	1	20	1	10	1	3	3	2	0	0
2	C	1	20	1	10	1	3	3	2	0	0
2	D	1	20	1	10	1	3	3	2	0	0
2	E	1	20	1	10	1	3	3	2	0	0
2	F	1	20	1	10	1	3	3	2	0	0
2	G	1	20	1	10	1	3	3	2	0	0
2	H	1	20	1	10	1	3	3	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	64	64	64	0	0
3	B	60	60	60	0	0
3	C	81	81	81	0	0
3	D	91	91	91	0	0

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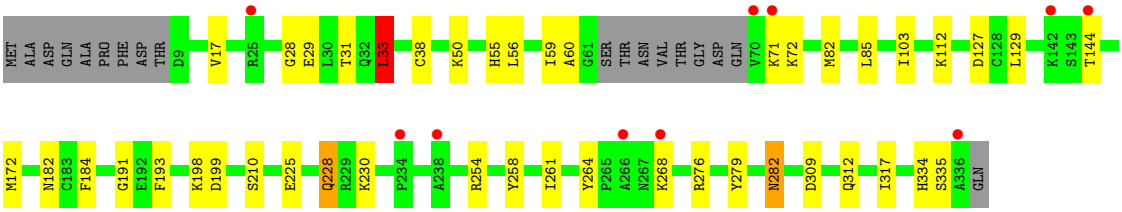
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	E	44	44	44	0	0
			Total	O		
3	F	46	46	46	0	0
			Total	O		
3	G	77	77	77	0	0
			Total	O		
3	H	71	71	71	0	0

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.

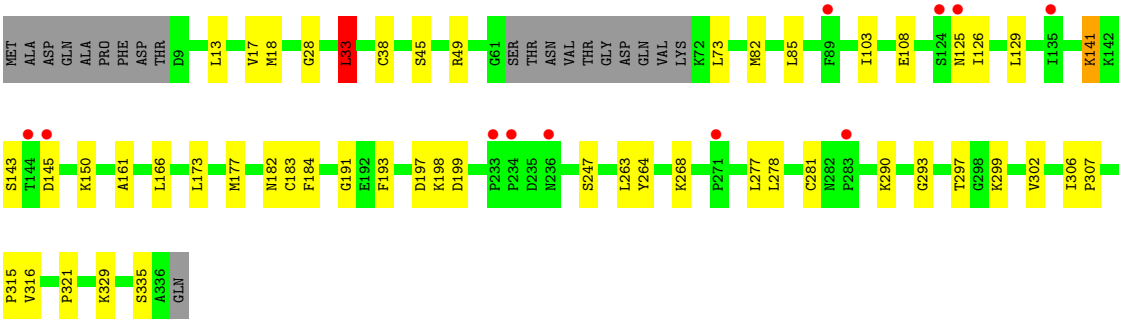
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain A:



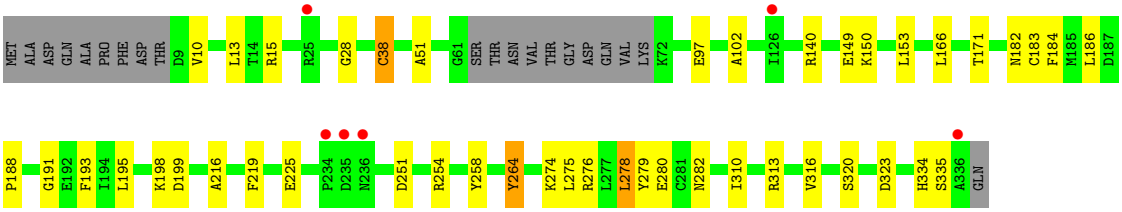
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain B:



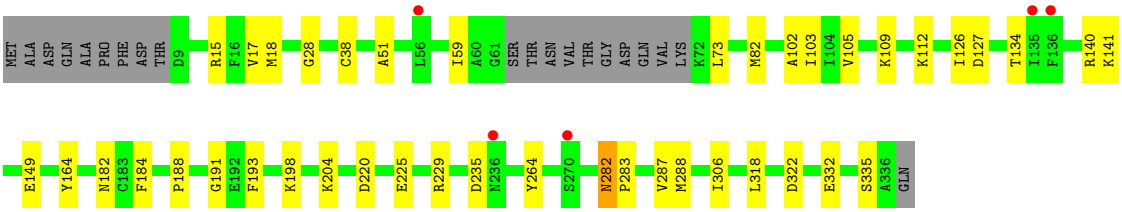
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain C:



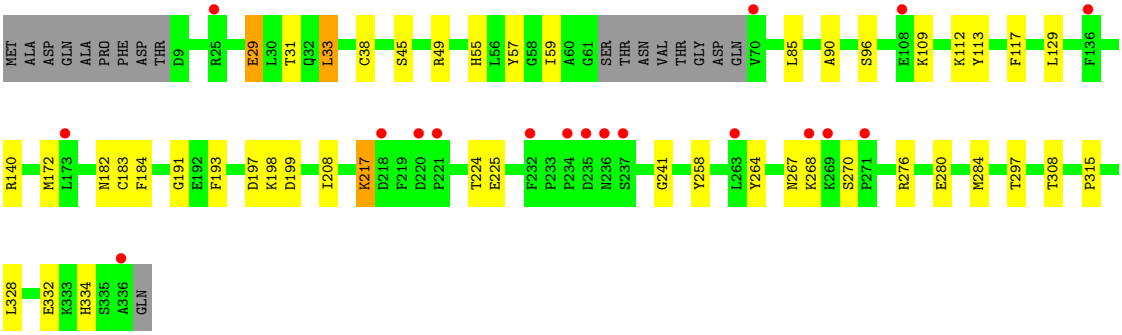
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain D:



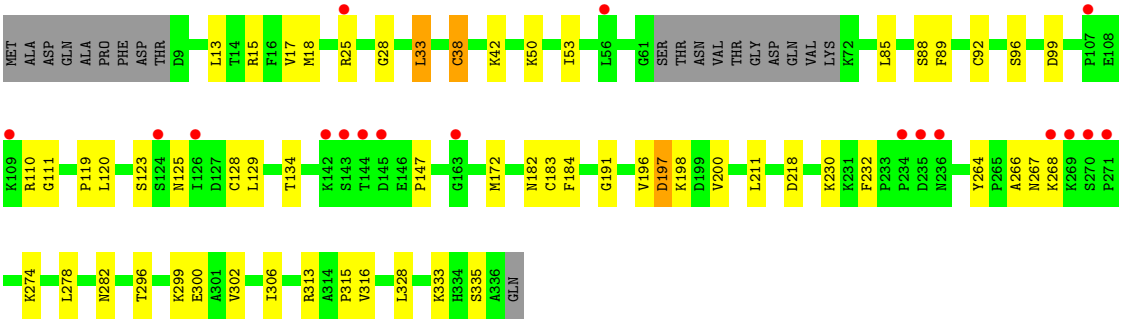
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain E:



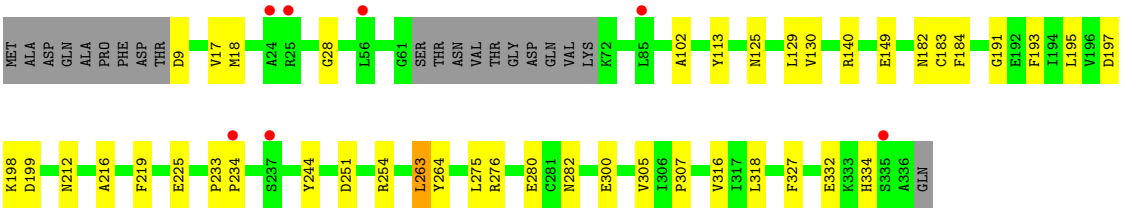
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain F:



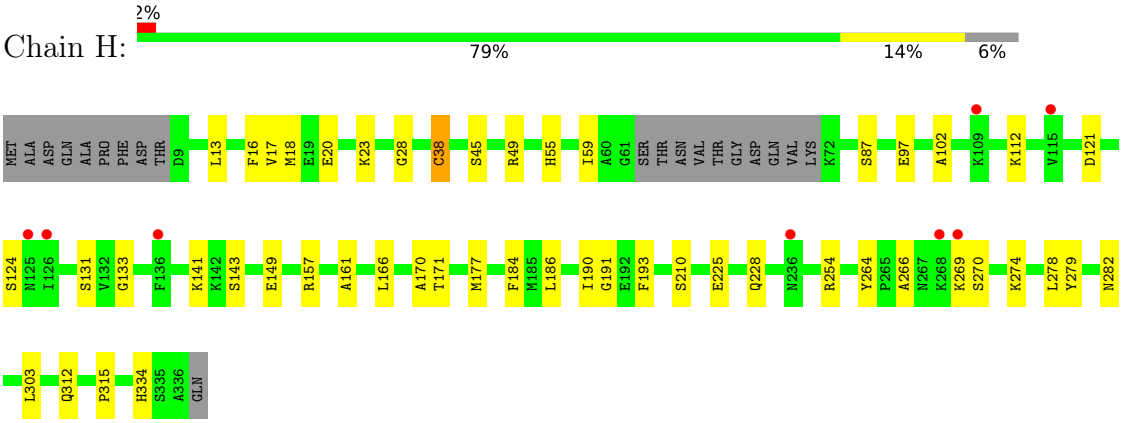
• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain G:



• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE 1

Chain H:


2%
79%
14%
6%
MET ALA ASP GLN ALA PRO PHE ASP THR D9 L13 F16 V17 M18 E19 E20 K23 G28 C38 S45 R49 H55 I59 A60 G61 SER THR ASN VAL THR GLY ASP GLN VAL LYS K72 S87 E97 A102 K109 K112 V115 D121
S124 M125 I126 S131 V132 G133 F136 K141 K142 S143 E149 R157 A161 L166 A170 T171 M177 F184 M185 L186 I190 G191 E192 F193 S210 E225 Q228 N236 R254 Y264 P265 A266 N267 K268 K269 S270 K274 L278 Y279 N282
L303 Q312 P315 H334 S335 A336 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.79Å 285.08Å 83.69Å 90.00° 97.30° 90.00°	Depositor
Resolution (Å)	142.86 – 2.20 24.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (142.86-2.20) 99.4 (24.89-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.205 , 0.254 0.201 , 0.247	Depositor DCC
R_{free} test set	7800 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20167	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: RO8

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	0.55	0/2496	0.66	1/3370 (0.0%)
1	B	0.53	0/2480	0.64	1/3349 (0.0%)
1	C	0.58	1/2469 (0.0%)	0.65	0/3335
1	D	0.57	0/2480	0.65	0/3349
1	E	0.50	0/2496	0.60	0/3370
1	F	0.49	0/2480	0.61	0/3349
1	G	0.55	0/2480	0.64	0/3349
1	H	0.54	0/2469	0.63	0/3335
All	All	0.54	1/19850 (0.0%)	0.63	2/26806 (0.0%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	183	CYS	CB-SG	-5.29	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	33	LEU	CA-CB-CG	5.70	128.41	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2447	0	2496	28	0
1	B	2432	0	2478	27	0
1	C	2426	0	2469	29	0
1	D	2432	0	2478	26	0
1	E	2448	0	2500	37	0
1	F	2431	0	2474	33	0
1	G	2431	0	2474	31	0
1	H	2426	0	2469	28	0
2	A	20	0	7	3	0
2	B	20	0	7	3	0
2	C	20	0	7	2	0
2	D	20	0	7	2	0
2	E	20	0	7	1	0
2	F	20	0	7	2	0
2	G	20	0	7	2	0
2	H	20	0	7	3	0
3	A	64	0	0	2	0
3	B	60	0	0	2	0
3	C	81	0	0	0	0
3	D	91	0	0	0	0
3	E	44	0	0	0	0
3	F	46	0	0	2	0
3	G	77	0	0	3	0
3	H	71	0	0	1	0
All	All	20167	0	19894	218	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 6.

All (218) 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:G:327:PHE:CZ	3:G:2050:HOH:O	2.00	1.14
1:E:140[B]:ARG:HG3	1:E:140[B]:ARG:HH11	1.21	1.04
1:E:140[B]:ARG:HH11	1:E:140[B]:ARG:CG	1.76	0.97
1:G:327:PHE:CE1	3:G:2050:HOH:O	2.14	0.95
3:A:2025:HOH:O	1:C:15:ARG:HD3	1.73	0.86
1:A:33:LEU:HD13	1:A:85:LEU:HD22	1.65	0.78
1:A:225:GLU:OE1	1:A:334:HIS:HE1	1.68	0.76
1:H:225:GLU:OE1	1:H:334:HIS:HE1	1.69	0.75
1:H:102:ALA:HB3	1:H:149:GLU:HG2	1.69	0.73
1:B:297:THR:HB	1:B:315:PRO:HG2	1.75	0.69
1:A:182:ASN:ND2	1:A:199:ASP:H	1.92	0.68
1:C:258:TYR:OH	1:D:127:ASP:HB2	1.94	0.67
1:E:140[B]:ARG:HG3	1:E:140[B]:ARG:NH1	2.00	0.66
1:C:225:GLU:OE1	1:C:334:HIS:HE1	1.79	0.66
1:H:45:SER:O	1:H:49:ARG:HD3	1.97	0.64
1:B:302:VAL:HG21	1:B:316:VAL:HG23	1.80	0.64
2:A:1000:RO8:O11	2:A:1000:RO8:S1	2.55	0.63
1:G:327:PHE:HZ	3:G:2050:HOH:O	1.55	0.63
1:C:184:PHE:HB3	1:C:193:PHE:HB3	1.81	0.63
1:H:225:GLU:OE1	1:H:334:HIS:CE1	2.50	0.62
1:E:217:LYS:HB2	1:F:232:PHE:CE2	2.34	0.62
1:F:120:LEU:HD23	1:F:123:SER:HB3	1.82	0.61
1:C:225:GLU:OE1	1:C:334:HIS:CE1	2.53	0.61
1:C:251:ASP:OD1	1:C:254:ARG:NH2	2.33	0.60
1:C:28:GLY:HA2	2:C:1000:RO8:C10	2.31	0.60
1:E:45:SER:O	1:E:49:ARG:HD3	2.02	0.60
1:H:266:ALA:HB2	1:H:315:PRO:HG3	1.83	0.60
1:E:140[B]:ARG:CG	1:E:140[B]:ARG:NH1	2.47	0.60
1:F:191:GLY:HA3	1:H:191:GLY:HA3	1.84	0.59
1:G:184:PHE:HB3	1:G:193:PHE:HB3	1.84	0.59
1:G:275:LEU:HD12	1:G:316:VAL:HG11	1.85	0.59
1:F:92:CYS:HB3	1:F:111:GLY:O	2.02	0.58
1:F:88:SER:O	1:F:89:PHE:HB2	2.03	0.58
1:A:33:LEU:HD13	1:A:85:LEU:CD2	2.32	0.58
1:G:275:LEU:HD12	1:G:316:VAL:CG1	2.33	0.58
1:B:293:GLY:HA2	1:B:321:PRO:HD3	1.86	0.58
1:C:195:LEU:HD21	1:C:198:LYS:HG2	1.86	0.58
1:B:141:LYS:HE3	1:B:143:SER:O	2.05	0.57
2:F:1000:RO8:O11	2:F:1000:RO8:S1	2.63	0.57
1:F:50:LYS:HD2	1:F:53:ILE:HD13	1.86	0.57
1:D:102:ALA:HB3	1:D:149:GLU:HG2	1.85	0.56
1:D:184:PHE:HB3	1:D:193:PHE:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLY:HA2	2:A:1000:RO8:C10	2.36	0.56
1:A:182:ASN:HD22	1:A:198:LYS:HA	1.69	0.56
1:D:182:ASN:HD22	1:D:198:LYS:HA	1.71	0.56
2:D:1000:RO8:O11	2:D:1000:RO8:S1	2.63	0.56
2:C:1000:RO8:O11	2:C:1000:RO8:S1	2.63	0.56
1:D:102:ALA:CB	1:D:149:GLU:HG2	2.36	0.56
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.88	0.56
1:B:182:ASN:ND2	1:B:199:ASP:H	2.04	0.55
1:E:182:ASN:ND2	1:E:199:ASP:H	2.03	0.55
1:B:17:VAL:HG13	2:B:1000:RO8:CL	2.44	0.55
1:A:276:ARG:HG3	1:A:279:TYR:CE1	2.42	0.55
1:B:13:LEU:HD22	1:B:173:LEU:CD2	2.37	0.55
1:B:73:LEU:HD23	1:B:126:ILE:HD13	1.88	0.54
2:H:1000:RO8:O11	2:H:1000:RO8:S1	2.64	0.54
1:H:17:VAL:HG13	2:H:1000:RO8:CL	2.45	0.54
1:H:141:LYS:HE3	1:H:143:SER:O	2.07	0.54
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.90	0.53
2:G:1000:RO8:O11	2:G:1000:RO8:S1	2.66	0.53
1:C:182:ASN:HD22	1:C:198:LYS:HA	1.73	0.53
1:F:296:THR:HG21	1:F:328:LEU:HD21	1.89	0.53
1:E:258:TYR:OH	1:F:125:ASN:HA	2.09	0.53
1:E:182:ASN:HD22	1:E:198:LYS:HA	1.74	0.53
1:A:182:ASN:HD21	1:A:199:ASP:H	1.54	0.53
1:H:161:ALA:HB2	1:H:177:MET:HG2	1.90	0.52
1:A:17:VAL:HG12	1:A:31:THR:OG1	2.09	0.52
1:C:182:ASN:ND2	1:C:199:ASP:H	2.07	0.52
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.91	0.52
1:E:31:THR:HG22	1:G:18:MET:CE	2.39	0.52
1:A:225:GLU:OE1	1:A:334:HIS:CE1	2.58	0.52
1:G:28:GLY:HA2	2:G:1000:RO8:C10	2.39	0.52
1:G:113:TYR:OH	1:G:140[B]:ARG:NH2	2.42	0.51
1:G:212:ASN:HB2	1:G:244:TYR:CE2	2.46	0.51
1:E:297:THR:HB	1:E:315:PRO:HG2	1.93	0.51
1:E:57:TYR:CZ	1:F:196:VAL:HG12	2.45	0.51
1:B:28:GLY:HA2	2:B:1000:RO8:C10	2.40	0.50
3:B:2018:HOH:O	1:D:15:ARG:HD3	2.11	0.50
1:D:82:MET:CE	1:D:103:ILE:HG13	2.41	0.50
1:E:31:THR:HG22	1:G:18:MET:HE1	1.94	0.50
1:H:278:LEU:HG	3:H:2029:HOH:O	2.11	0.50
1:E:31:THR:CG2	1:G:18:MET:CE	2.90	0.50
1:F:333:LYS:C	1:F:335:SER:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:MET:HE3	1:H:18:MET:HE3	1.93	0.50
1:F:110:ARG:HD3	1:F:147:PRO:HG2	1.94	0.50
1:A:82:MET:HE3	1:A:103:ILE:HD13	1.94	0.50
1:E:29:GLU:OE2	1:E:112:LYS:HG2	2.12	0.49
1:F:183:CYS:HB2	1:F:197:ASP:HB2	1.94	0.49
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.12	0.49
1:H:121:ASP:N	1:H:133:GLY:O	2.45	0.49
1:F:15:ARG:NH1	1:H:87:SER:OG	2.44	0.49
1:H:97:GLU:HG2	1:H:279:TYR:CE1	2.46	0.49
1:D:140[B]:ARG:HD3	1:D:141:LYS:O	2.12	0.49
1:E:208:ILE:HA	1:E:241:GLY:O	2.13	0.49
1:B:13:LEU:HD22	1:B:173:LEU:HD22	1.94	0.49
1:B:33:LEU:HD13	1:B:85:LEU:HD22	1.95	0.49
1:B:18:MET:HE3	1:D:18:MET:HE3	1.94	0.48
1:C:320:SER:HB2	1:C:323:ASP:OD2	2.13	0.48
1:E:258:TYR:CE1	1:F:128:CYS:HB3	2.47	0.48
1:E:33:LEU:O	1:E:33:LEU:HD12	2.12	0.48
1:E:267:ASN:OD1	1:E:270:SER:N	2.38	0.48
1:A:309:ASP:HB3	1:A:312:GLN:HB3	1.95	0.48
1:E:31:THR:CG2	1:G:18:MET:HE1	2.44	0.48
1:F:28:GLY:HA2	2:F:1000:RO8:C10	2.43	0.48
1:C:188:PRO:HD2	1:D:51:ALA:HA	1.95	0.48
1:C:264:TYR:CZ	1:C:274:LYS:HG2	2.48	0.48
1:E:184:PHE:HB3	1:E:193:PHE:HB3	1.94	0.47
1:E:276:ARG:O	1:E:280:GLU:HB2	2.14	0.47
1:G:129:LEU:HD22	1:H:170:ALA:HB3	1.95	0.47
1:G:182:ASN:ND2	1:G:199:ASP:H	2.12	0.47
1:G:183:CYS:HB2	1:G:197:ASP:HB2	1.96	0.47
1:E:258:TYR:HE1	1:F:128:CYS:HB3	1.79	0.47
1:F:274:LYS:HA	1:F:313:ARG:HD3	1.96	0.47
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.96	0.47
1:D:73:LEU:HD23	1:D:126:ILE:HD13	1.97	0.47
1:F:230:LYS:NZ	3:F:2030:HOH:O	2.42	0.47
1:B:82:MET:CE	1:B:103:ILE:HG13	2.45	0.47
1:D:225:GLU:OE2	1:D:229:ARG:NH2	2.45	0.47
1:G:125:ASN:O	1:G:130:VAL:HG12	2.15	0.47
1:G:195:LEU:HD21	1:G:198:LYS:HG2	1.97	0.47
1:B:277:LEU:HA	1:B:281:CYS:HB2	1.96	0.46
1:E:109:LYS:NZ	1:G:9:ASP:OD2	2.48	0.46
1:A:17:VAL:HG13	2:A:1000:RO8:CL	2.53	0.46
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:MET:HG3	1:F:184:PHE:O	2.16	0.46
1:B:290:LYS:HA	1:B:290:LYS:HD3	1.67	0.46
1:G:251:ASP:OD1	1:G:254:ARG:NH2	2.47	0.46
1:A:282:ASN:HD22	1:A:282:ASN:HA	1.58	0.46
1:F:42:LYS:HD2	1:H:190:ILE:O	2.15	0.45
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.97	0.45
1:C:13:LEU:CD2	1:C:38:CYS:HB2	2.47	0.45
1:A:50:LYS:NZ	3:A:2014:HOH:O	2.49	0.45
1:H:171:THR:HB	1:H:186:LEU:HB3	1.99	0.45
1:A:230:LYS:HE2	1:A:230:LYS:HA	1.99	0.45
2:E:1000:RO8:S1	2:E:1000:RO8:O11	2.75	0.45
1:B:306:ILE:HA	1:B:307:PRO:HD3	1.84	0.44
1:C:186:LEU:O	1:C:188:PRO:HD3	2.17	0.44
1:B:18:MET:HE3	1:D:18:MET:CE	2.47	0.44
1:D:105:VAL:CG1	1:D:109:LYS:HB2	2.47	0.44
1:E:96:SER:HB2	1:E:117:PHE:CZ	2.52	0.44
1:A:129:LEU:HD12	1:B:166:LEU:HD23	2.00	0.44
1:C:282:ASN:HD22	1:C:282:ASN:HA	1.71	0.44
1:D:288:MET:HG3	1:D:318:LEU:HD13	1.98	0.44
1:D:134:THR:O	1:D:164:TYR:HA	2.18	0.44
1:A:182:ASN:ND2	1:A:198:LYS:HA	2.33	0.44
1:G:182:ASN:HD22	1:G:198:LYS:HA	1.83	0.44
2:B:1000:RO8:O11	2:B:1000:RO8:S1	2.76	0.44
1:D:182:ASN:ND2	1:D:198:LYS:HA	2.32	0.44
1:D:282:ASN:HD22	1:D:282:ASN:HA	1.61	0.44
1:G:102:ALA:HB2	1:G:149:GLU:HG3	2.00	0.43
1:G:216:ALA:HA	1:G:219:PHE:CD2	2.53	0.43
1:D:283:PRO:O	1:D:287:VAL:HG23	2.19	0.43
1:G:318:LEU:C	1:G:318:LEU:HD12	2.39	0.43
1:B:247:SER:OG	3:B:2046:HOH:O	2.21	0.43
1:E:33:LEU:CD1	1:E:85:LEU:HD22	2.48	0.43
1:F:266:ALA:HB2	1:F:315:PRO:HG3	2.00	0.43
1:B:182:ASN:HD22	1:B:198:LYS:HA	1.83	0.43
1:F:333:LYS:C	1:F:335:SER:N	2.71	0.43
1:H:157:ARG:HG2	1:H:303:LEU:O	2.18	0.43
1:H:13:LEU:HD23	1:H:38:CYS:HB2	2.00	0.43
1:A:261:ILE:HD11	1:A:317:ILE:CG2	2.48	0.43
1:B:183:CYS:HB2	1:B:197:ASP:HB2	2.00	0.43
1:D:112:LYS:HB2	1:D:140[B]:ARG:CZ	2.49	0.43
1:A:55:HIS:HA	1:A:59:ILE:HG22	2.01	0.43
1:F:119:PRO:HA	1:F:134:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:LEU:N	1:G:263:LEU:HD12	2.33	0.43
1:E:225:GLU:OE1	1:E:334:HIS:HE1	2.02	0.42
1:B:161:ALA:HB2	1:B:177:MET:HG2	2.00	0.42
1:D:235:ASP:OD1	1:D:235:ASP:N	2.45	0.42
1:H:97:GLU:HG2	1:H:279:TYR:HE1	1.83	0.42
1:H:266:ALA:HB2	1:H:315:PRO:CG	2.48	0.42
1:H:282:ASN:HD22	1:H:282:ASN:HA	1.64	0.42
1:C:10:VAL:HG11	1:D:59:ILE:HA	2.02	0.42
1:G:225:GLU:OE1	1:G:334:HIS:HE1	2.02	0.42
1:F:33:LEU:HD13	1:F:85:LEU:HD22	2.02	0.42
1:A:172:MET:HB2	1:B:129:LEU:HD11	2.00	0.42
1:B:45:SER:O	1:B:49:ARG:HD3	2.20	0.42
1:C:275:LEU:HD12	1:C:316:VAL:CG1	2.50	0.42
1:E:172:MET:SD	1:E:183:CYS:HB3	2.60	0.42
1:E:183:CYS:HB2	1:E:197:ASP:HB2	2.01	0.42
1:F:183:CYS:SG	1:F:200:VAL:HG21	2.60	0.41
1:C:51:ALA:HA	1:D:188:PRO:HD2	2.01	0.41
1:D:28:GLY:HA2	2:D:1000:RO8:C10	2.50	0.41
1:F:13:LEU:HD23	1:F:38:CYS:HB2	2.02	0.41
1:H:16:PHE:O	1:H:20:GLU:HG2	2.20	0.41
1:G:233:PRO:HA	1:G:234:PRO:HD3	1.85	0.41
1:A:258:TYR:OH	1:B:125:ASN:HA	2.20	0.41
1:C:166:LEU:O	1:C:171:THR:HA	2.21	0.41
1:C:184:PHE:CE2	1:C:195:LEU:HB2	2.55	0.41
1:G:282:ASN:HD22	1:G:282:ASN:HA	1.76	0.41
1:E:129:LEU:HD11	1:F:172:MET:HB2	2.01	0.41
1:A:276:ARG:HG3	1:A:279:TYR:HE1	1.84	0.41
1:C:97:GLU:HG2	1:C:279:TYR:CE1	2.55	0.41
1:E:33:LEU:HD13	1:E:85:LEU:HD22	2.01	0.41
1:E:328:LEU:HD23	1:E:328:LEU:HA	1.89	0.41
1:F:306:ILE:O	3:F:2042:HOH:O	2.21	0.41
1:G:305:VAL:O	1:G:307:PRO:HD3	2.20	0.41
1:A:210:SER:HB2	1:A:254:ARG:NH2	2.35	0.41
1:A:228:GLN:HE21	1:A:228:GLN:HB3	1.65	0.41
1:C:278:LEU:HG	1:C:310:ILE:O	2.21	0.41
1:E:90:ALA:O	1:E:113:TYR:HB2	2.21	0.41
1:F:96:SER:HB3	1:F:99:ASP:OD2	2.21	0.41
1:G:276:ARG:O	1:G:280:GLU:HB2	2.20	0.41
1:H:28:GLY:HA2	2:H:1000:RO8:C10	2.50	0.41
1:C:274:LYS:O	1:C:313:ARG:NH1	2.52	0.41
1:D:204:LYS:HE3	1:D:322:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:HIS:HA	1:E:59:ILE:HG22	2.03	0.41
1:E:172:MET:HB2	1:F:129:LEU:HD11	2.02	0.41
1:C:150:LYS:HA	1:C:153:LEU:HD12	2.03	0.40
1:C:276:ARG:O	1:C:280:GLU:HB2	2.20	0.40
1:E:280:GLU:O	1:E:284:MET:HG2	2.22	0.40
1:F:182:ASN:HD22	1:F:198:LYS:HA	1.85	0.40
1:H:55:HIS:HA	1:H:59:ILE:HG22	2.04	0.40
1:C:102:ALA:HB2	1:C:149:GLU:HG3	2.04	0.40
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.56	0.40
1:F:282:ASN:ND2	1:F:302:VAL:HG12	2.36	0.40
1:H:131:SER:HB3	1:H:166:LEU:HD11	2.02	0.40
1:H:210:SER:HB2	1:H:254:ARG:NH2	2.36	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	317/338 (94%)	303 (96%)	13 (4%)	1 (0%)	41 46
1	B	315/338 (93%)	305 (97%)	10 (3%)	0	100 100
1	C	314/338 (93%)	307 (98%)	6 (2%)	1 (0%)	41 46
1	D	315/338 (93%)	308 (98%)	7 (2%)	0	100 100
1	E	317/338 (94%)	304 (96%)	13 (4%)	0	100 100
1	F	315/338 (93%)	295 (94%)	20 (6%)	0	100 100
1	G	315/338 (93%)	303 (96%)	12 (4%)	0	100 100
1	H	314/338 (93%)	299 (95%)	15 (5%)	0	100 100
All	All	2522/2704 (93%)	2424 (96%)	96 (4%)	2 (0%)	51 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	335	SER
1	A	335	SER

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	267/281 (95%)	256 (96%)	11 (4%)	30	39
1	B	265/281 (94%)	252 (95%)	13 (5%)	25	31
1	C	264/281 (94%)	260 (98%)	4 (2%)	65	78
1	D	265/281 (94%)	257 (97%)	8 (3%)	41	53
1	E	267/281 (95%)	258 (97%)	9 (3%)	37	47
1	F	265/281 (94%)	251 (95%)	14 (5%)	22	27
1	G	265/281 (94%)	260 (98%)	5 (2%)	57	71
1	H	264/281 (94%)	254 (96%)	10 (4%)	33	42
All	All	2122/2248 (94%)	2048 (96%)	74 (4%)	36	46

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	38	CYS
1	A	56	LEU
1	A	71	LYS
1	A	72	LYS
1	A	127	ASP
1	A	144	THR
1	A	228	GLN
1	A	264	TYR
1	A	268	LYS
1	A	282	ASN
1	B	33	LEU
1	B	38	CYS
1	B	108	GLU

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Mol	Chain	Res	Type
1	B	141	LYS
1	B	145	ASP
1	B	150	LYS
1	B	263	LEU
1	B	264	TYR
1	B	268	LYS
1	B	278	LEU
1	B	299	LYS
1	B	329	LYS
1	B	335	SER
1	C	38	CYS
1	C	140	ARG
1	C	264	TYR
1	C	278	LEU
1	D	17	VAL
1	D	38	CYS
1	D	220	ASP
1	D	264	TYR
1	D	282	ASN
1	D	306	ILE
1	D	332	GLU
1	D	335	SER
1	E	29	GLU
1	E	33	LEU
1	E	38	CYS
1	E	217	LYS
1	E	224	THR
1	E	264	TYR
1	E	268	LYS
1	E	308	THR
1	E	332	GLU
1	F	17	VAL
1	F	25	ARG
1	F	33	LEU
1	F	38	CYS
1	F	197	ASP
1	F	211	LEU
1	F	218	ASP
1	F	264	TYR
1	F	267	ASN
1	F	268	LYS
1	F	278	LEU

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Mol	Chain	Res	Type
1	F	299	LYS
1	F	300	GLU
1	F	316	VAL
1	G	17	VAL
1	G	263	LEU
1	G	264	TYR
1	G	300	GLU
1	G	332	GLU
1	H	23	LYS
1	H	38	CYS
1	H	112	LYS
1	H	124	SER
1	H	228	GLN
1	H	264	TYR
1	H	269	LYS
1	H	270	SER
1	H	274	LYS
1	H	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	228	GLN
1	A	282	ASN
1	A	334	HIS
1	B	182	ASN
1	B	282	ASN
1	C	125	ASN
1	C	182	ASN
1	C	282	ASN
1	C	334	HIS
1	D	125	ASN
1	D	182	ASN
1	D	282	ASN
1	D	334	HIS
1	E	101	HIS
1	E	182	ASN
1	E	228	GLN
1	E	282	ASN
1	E	334	HIS
1	F	125	ASN

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Mol	Chain	Res	Type
1	F	182	ASN
1	F	267	ASN
1	F	282	ASN
1	G	182	ASN
1	G	282	ASN
1	G	334	HIS
1	H	182	ASN
1	H	282	ASN
1	H	334	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RO8	H	1000	-	20,21,21	1.95	5 (25%)	26,30,30	2.77	6 (23%)
2	RO8	B	1000	-	20,21,21	1.89	5 (25%)	26,30,30	2.87	6 (23%)
2	RO8	E	1000	-	20,21,21	1.91	6 (30%)	26,30,30	2.63	6 (23%)
2	RO8	D	1000	-	20,21,21	2.13	6 (30%)	26,30,30	2.43	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RO8	F	1000	-	20,21,21	1.85	5 (25%)	26,30,30	2.74	7 (26%)
2	RO8	G	1000	-	20,21,21	1.93	6 (30%)	26,30,30	2.53	7 (26%)
2	RO8	C	1000	-	20,21,21	2.20	6 (30%)	26,30,30	2.59	7 (26%)
2	RO8	A	1000	-	20,21,21	1.92	5 (25%)	26,30,30	2.49	7 (26%)

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	RO8	H	1000	-	-	0/14/15/15	0/2/2/2
2	RO8	B	1000	-	-	0/14/15/15	0/2/2/2
2	RO8	E	1000	-	-	0/14/15/15	0/2/2/2
2	RO8	D	1000	-	-	2/14/15/15	0/2/2/2
2	RO8	F	1000	-	-	0/14/15/15	0/2/2/2
2	RO8	G	1000	-	-	0/14/15/15	0/2/2/2
2	RO8	C	1000	-	-	0/14/15/15	0/2/2/2
2	RO8	A	1000	-	-	0/14/15/15	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1000	RO8	S8-N9	-5.69	1.52	1.64
2	C	1000	RO8	S8-N9	-5.57	1.52	1.64
2	E	1000	RO8	S8-N9	-5.53	1.52	1.64
2	D	1000	RO8	S8-N9	-5.53	1.52	1.64
2	B	1000	RO8	S8-N9	-5.47	1.52	1.64
2	F	1000	RO8	S8-N9	-5.47	1.52	1.64
2	A	1000	RO8	S8-N9	-5.23	1.53	1.64
2	C	1000	RO8	C14-S8	-5.10	1.68	1.76
2	D	1000	RO8	C14-S8	-4.93	1.68	1.76
2	G	1000	RO8	S8-N9	-4.92	1.54	1.64
2	B	1000	RO8	C14-S8	-4.05	1.70	1.76
2	G	1000	RO8	C14-S8	-3.68	1.70	1.76
2	A	1000	RO8	C14-S8	-3.32	1.71	1.76
2	F	1000	RO8	C14-S8	-3.24	1.71	1.76
2	H	1000	RO8	C14-S8	-3.22	1.71	1.76
2	A	1000	RO8	C10-N7	-3.20	1.33	1.38
2	C	1000	RO8	C2-N3	3.15	1.37	1.34
2	H	1000	RO8	BR6-C5	3.01	1.93	1.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	RO8	BR6-C5	2.95	1.93	1.87
2	G	1000	RO8	C2-N3	2.94	1.37	1.34
2	F	1000	RO8	BR6-C5	2.91	1.93	1.87
2	E	1000	RO8	C14-S8	-2.88	1.72	1.76
2	E	1000	RO8	C17-CL	2.84	1.80	1.74
2	D	1000	RO8	BR6-C5	2.79	1.92	1.87
2	H	1000	RO8	C10-N7	-2.67	1.34	1.38
2	D	1000	RO8	C10-N7	-2.66	1.34	1.38
2	A	1000	RO8	BR6-C5	2.62	1.92	1.87
2	A	1000	RO8	C2-N3	2.60	1.36	1.34
2	E	1000	RO8	C2-N3	2.60	1.36	1.34
2	G	1000	RO8	BR6-C5	2.59	1.92	1.87
2	B	1000	RO8	C2-N3	2.50	1.36	1.34
2	H	1000	RO8	C17-CL	2.42	1.79	1.74
2	C	1000	RO8	C17-CL	2.41	1.79	1.74
2	G	1000	RO8	C10-N7	-2.36	1.34	1.38
2	E	1000	RO8	C10-N7	-2.35	1.34	1.38
2	D	1000	RO8	C17-CL	2.30	1.79	1.74
2	C	1000	RO8	C10-N7	-2.30	1.34	1.38
2	F	1000	RO8	C10-N7	-2.26	1.34	1.38
2	E	1000	RO8	BR6-C5	2.25	1.91	1.87
2	B	1000	RO8	BR6-C5	2.22	1.91	1.87
2	B	1000	RO8	C10-N7	-2.21	1.34	1.38
2	F	1000	RO8	C17-CL	2.19	1.79	1.74
2	G	1000	RO8	C17-CL	2.11	1.79	1.74
2	D	1000	RO8	C10-N9	-2.08	1.32	1.36

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	RO8	O13-S8-O12	-11.43	105.50	119.55
2	F	1000	RO8	O13-S8-O12	-9.84	107.46	119.55
2	A	1000	RO8	O13-S8-O12	-9.77	107.53	119.55
2	E	1000	RO8	O13-S8-O12	-9.77	107.54	119.55
2	H	1000	RO8	O13-S8-O12	-9.50	107.87	119.55
2	C	1000	RO8	O13-S8-O12	-8.72	108.83	119.55
2	G	1000	RO8	O13-S8-O12	-8.66	108.91	119.55
2	D	1000	RO8	O13-S8-O12	-8.11	109.57	119.55
2	H	1000	RO8	C14-S8-N9	5.61	114.46	105.97
2	C	1000	RO8	C14-S8-N9	5.54	114.37	105.97
2	E	1000	RO8	C14-S8-N9	5.52	114.34	105.97
2	F	1000	RO8	C14-S8-N9	5.46	114.23	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	RO8	C14-S8-N9	5.24	113.91	105.97
2	G	1000	RO8	N9-C10-N7	4.51	117.97	110.93
2	G	1000	RO8	C14-S8-N9	4.48	112.76	105.97
2	B	1000	RO8	C2-N7-C10	4.39	128.22	116.50
2	D	1000	RO8	C14-S8-N9	4.34	112.55	105.97
2	E	1000	RO8	C2-N7-C10	4.34	128.07	116.50
2	H	1000	RO8	N9-C10-N7	4.06	117.27	110.93
2	D	1000	RO8	N9-C10-N7	3.86	116.96	110.93
2	G	1000	RO8	C2-N7-C10	3.85	126.78	116.50
2	H	1000	RO8	BR6-C5-S1	3.61	124.54	119.67
2	F	1000	RO8	N9-C10-N7	3.59	116.53	110.93
2	A	1000	RO8	C14-S8-N9	3.54	111.34	105.97
2	H	1000	RO8	C5-C4-N3	3.53	114.59	109.39
2	F	1000	RO8	C5-C4-N3	3.51	114.56	109.39
2	H	1000	RO8	C2-N7-C10	3.41	125.58	116.50
2	C	1000	RO8	C2-N7-C10	3.40	125.55	116.50
2	D	1000	RO8	BR6-C5-S1	3.38	124.23	119.67
2	F	1000	RO8	C2-N7-C10	3.31	125.33	116.50
2	D	1000	RO8	C5-C4-N3	3.27	114.21	109.39
2	C	1000	RO8	C5-C4-N3	3.21	114.12	109.39
2	D	1000	RO8	C2-N7-C10	3.07	124.69	116.50
2	A	1000	RO8	C2-N7-C10	2.94	124.34	116.50
2	C	1000	RO8	N3-C2-N7	2.84	126.01	120.29
2	G	1000	RO8	C5-C4-N3	2.83	113.56	109.39
2	C	1000	RO8	C15-C14-S8	-2.83	115.91	119.08
2	E	1000	RO8	N9-C10-N7	2.81	115.32	110.93
2	F	1000	RO8	O12-S8-C14	2.81	111.42	107.97
2	A	1000	RO8	N9-C10-N7	2.79	115.28	110.93
2	A	1000	RO8	C5-C4-N3	2.74	113.42	109.39
2	C	1000	RO8	N9-C10-N7	2.69	115.12	110.93
2	B	1000	RO8	N9-C10-N7	2.56	114.92	110.93
2	B	1000	RO8	C5-C4-N3	2.56	113.16	109.39
2	G	1000	RO8	N3-C2-N7	2.30	124.94	120.29
2	E	1000	RO8	C5-C4-N3	2.25	112.71	109.39
2	B	1000	RO8	N3-C2-N7	2.18	124.69	120.29
2	F	1000	RO8	N3-C2-N7	2.16	124.64	120.29
2	G	1000	RO8	O11-C10-N7	-2.15	120.79	125.62
2	E	1000	RO8	N3-C2-N7	2.15	124.63	120.29
2	A	1000	RO8	C18-C16-C14	2.11	121.15	118.95
2	A	1000	RO8	C4-C5-S1	2.03	115.23	113.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

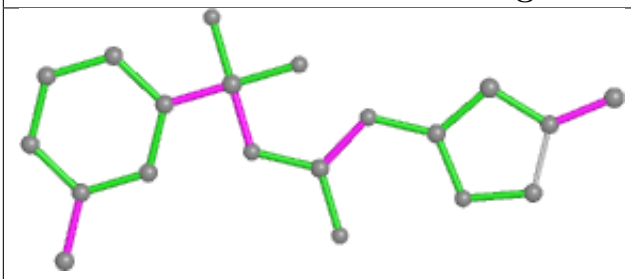
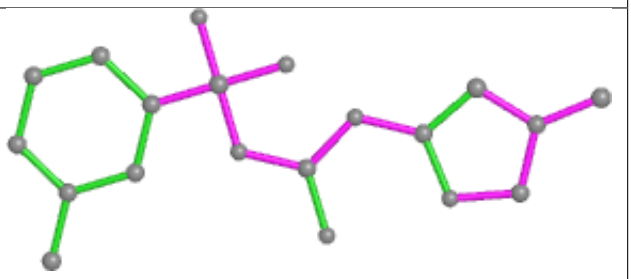
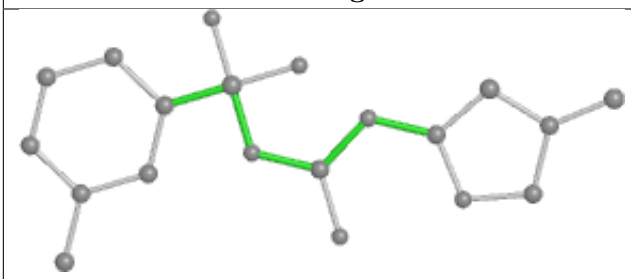
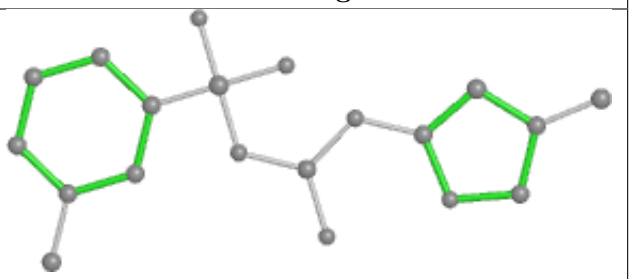
Mol	Chain	Res	Type	Atoms
2	D	1000	RO8	N3-C2-N7-C10
2	D	1000	RO8	C10-N9-S8-O13

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1000	RO8	3	0
2	B	1000	RO8	3	0
2	E	1000	RO8	1	0
2	D	1000	RO8	2	0
2	F	1000	RO8	2	0
2	G	1000	RO8	2	0
2	C	1000	RO8	2	0
2	A	1000	RO8	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 then 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 RO8 H 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

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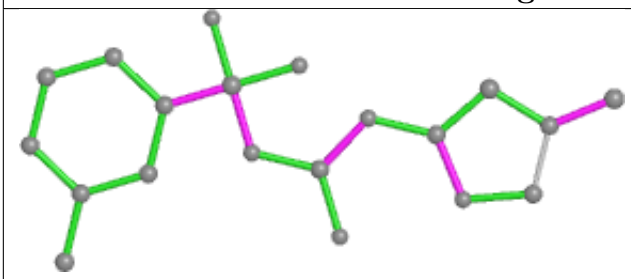
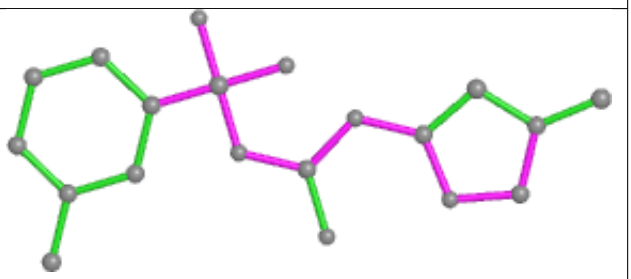
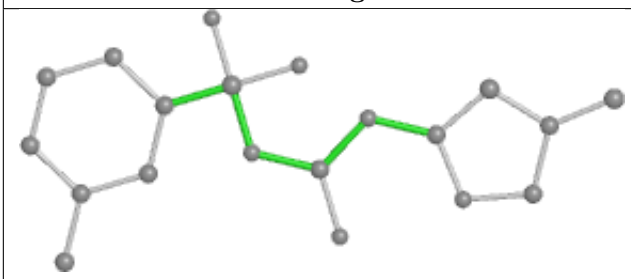
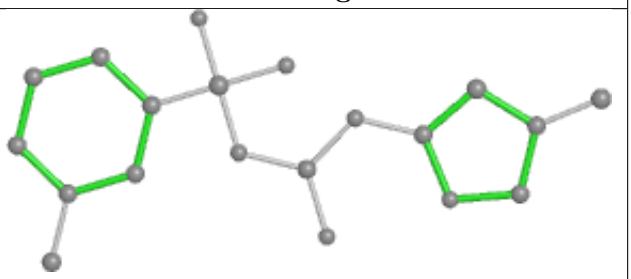
 Bond lengths	 Bond angles
 Torsions	 Rings

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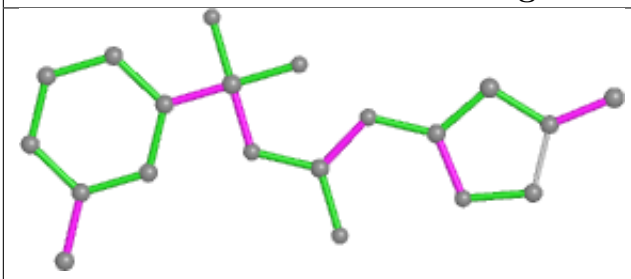
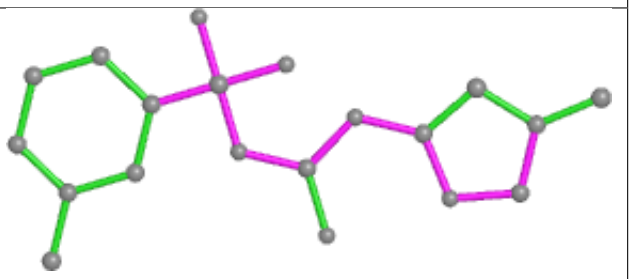
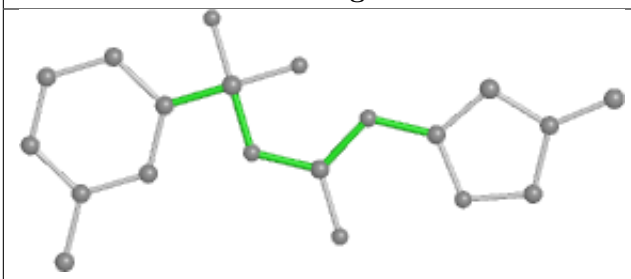
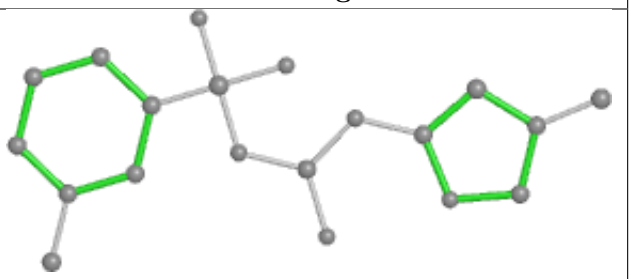
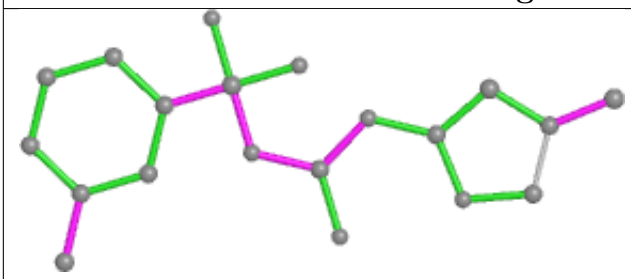
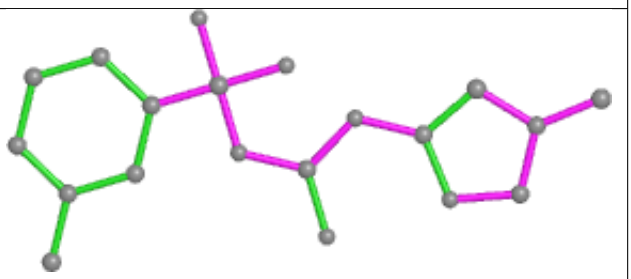
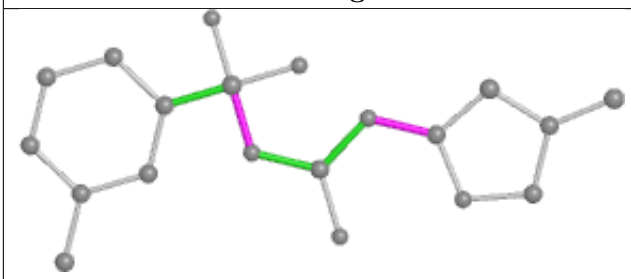
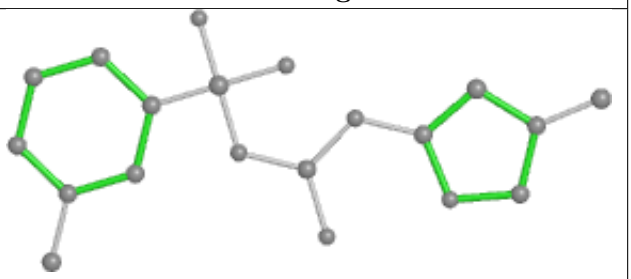
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RO8 D 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

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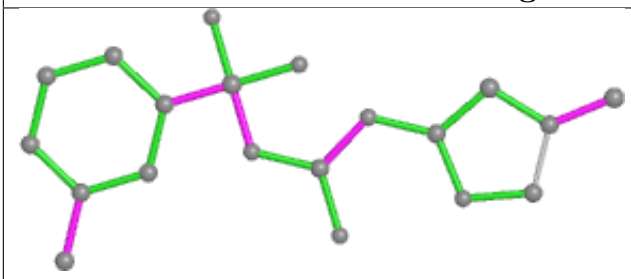
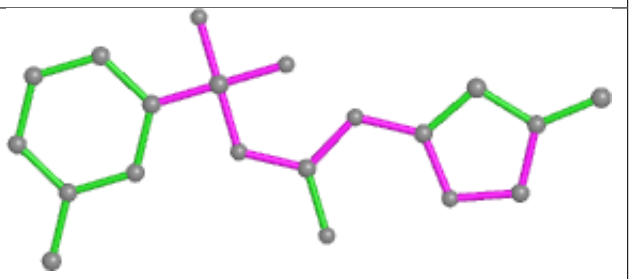
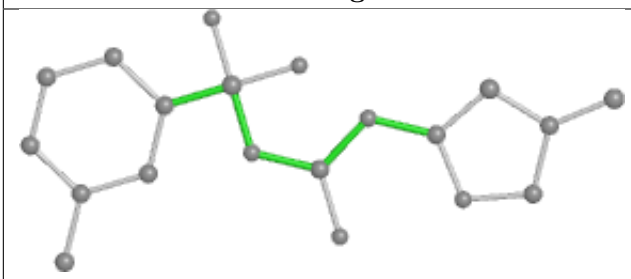
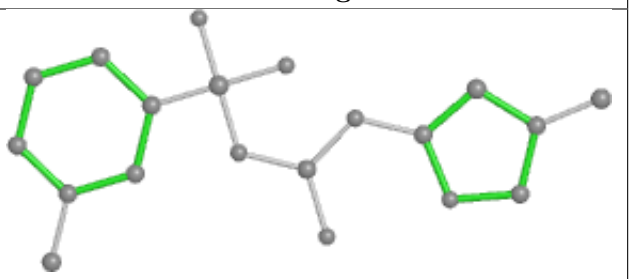
 Bond lengths	 Bond angles
 Torsions	 Rings

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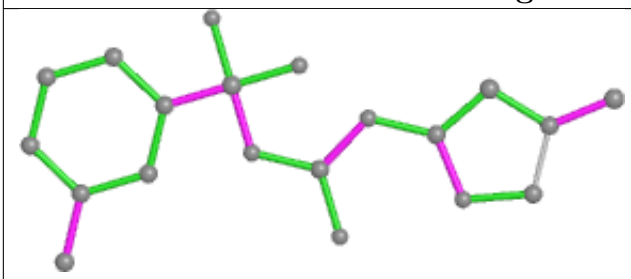
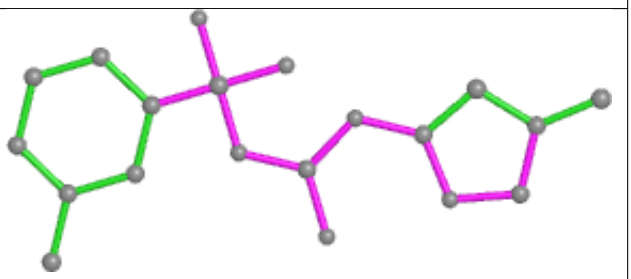
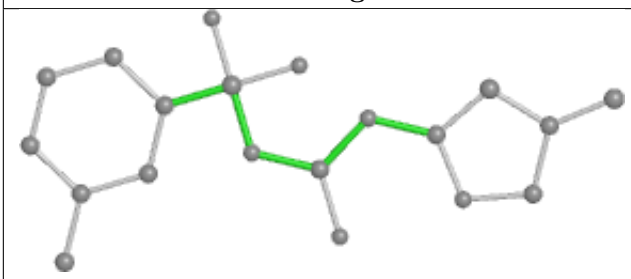
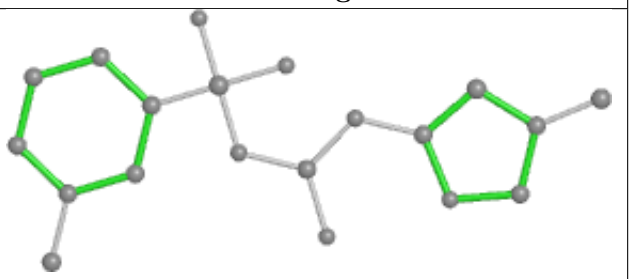
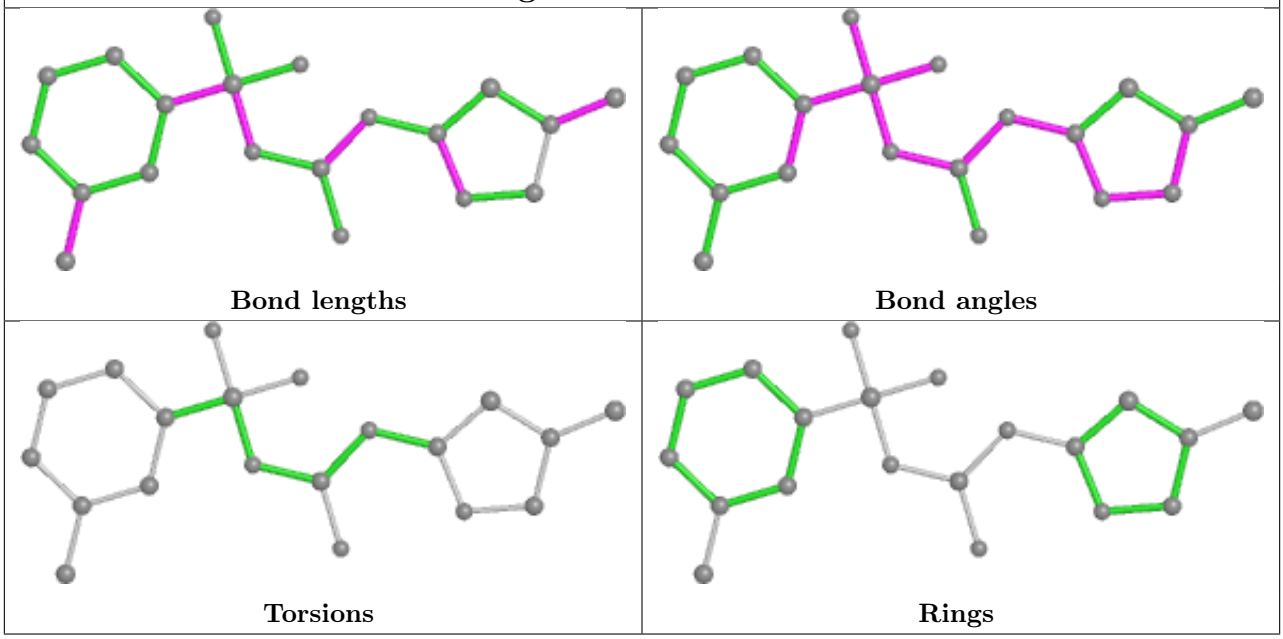
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RO8 C 1000



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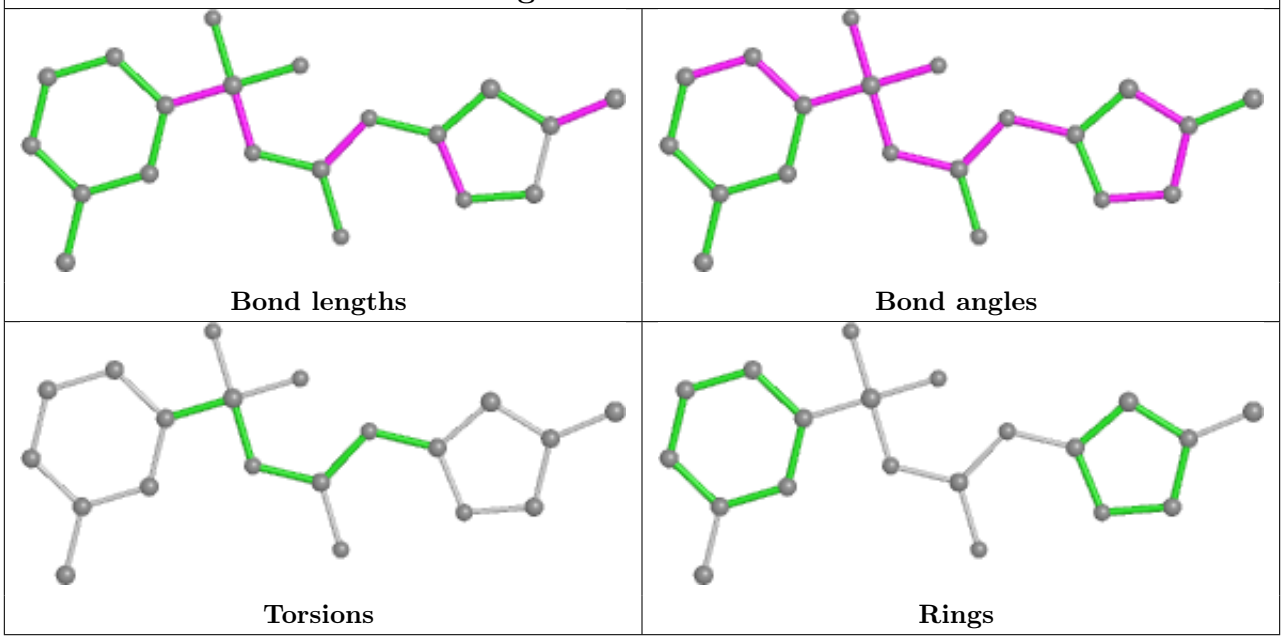

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	320/338 (94%)	0.05	10 (3%)	49	47	29, 44, 79, 119	0
1	B	318/338 (94%)	0.09	11 (3%)	44	42	28, 46, 80, 113	0
1	C	318/338 (94%)	-0.09	6 (1%)	66	65	26, 41, 65, 97	0
1	D	318/338 (94%)	-0.17	5 (1%)	72	70	24, 37, 61, 80	0
1	E	320/338 (94%)	0.20	18 (5%)	24	23	33, 52, 89, 116	0
1	F	318/338 (94%)	0.19	18 (5%)	23	22	32, 51, 89, 120	0
1	G	318/338 (94%)	-0.05	7 (2%)	62	59	29, 43, 70, 93	0
1	H	318/338 (94%)	-0.11	8 (2%)	57	55	28, 43, 72, 91	0
All	All	2548/2704 (94%)	0.01	83 (3%)	46	44	24, 44, 78, 120	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	7.2
1	E	70	VAL	6.0
1	B	236	ASN	5.6
1	F	144	THR	4.9
1	C	236	ASN	4.6
1	B	234	PRO	4.2
1	E	234	PRO	4.0
1	F	143	SER	3.9
1	F	56	LEU	3.9
1	F	109	LYS	3.8
1	E	235	ASP	3.7
1	F	236	ASN	3.7
1	F	234	PRO	3.6
1	D	236	ASN	3.6
1	F	142	LYS	3.6
1	E	232	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	336	ALA	3.5
1	G	335	SER	3.5
1	G	25	ARG	3.3
1	A	336	ALA	3.3
1	F	25	ARG	3.1
1	A	25	ARG	3.1
1	E	336	ALA	3.1
1	F	269	LYS	3.0
1	H	236	ASN	3.0
1	E	25	ARG	3.0
1	A	234	PRO	2.9
1	A	71	LYS	2.9
1	F	268	LYS	2.9
1	E	269	LYS	2.8
1	F	107	PRO	2.8
1	A	268	LYS	2.8
1	E	271	PRO	2.7
1	H	126	ILE	2.7
1	F	145	ASP	2.7
1	H	269	LYS	2.7
1	G	85	LEU	2.7
1	B	124	SER	2.7
1	C	25	ARG	2.6
1	E	236	ASN	2.6
1	C	234	PRO	2.6
1	E	218	ASP	2.6
1	B	145	ASP	2.6
1	D	270	SER	2.5
1	A	142	LYS	2.5
1	F	271	PRO	2.5
1	B	89	PHE	2.5
1	E	263	LEU	2.5
1	F	235	ASP	2.5
1	C	126	ILE	2.4
1	E	268	LYS	2.4
1	A	144	THR	2.4
1	B	283	PRO	2.4
1	E	221	PRO	2.4
1	E	237	SER	2.4
1	D	136	PHE	2.4
1	E	173	LEU	2.3
1	A	266	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	144	THR	2.3
1	H	136	PHE	2.3
1	A	238	ALA	2.3
1	H	125	ASN	2.3
1	F	270	SER	2.3
1	G	24	ALA	2.3
1	E	108	GLU	2.2
1	F	126	ILE	2.2
1	B	233	PRO	2.2
1	B	125	ASN	2.2
1	G	234	PRO	2.2
1	E	136	PHE	2.2
1	H	109	LYS	2.1
1	G	237	SER	2.1
1	D	135	ILE	2.1
1	E	220	ASP	2.1
1	B	271	PRO	2.1
1	F	163	GLY	2.1
1	D	56	LEU	2.1
1	H	115	VAL	2.1
1	B	135	ILE	2.0
1	H	268	LYS	2.0
1	G	56	LEU	2.0
1	F	124	SER	2.0
1	C	235	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

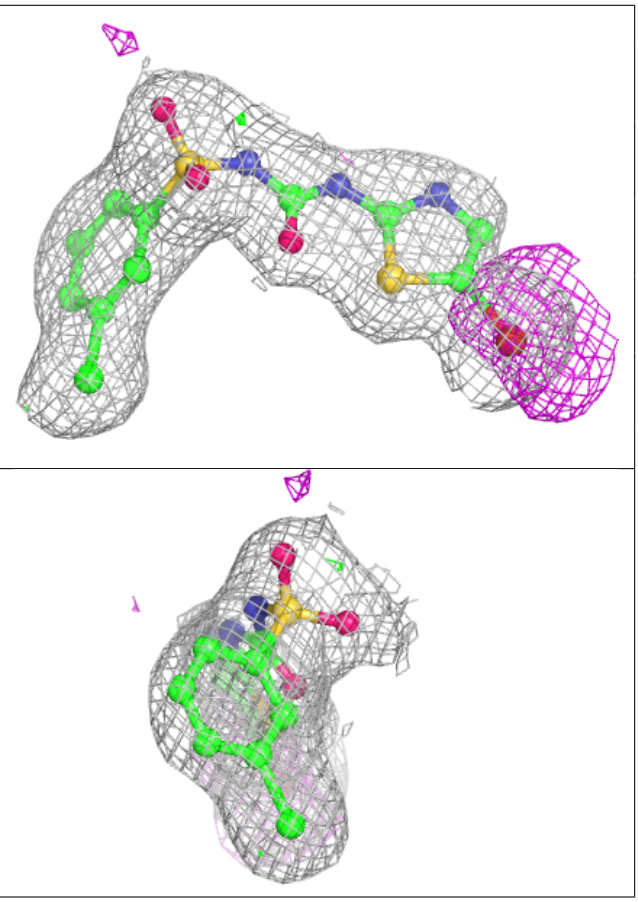
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	RO8	A	1000	20/20	0.95	0.09	34,43,61,63	0
2	RO8	G	1000	20/20	0.95	0.10	40,50,68,75	0
2	RO8	C	1000	20/20	0.96	0.10	33,43,62,66	0
2	RO8	D	1000	20/20	0.96	0.09	35,40,58,61	0
2	RO8	E	1000	20/20	0.96	0.12	43,51,61,63	0
2	RO8	B	1000	20/20	0.96	0.08	41,48,63,63	0
2	RO8	F	1000	20/20	0.97	0.12	50,55,61,70	0
2	RO8	H	1000	20/20	0.97	0.13	49,55,63,77	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.

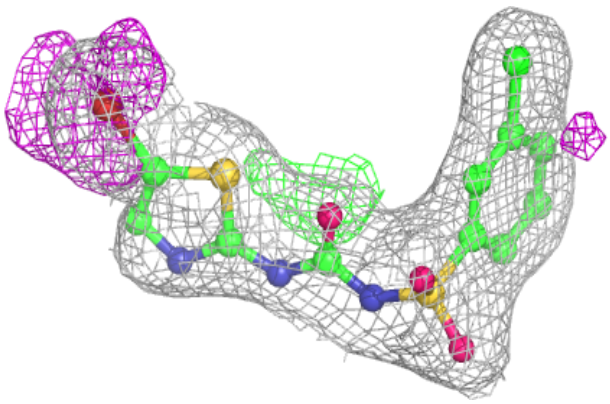
Electron density around RO8 A 1000:

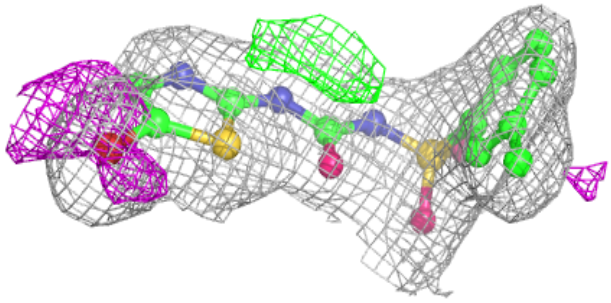
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

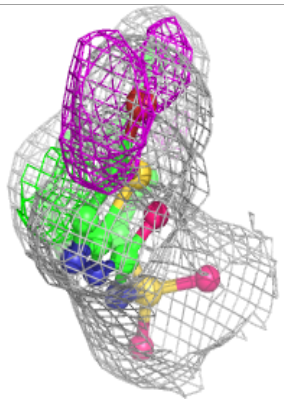


Electron density around RO8 G 1000:

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

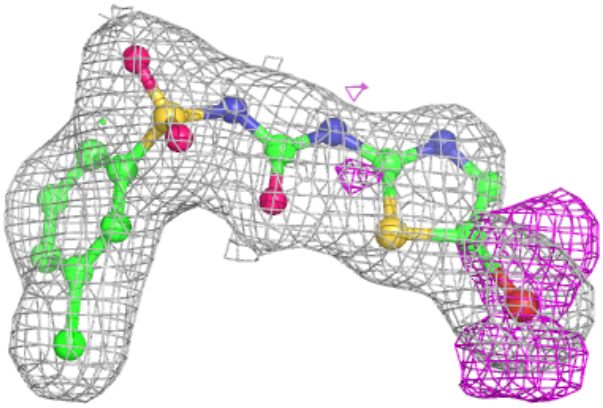


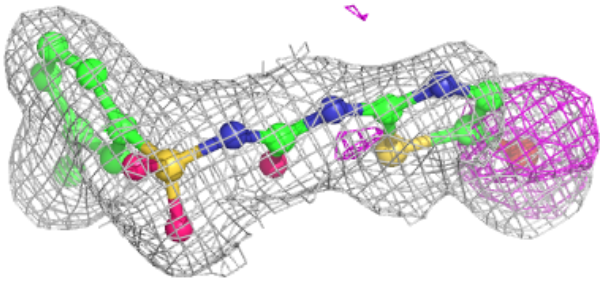


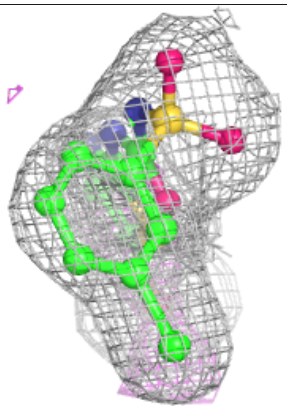


Electron density around RO8 C 1000:

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

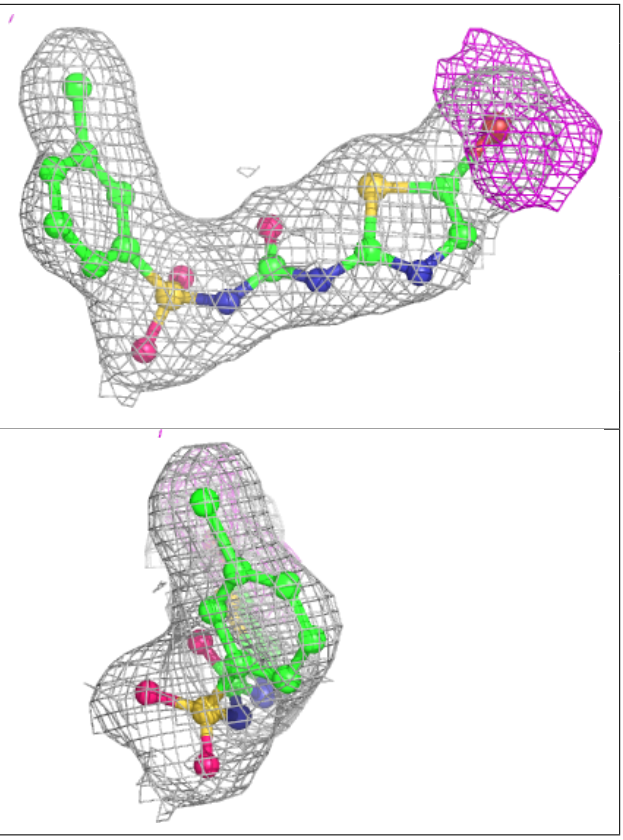


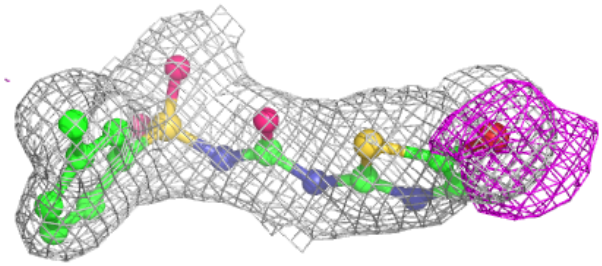




Electron density around RO8 D 1000:

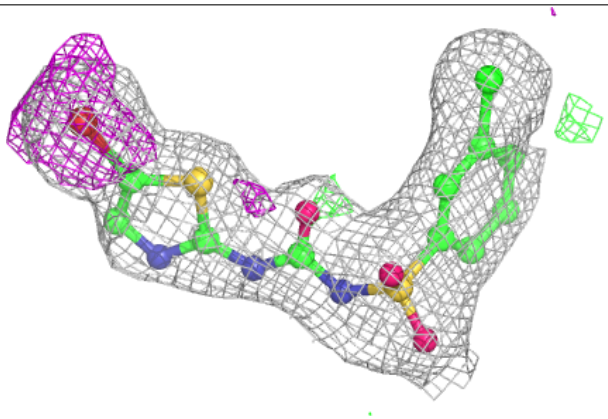
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

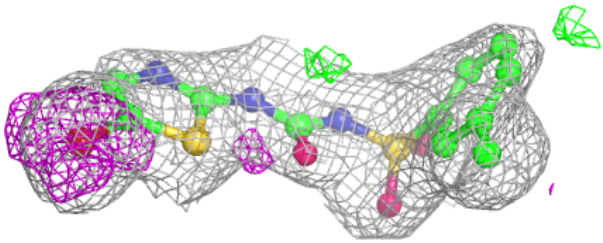


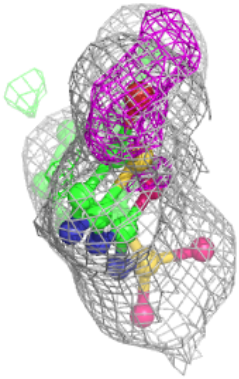


Electron density around RO8 E 1000:

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

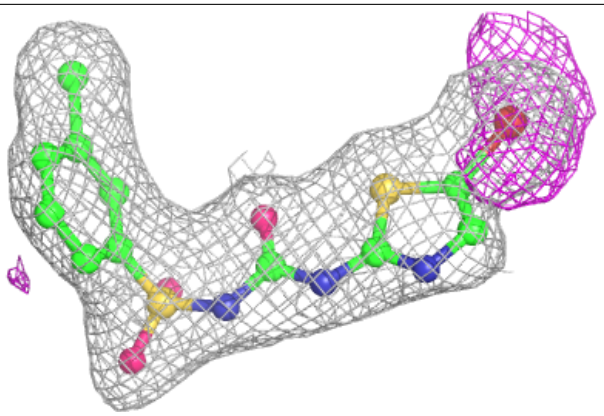


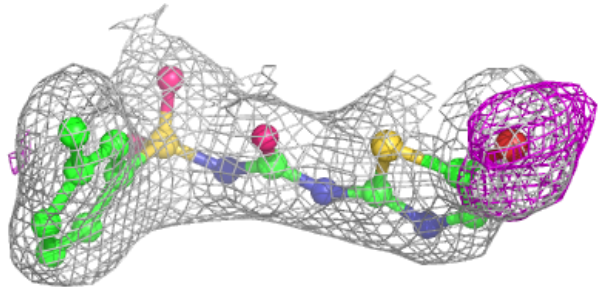


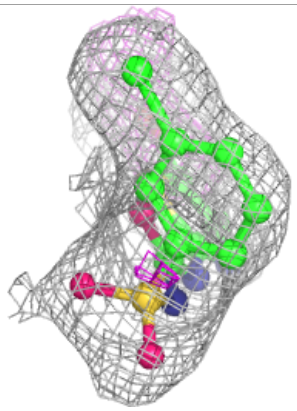


Electron density around RO8 B 1000:

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

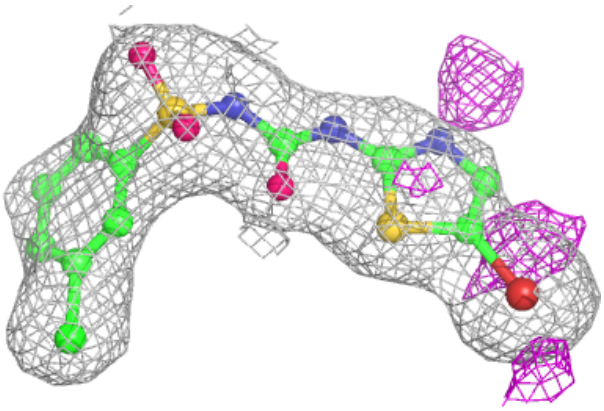


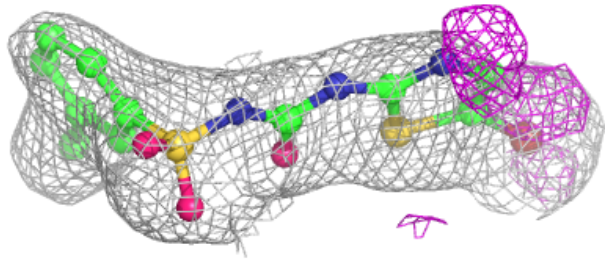


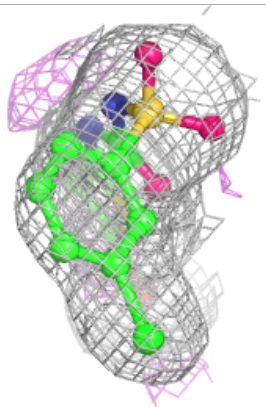


Electron density around RO8 F 1000:

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

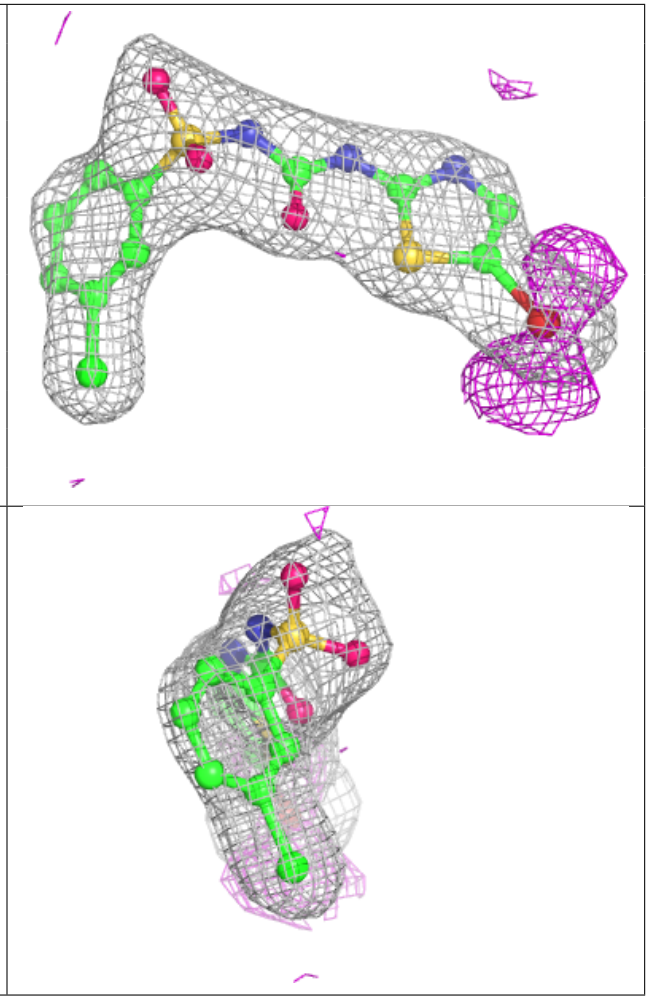






Electron density around RO8 H 1000:

$2mF_o$-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.