Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 01:40 AM EDT

PDB ID	:	1G3L
Title	:	THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). TDP-L-RHAMNOSE COMPLEX.
Authors	:	Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naismith, J.H.
Deposited on	:	2000-10-24
Resolution	:	2.70 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:

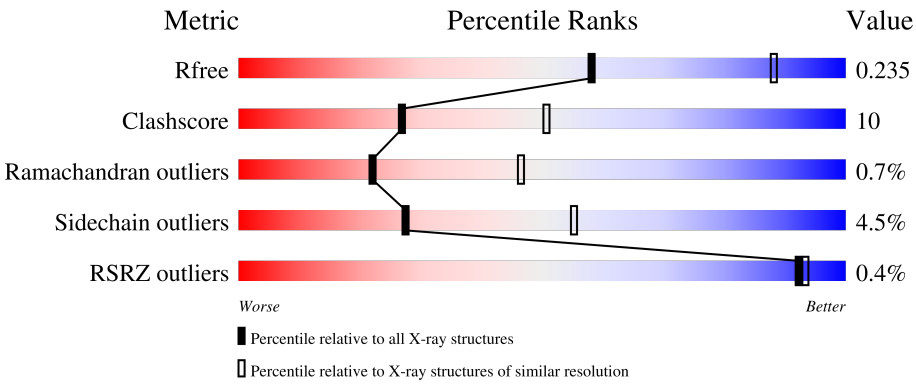
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	293	73% 25% •
1	B	293	% 77% 19% • •
1	C	293	78% 17% •
1	D	293	77% 19% • •

2 Entry composition (i)

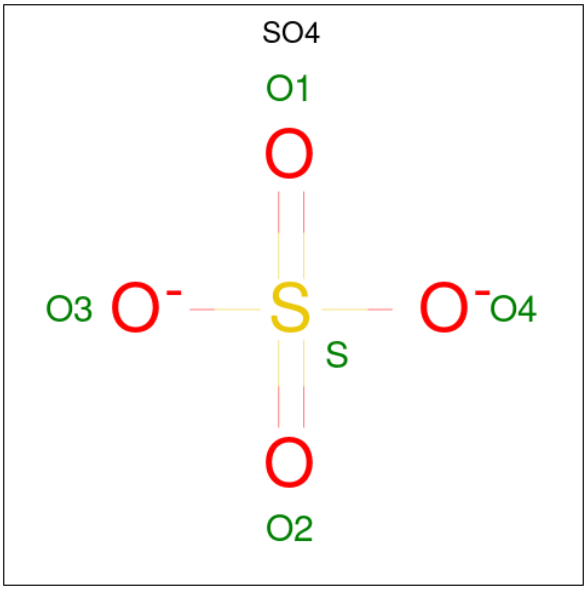
There are 3 unique types of molecules in this entry. The entry contains 9453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2285	1462	385	434	4	0	0	0
1	B	292	2285	1462	385	434	4	0	0	0
1	C	292	2285	1462	385	434	4	0	0	0
1	D	293	2293	1467	386	435	5	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0

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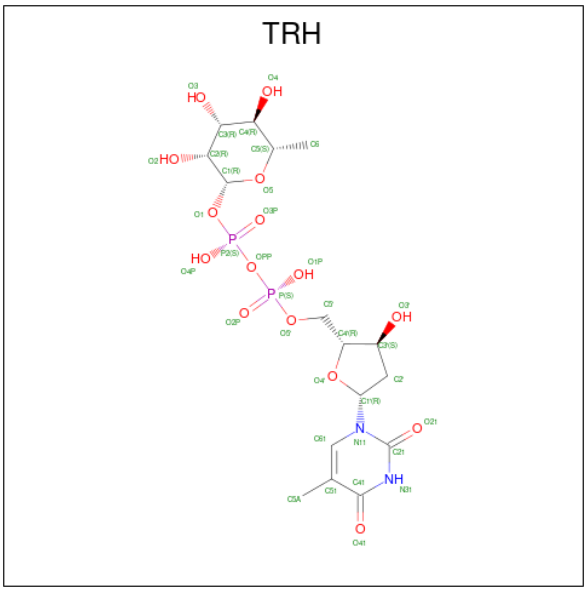
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0

- Molecule 3 is 2'-DEOXY-THYMIDINE-BETA-L-RHAMNOSE (three-letter code: TRH) (formula: $C_{16}H_{26}N_2O_{15}P_2$).



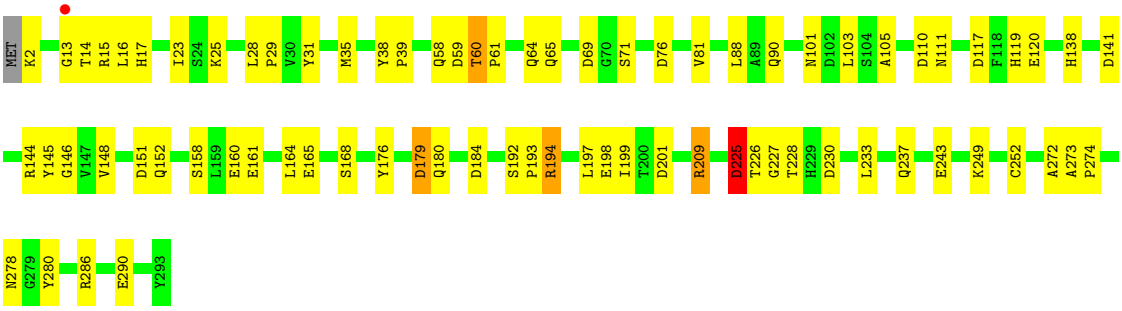
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	35	16	2	15	2	0	0
			Total	C	N	O	P		
3	A	1	35	16	2	15	2	0	0
			Total	C	N	O	P		
3	B	1	35	16	2	15	2	0	0
			Total	C	N	O	P		
3	B	1	35	16	2	15	2	0	0
			Total	C	N	O	P		
3	C	1	35	16	2	15	2	0	0
			Total	C	N	O	P		
3	C	1	35	16	2	15	2	0	0
			Total	C	N	O	P		
3	D	1	35	16	2	15	2	0	0
			Total	C	N	O	P		
3	D	1	35	16	2	15	2	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.

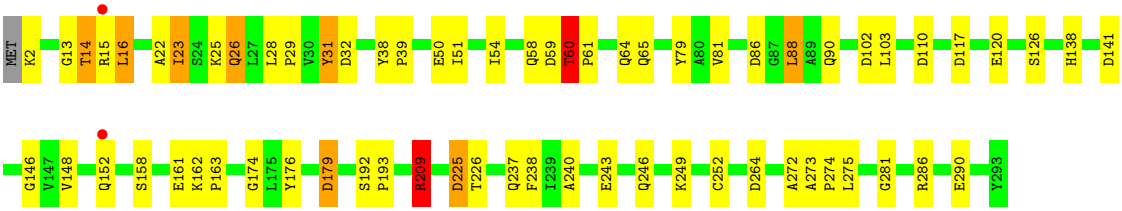
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain A:



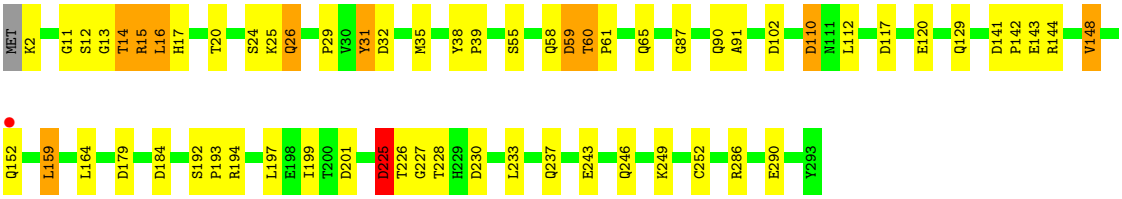
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



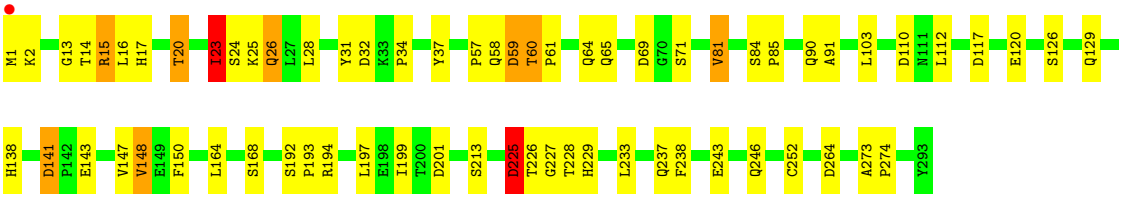
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain C:



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain D:


M1
K2
G13
T14
R15
L16
H17
T20
I23
S24
K25
Q26
L27
L28
Y31
D32
K33
P34
Y37
P57
Q58
D59
T60
P61
Q64
Q65
D69
G70
S71
V81
S84
P85
Q90
A91
L103
D110
N111
L112
D117
E120
S126
Q129
H138
D141
P142
E143
V147
V148
E149
F150
L164
S168
S192
P193
R194
L197
E198
I199
T200
D201
S213
D226
T226
G227
T228
H229
L233
Q237
F238
E243
Q246
C252
D264
A273
P274
Y293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.09Å 138.56Å 139.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 49.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.8 (100.00-2.70) 93.8 (49.82-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.81 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.230 0.213 , 0.235	Depositor DCC
R_{free} test set	1815 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9453	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9405e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: TRH, SO4

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	0.91	0/2335	1.01	10/3168 (0.3%)
1	B	0.89	1/2335 (0.0%)	1.02	12/3168 (0.4%)
1	C	0.86	0/2335	1.03	13/3168 (0.4%)
1	D	0.89	1/2343 (0.0%)	1.01	10/3178 (0.3%)
All	All	0.89	2/9348 (0.0%)	1.02	45/12682 (0.4%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ARG	CB-CG	-5.11	1.38	1.52
1	D	23	ILE	CA-CB	-5.03	1.43	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	102	ASP	CB-CG-OD2	8.76	126.18	118.30
1	C	59	ASP	CB-CG-OD2	7.28	124.85	118.30
1	A	184	ASP	CB-CG-OD2	7.07	124.67	118.30
1	B	59	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	225	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	152	GLN	CA-CB-CG	-6.77	98.51	113.40
1	C	110	ASP	CB-CG-OD2	6.64	124.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	184	ASP	CB-CG-OD2	6.62	124.26	118.30
1	D	59	ASP	CB-CG-OD2	6.51	124.16	118.30
1	D	117	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	209	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	209	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	201	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	152	GLN	CA-CB-CG	-6.04	100.12	113.40
1	A	76	ASP	CB-CG-OD2	5.98	123.69	118.30
1	D	110	ASP	CB-CG-OD2	5.95	123.65	118.30
1	D	201	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	179	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	102	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	141	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	15	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	110	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	194	ARG	CB-CA-C	-5.70	99.00	110.40
1	B	141	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	201	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	117	ASP	CB-CG-OD2	5.57	123.32	118.30
1	C	117	ASP	CB-CG-OD2	5.57	123.32	118.30
1	C	230	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	194	ARG	CB-CA-C	-5.49	99.43	110.40
1	D	225	ASP	CB-CA-C	5.48	121.36	110.40
1	C	194	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	117	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	16	LEU	CA-CB-CG	5.40	127.73	115.30
1	B	60	THR	OG1-CB-CG2	-5.34	97.72	110.00
1	B	179	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	194	ARG	CB-CA-C	-5.27	99.86	110.40
1	A	230	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	225	ASP	CB-CA-C	5.24	120.87	110.40
1	B	86	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	209	ARG	CB-CA-C	-5.13	100.14	110.40
1	D	141	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	59	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	264	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	159	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	D	15	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	HIS	Sidechain
1	A	17	HIS	Sidechain

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	2285	0	2272	50	0
1	B	2285	0	2272	49	0
1	C	2285	0	2272	55	0
1	D	2293	0	2284	56	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	70	0	48	1	0
3	B	70	0	48	0	0
3	C	70	0	48	3	0
3	D	70	0	48	1	0
All	All	9453	0	9292	192	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 10.

All (192) 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:B:120:GLU:N	1:B:120:GLU:OE1	2.07	0.88
1:C:58:GLN:HE22	1:D:65:GLN:HE22	1.23	0.84
1:C:141:ASP:OD2	1:C:144:ARG:HD3	1.78	0.83
1:D:120:GLU:N	1:D:120:GLU:OE1	2.17	0.78
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.66	0.78
1:C:58:GLN:NE2	1:D:65:GLN:HE22	1.81	0.78
1:C:26:GLN:NE2	1:C:26:GLN:H	1.82	0.77
1:A:237:GLN:OE1	1:B:237:GLN:NE2	2.17	0.76
1:D:26:GLN:HE21	1:D:26:GLN:H	1.32	0.75
1:A:13:GLY:O	1:A:16:LEU:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ASP:OD1	1:D:71:SER:OG	2.06	0.73
1:A:120:GLU:N	1:A:120:GLU:OE1	2.21	0.73
1:C:120:GLU:N	1:C:120:GLU:OE1	2.21	0.72
1:C:60:THR:HB	1:C:61:PRO:HD3	1.73	0.71
1:D:13:GLY:O	1:D:16:LEU:N	2.23	0.70
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.73	0.70
1:C:141:ASP:HB2	1:C:143:GLU:OE2	1.91	0.70
1:A:25:LYS:NZ	1:A:226:THR:O	2.24	0.69
1:B:88:LEU:N	1:B:88:LEU:HD23	2.08	0.68
1:C:26:GLN:H	1:C:26:GLN:HE21	1.41	0.67
1:B:60:THR:HG22	1:B:61:PRO:N	2.10	0.67
1:A:58:GLN:HE22	1:B:65:GLN:HE22	1.41	0.67
1:A:65:GLN:HE22	1:B:58:GLN:HE22	1.40	0.67
1:A:25:LYS:HE3	1:A:226:THR:O	1.96	0.66
1:C:2:LYS:O	1:C:2:LYS:HG3	1.96	0.65
1:D:26:GLN:H	1:D:26:GLN:NE2	1.94	0.65
1:B:13:GLY:O	1:B:14:THR:C	2.35	0.63
1:D:1:MET:N	1:D:129:GLN:HE21	1.97	0.63
1:D:25:LYS:HE3	1:D:226:THR:O	1.99	0.63
1:A:28:LEU:HD22	1:B:29:PRO:HD3	1.81	0.62
1:B:209:ARG:HG2	1:B:209:ARG:HH11	1.63	0.62
1:C:58:GLN:HE22	1:D:65:GLN:NE2	1.96	0.61
1:A:225:ASP:OD1	1:A:225:ASP:C	2.39	0.60
1:A:144:ARG:NH2	1:A:145:TYR:OH	2.34	0.60
1:A:60:THR:HB	1:A:61:PRO:HD3	1.84	0.60
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.82	0.60
1:D:1:MET:CE	1:D:103:LEU:HD21	2.31	0.59
1:A:25:LYS:CE	1:A:226:THR:O	2.51	0.59
1:D:25:LYS:NZ	1:D:226:THR:O	2.36	0.59
1:C:11:GLY:HA3	3:C:504:TRH:H2'1	1.85	0.58
1:B:64:GLN:HG2	1:B:79:TYR:CE1	2.39	0.58
1:D:25:LYS:CE	1:D:226:THR:O	2.51	0.58
1:A:23:ILE:HG12	1:B:23:ILE:HG12	1.86	0.58
1:A:13:GLY:O	1:A:14:THR:C	2.43	0.57
1:A:14:THR:O	1:A:15:ARG:C	2.40	0.57
1:C:60:THR:HG22	1:C:61:PRO:N	2.18	0.57
1:C:142:PRO:HD2	1:C:143:GLU:OE1	2.04	0.57
1:A:60:THR:HG22	1:A:61:PRO:N	2.15	0.56
1:B:192:SER:HB2	1:B:193:PRO:CD	2.36	0.56
1:C:60:THR:CB	1:C:61:PRO:HD3	2.35	0.56
1:A:101:ASN:O	1:A:180:GLN:NE2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD12	1:B:25:LYS:HD3	1.89	0.55
1:D:23:ILE:HD12	1:D:28:LEU:HD21	1.87	0.55
1:A:69:ASP:OD1	1:A:71:SER:OG	2.15	0.55
1:B:23:ILE:HD12	1:B:23:ILE:H	1.72	0.55
1:D:13:GLY:O	1:D:14:THR:C	2.44	0.55
1:D:1:MET:HE3	1:D:103:LEU:HD21	1.88	0.54
1:C:25:LYS:HE2	1:C:110:ASP:HB2	1.89	0.54
1:C:129:GLN:N	2:C:703:SO4:O4	2.39	0.54
1:A:110:ASP:OD2	3:A:500:TRH:O3'	2.16	0.53
1:C:179:ASP:OD1	1:C:179:ASP:C	2.46	0.53
1:C:29:PRO:HD3	1:D:28:LEU:HD22	1.92	0.53
1:D:60:THR:HG23	1:D:64:GLN:OE1	2.08	0.52
1:C:24:SER:HB3	1:C:26:GLN:HE22	1.73	0.52
1:D:60:THR:HG22	1:D:61:PRO:N	2.23	0.52
1:B:179:ASP:OD1	1:B:179:ASP:C	2.48	0.52
1:D:32:ASP:OD2	1:D:243:GLU:OE1	2.28	0.52
1:B:243:GLU:HG2	1:B:249:LYS:HA	1.92	0.52
1:C:225:ASP:OD1	1:C:225:ASP:C	2.48	0.52
1:A:65:GLN:NE2	1:B:58:GLN:HE22	2.06	0.52
1:D:1:MET:HB2	1:D:103:LEU:HD11	1.92	0.52
1:D:129:GLN:N	2:D:704:SO4:O1	2.23	0.52
1:C:14:THR:O	1:C:15:ARG:O	2.28	0.52
1:C:14:THR:O	1:C:15:ARG:C	2.47	0.52
1:C:31:TYR:CE1	1:D:229:HIS:HB3	2.46	0.51
1:C:112:LEU:C	1:C:112:LEU:HD23	2.30	0.51
1:A:286:ARG:NH1	1:A:290:GLU:OE1	2.40	0.51
1:B:14:THR:O	1:B:15:ARG:C	2.49	0.51
1:B:138:HIS:ND1	1:D:246:GLN:O	2.43	0.51
1:C:38:TYR:HB2	1:C:39:PRO:CD	2.40	0.51
1:B:225:ASP:C	1:B:225:ASP:OD1	2.49	0.51
1:A:2:LYS:O	1:A:2:LYS:HG3	2.09	0.51
1:D:273:ALA:N	1:D:274:PRO:CD	2.74	0.51
1:B:103:LEU:HD23	1:B:179:ASP:HA	1.93	0.51
1:C:25:LYS:HE2	1:C:110:ASP:CB	2.41	0.50
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.93	0.50
1:A:278:ASN:OD1	1:A:280:TYR:N	2.45	0.50
1:D:141:ASP:HB3	1:D:143:GLU:OE2	2.11	0.50
1:A:38:TYR:HB2	1:A:39:PRO:CD	2.43	0.49
1:A:194:ARG:NH2	1:A:198:GLU:OE1	2.41	0.49
1:D:24:SER:OG	1:D:59:ASP:OD2	2.17	0.49
1:A:273:ALA:N	1:A:274:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:H3	1:D:129:GLN:HE21	1.61	0.49
1:C:13:GLY:O	1:C:14:THR:C	2.49	0.48
1:A:29:PRO:HD3	1:B:28:LEU:HD22	1.96	0.48
1:D:60:THR:N	1:D:61:PRO:HD2	2.29	0.48
1:C:60:THR:CB	1:C:61:PRO:CD	2.91	0.48
1:A:272:ALA:O	1:A:273:ALA:C	2.52	0.48
1:C:227:GLY:C	1:C:228:THR:CG2	2.81	0.48
1:D:112:LEU:C	1:D:112:LEU:HD23	2.34	0.48
1:B:2:LYS:HG3	1:B:2:LYS:O	2.12	0.47
1:B:162:LYS:N	1:B:163:PRO:CD	2.77	0.47
1:A:227:GLY:O	1:A:228:THR:HG22	2.14	0.47
1:B:146:GLY:HA2	1:B:161:GLU:HA	1.96	0.47
1:A:164:LEU:C	1:A:165:GLU:HG2	2.34	0.47
1:B:246:GLN:O	1:D:138:HIS:ND1	2.41	0.47
1:D:60:THR:N	1:D:61:PRO:CD	2.77	0.47
1:D:164:LEU:HD23	1:D:164:LEU:HA	1.83	0.47
1:B:50:GLU:C	1:B:51:ILE:HG13	2.35	0.47
1:B:23:ILE:HD12	1:B:23:ILE:N	2.31	0.46
1:C:60:THR:O	1:C:61:PRO:C	2.52	0.46
1:A:105:ALA:HA	1:A:176:TYR:O	2.15	0.46
1:A:35:MET:SD	1:A:110:ASP:HA	2.55	0.46
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.48	0.46
1:A:25:LYS:HZ2	1:A:226:THR:C	2.19	0.46
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.98	0.46
1:A:103:LEU:HD23	1:A:179:ASP:HA	1.98	0.46
1:B:209:ARG:HG2	1:B:209:ARG:NH1	2.30	0.45
1:A:60:THR:CB	1:A:61:PRO:HD3	2.45	0.45
1:C:233:LEU:HA	1:C:233:LEU:HD12	1.57	0.45
1:D:90:GLN:O	1:D:91:ALA:C	2.54	0.45
1:C:24:SER:OG	1:C:59:ASP:OD2	2.24	0.45
1:C:90:GLN:HG3	1:C:197:LEU:HD12	1.99	0.44
1:D:225:ASP:OD1	1:D:225:ASP:C	2.55	0.44
1:B:60:THR:N	1:B:61:PRO:HD2	2.32	0.44
1:A:243:GLU:HG2	1:A:249:LYS:HA	1.99	0.44
1:D:1:MET:HB2	1:D:103:LEU:CD1	2.48	0.44
1:A:60:THR:CG2	1:A:64:GLN:NE2	2.81	0.44
1:B:174:GLY:HA2	1:B:176:TYR:CZ	2.53	0.44
1:D:90:GLN:HG3	1:D:197:LEU:HD12	1.99	0.44
1:B:275:LEU:O	1:B:281:GLY:HA3	2.18	0.44
1:A:16:LEU:HD12	1:A:25:LYS:HD2	1.99	0.44
1:D:17:HIS:HD2	1:D:20:THR:OG1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:506:TRH:O5'	3:D:506:TRH:H2'2	2.18	0.44
1:B:32:ASP:OD2	1:B:243:GLU:OE1	2.35	0.43
1:C:35:MET:O	1:C:39:PRO:HD2	2.17	0.43
1:D:227:GLY:C	1:D:228:THR:CG2	2.85	0.43
1:D:14:THR:O	1:D:15:ARG:C	2.55	0.43
1:A:88:LEU:N	1:A:88:LEU:HD23	2.33	0.43
1:B:272:ALA:O	1:B:273:ALA:C	2.55	0.43
1:C:65:GLN:HE22	1:D:58:GLN:HE22	1.66	0.43
1:B:22:ALA:C	1:B:23:ILE:HG13	2.39	0.43
1:C:286:ARG:NH1	1:C:290:GLU:OE1	2.45	0.43
1:D:228:THR:O	1:D:229:HIS:C	2.57	0.43
1:B:31:TYR:CD1	1:B:240:ALA:HB2	2.53	0.42
1:B:38:TYR:HB2	1:B:39:PRO:CD	2.49	0.42
1:B:60:THR:CB	1:B:61:PRO:HD3	2.49	0.42
1:C:87:GLY:HA2	3:C:504:TRH:HCA2	2.00	0.42
1:B:238:PHE:CE1	1:D:238:PHE:CE1	3.07	0.42
1:C:24:SER:HB3	1:C:26:GLN:NE2	2.33	0.42
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.93	0.42
1:C:192:SER:HB2	1:C:193:PRO:HD2	2.01	0.42
1:D:192:SER:HB2	1:D:193:PRO:CD	2.50	0.42
1:B:16:LEU:CD1	1:B:25:LYS:HD3	2.49	0.42
1:D:57:PRO:HA	1:D:81:VAL:HG22	2.01	0.42
1:D:84:SER:HA	1:D:85:PRO:HD3	1.93	0.42
1:A:90:GLN:HG3	1:A:197:LEU:HD12	2.01	0.42
1:C:237:GLN:HE22	1:D:237:GLN:HE21	1.68	0.42
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.45	0.42
1:A:138:HIS:ND1	1:C:246:GLN:O	2.47	0.42
1:A:199:ILE:HD12	1:A:199:ILE:HA	1.89	0.42
1:C:35:MET:SD	1:C:110:ASP:HA	2.59	0.42
1:D:1:MET:N	1:D:129:GLN:NE2	2.66	0.42
1:B:286:ARG:NH1	1:B:290:GLU:OE1	2.52	0.41
1:C:11:GLY:HA3	3:C:504:TRH:C2'	2.49	0.41
1:C:199:ILE:HD12	1:C:199:ILE:HA	1.91	0.41
1:D:60:THR:CG2	1:D:64:GLN:OE1	2.69	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.77	0.41
1:C:58:GLN:O	1:C:58:GLN:HG2	2.20	0.41
1:A:146:GLY:HA2	1:A:161:GLU:HA	2.03	0.41
1:A:151:ASP:OD1	1:A:151:ASP:C	2.59	0.41
1:B:26:GLN:HE21	1:B:26:GLN:HB2	1.55	0.41
1:D:148:VAL:HG22	1:D:150:PHE:CE1	2.55	0.41
1:C:148:VAL:HB	1:C:159:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:HD12	1:D:233:LEU:HA	1.70	0.41
1:D:199:ILE:HD12	1:D:199:ILE:HA	1.88	0.41
1:C:32:ASP:OD2	1:C:243:GLU:OE1	2.38	0.41
1:C:60:THR:N	1:C:61:PRO:CD	2.83	0.41
1:A:209:ARG:HH11	1:A:209:ARG:HD3	1.70	0.41
1:D:34:PRO:O	1:D:37:TYR:HB2	2.21	0.41
1:B:25:LYS:NZ	1:B:226:THR:O	2.46	0.40
1:B:264:ASP:C	1:B:264:ASP:OD1	2.59	0.40
1:C:243:GLU:HG2	1:C:249:LYS:HA	2.01	0.40
1:C:26:GLN:NE2	1:C:26:GLN:N	2.61	0.40
1:C:90:GLN:O	1:C:91:ALA:C	2.57	0.40
1:B:23:ILE:N	1:B:23:ILE:CD1	2.82	0.40
1:C:17:HIS:HD2	1:C:20:THR:OG1	2.05	0.40
1:C:25:LYS:NZ	1:C:226:THR:O	2.49	0.40
1:C:65:GLN:HE22	1:D:58:GLN:NE2	2.20	0.40
1:D:147:VAL:HG12	1:D:148:VAL:N	2.37	0.40
1:A:227:GLY:C	1:A:228:THR:CG2	2.87	0.40
1:B:54:ILE:HG21	1:B:54:ILE:HD13	1.83	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	290/293 (99%)	278 (96%)	11 (4%)	1 (0%)	41 66
1	B	290/293 (99%)	279 (96%)	9 (3%)	2 (1%)	22 46
1	C	290/293 (99%)	277 (96%)	9 (3%)	4 (1%)	11 28
1	D	291/293 (99%)	281 (97%)	9 (3%)	1 (0%)	41 66
All	All	1161/1172 (99%)	1115 (96%)	38 (3%)	8 (1%)	22 46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	16	LEU
1	B	31	TYR
1	C	31	TYR
1	A	31	TYR
1	B	16	LEU
1	C	12	SER
1	D	31	TYR

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	239/240 (100%)	228 (95%)	11 (5%)	27	54
1	B	239/240 (100%)	226 (95%)	13 (5%)	22	47
1	C	239/240 (100%)	232 (97%)	7 (3%)	42	71
1	D	240/240 (100%)	228 (95%)	12 (5%)	24	51
All	All	957/960 (100%)	914 (96%)	43 (4%)	27	55

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	81	VAL
1	A	111	ASN
1	A	148	VAL
1	A	152	GLN
1	A	158	SER
1	A	160	GLU
1	A	168	SER
1	A	209	ARG
1	A	225	ASP
1	A	252	CYS
1	B	14	THR
1	B	23	ILE
1	B	26	GLN

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Mol	Chain	Res	Type
1	B	60	THR
1	B	81	VAL
1	B	88	LEU
1	B	90	GLN
1	B	126	SER
1	B	148	VAL
1	B	158	SER
1	B	209	ARG
1	B	225	ASP
1	B	252	CYS
1	C	14	THR
1	C	26	GLN
1	C	55	SER
1	C	60	THR
1	C	148	VAL
1	C	225	ASP
1	C	252	CYS
1	D	2	LYS
1	D	20	THR
1	D	23	ILE
1	D	26	GLN
1	D	60	THR
1	D	81	VAL
1	D	126	SER
1	D	148	VAL
1	D	168	SER
1	D	213	SER
1	D	225	ASP
1	D	252	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	B	17	HIS
1	B	26	GLN
1	B	58	GLN
1	B	116	HIS
1	C	17	HIS
1	C	26	GLN
1	C	58	GLN
1	C	65	GLN

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Mol	Chain	Res	Type
1	D	17	HIS
1	D	26	GLN
1	D	129	GLN
1	D	237	GLN

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)

13 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	SO4	B	702	-	4,4,4	0.17	0	6,6,6	0.77	0
2	SO4	C	703	-	4,4,4	0.20	0	6,6,6	0.80	0
3	TRH	C	505	-	34,37,37	2.18	9 (26%)	52,57,57	4.14	25 (48%)
3	TRH	D	507	-	34,37,37	2.01	9 (26%)	52,57,57	3.67	18 (34%)
3	TRH	A	500	-	34,37,37	2.16	11 (32%)	52,57,57	3.44	24 (46%)
3	TRH	B	503	-	34,37,37	1.97	10 (29%)	52,57,57	4.21	23 (44%)
3	TRH	C	504	-	34,37,37	2.01	9 (26%)	52,57,57	4.21	26 (50%)
2	SO4	D	704	-	4,4,4	0.23	0	6,6,6	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TRH	A	501	-	34,37,37	1.98	10 (29%)	52,57,57	3.80	20 (38%)
3	TRH	D	506	-	34,37,37	1.87	9 (26%)	52,57,57	3.79	21 (40%)
3	TRH	B	502	-	34,37,37	1.99	7 (20%)	52,57,57	3.95	25 (48%)
2	SO4	A	701	-	4,4,4	0.28	0	6,6,6	0.84	0
2	SO4	B	700	-	4,4,4	0.30	0	6,6,6	0.90	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
3	TRH	C	505	-	-	4/21/53/53	0/3/3/3
3	TRH	D	507	-	-	4/21/53/53	0/3/3/3
3	TRH	A	500	-	-	5/21/53/53	0/3/3/3
3	TRH	B	503	-	-	4/21/53/53	0/3/3/3
3	TRH	C	504	-	-	6/21/53/53	0/3/3/3
3	TRH	A	501	-	-	5/21/53/53	0/3/3/3
3	TRH	D	506	-	-	2/21/53/53	0/3/3/3
3	TRH	B	502	-	-	5/21/53/53	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	TRH	O41-C41	6.21	1.35	1.23
3	A	500	TRH	O41-C41	5.80	1.34	1.23
3	C	504	TRH	O41-C41	5.54	1.34	1.23
3	A	501	TRH	O21-C21	5.43	1.33	1.23
3	C	505	TRH	O21-C21	5.41	1.32	1.23
3	D	507	TRH	O21-C21	5.41	1.32	1.23
3	C	505	TRH	C41-C51	-5.31	1.36	1.44
3	A	500	TRH	C41-C51	-5.07	1.36	1.44
3	B	502	TRH	C41-C51	-5.04	1.36	1.44
3	C	504	TRH	O21-C21	4.91	1.32	1.23
3	C	505	TRH	O41-C41	4.87	1.32	1.23
3	A	501	TRH	O41-C41	4.85	1.32	1.23
3	B	503	TRH	C41-C51	-4.82	1.36	1.44
3	B	503	TRH	O21-C21	4.74	1.31	1.23
3	D	506	TRH	O41-C41	4.58	1.32	1.23
3	D	507	TRH	O41-C41	4.57	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	TRH	C41-C51	-4.50	1.37	1.44
3	A	501	TRH	C41-C51	-4.41	1.37	1.44
3	C	505	TRH	C61-N11	-4.40	1.30	1.38
3	A	500	TRH	O21-C21	4.40	1.31	1.23
3	B	502	TRH	O21-C21	4.39	1.31	1.23
3	D	506	TRH	C41-C51	-4.38	1.37	1.44
3	B	503	TRH	O41-C41	4.36	1.31	1.23
3	D	506	TRH	O21-C21	4.35	1.31	1.23
3	A	500	TRH	O5-C5	-4.00	1.35	1.44
3	C	504	TRH	C61-C51	3.72	1.40	1.34
3	A	500	TRH	C21-N11	-3.51	1.32	1.38
3	C	505	TRH	C21-N31	-3.34	1.32	1.38
3	B	503	TRH	C61-N11	-3.32	1.32	1.38
3	D	507	TRH	C21-N31	-3.25	1.32	1.38
3	C	505	TRH	P2-O3P	3.22	1.62	1.50
3	C	504	TRH	C41-N31	-3.20	1.32	1.38
3	D	507	TRH	P2-O3P	3.19	1.62	1.50
3	A	501	TRH	C41-N31	-3.09	1.33	1.38
3	D	507	TRH	C41-N31	-3.04	1.33	1.38
3	C	504	TRH	C41-C51	-3.02	1.39	1.44
3	C	505	TRH	O4'-C4'	-3.01	1.38	1.45
3	A	500	TRH	C61-N11	-2.98	1.33	1.38
3	D	507	TRH	P-O2P	2.97	1.61	1.50
3	B	502	TRH	C61-N11	-2.94	1.33	1.38
3	D	506	TRH	C61-N11	-2.93	1.33	1.38
3	B	502	TRH	P-O2P	2.87	1.61	1.50
3	B	503	TRH	C61-C51	2.82	1.39	1.34
3	B	503	TRH	C41-N31	-2.80	1.33	1.38
3	B	502	TRH	C21-N31	-2.79	1.33	1.38
3	C	504	TRH	P-O2P	2.78	1.60	1.50
3	C	504	TRH	P2-O3P	2.77	1.60	1.50
3	D	506	TRH	C21-N31	-2.71	1.33	1.38
3	A	501	TRH	P-O2P	2.71	1.60	1.50
3	A	500	TRH	P2-O3P	2.70	1.60	1.50
3	B	503	TRH	P-O2P	2.69	1.60	1.50
3	A	501	TRH	C61-C51	2.63	1.38	1.34
3	A	501	TRH	C21-N31	-2.57	1.33	1.38
3	A	500	TRH	C21-N31	-2.52	1.33	1.38
3	C	504	TRH	O4'-C4'	-2.51	1.39	1.45
3	B	502	TRH	P2-O3P	2.51	1.59	1.50
3	A	501	TRH	P2-O3P	2.47	1.59	1.50
3	D	506	TRH	C2'-C3'	-2.41	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	TRH	C61-N11	-2.37	1.34	1.38
3	C	504	TRH	C21-N11	-2.34	1.34	1.38
3	A	500	TRH	P-O2P	2.30	1.59	1.50
3	D	506	TRH	O4'-C4'	-2.29	1.39	1.45
3	A	501	TRH	C61-N11	-2.26	1.34	1.38
3	A	500	TRH	O4'-C4'	-2.26	1.39	1.45
3	A	500	TRH	C41-N31	-2.26	1.34	1.38
3	C	505	TRH	C41-N31	-2.25	1.34	1.38
3	B	503	TRH	O4'-C4'	-2.25	1.40	1.45
3	B	503	TRH	C21-N31	-2.21	1.34	1.38
3	B	503	TRH	C3'-C4'	-2.14	1.47	1.53
3	D	507	TRH	O4'-C4'	-2.11	1.40	1.45
3	D	506	TRH	C41-N31	-2.10	1.34	1.38
3	D	506	TRH	C61-C51	2.07	1.38	1.34
3	A	501	TRH	O4'-C4'	-2.06	1.40	1.45
3	C	505	TRH	P2-O1	-2.03	1.55	1.60

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	TRH	O5-C1-O1	-18.69	86.94	111.36
3	B	502	TRH	O5-C1-O1	-18.31	87.43	111.36
3	C	505	TRH	O5-C1-O1	-17.92	87.94	111.36
3	A	501	TRH	O5-C1-O1	-16.41	89.92	111.36
3	C	504	TRH	O5-C1-O1	-16.31	90.05	111.36
3	D	506	TRH	O5-C1-O1	-15.95	90.52	111.36
3	D	507	TRH	O5-C1-O1	-14.67	92.19	111.36
3	C	504	TRH	C1-O5-C5	-13.82	89.90	113.67
3	C	505	TRH	C1-O5-C5	-13.52	90.42	113.67
3	B	503	TRH	C1-O5-C5	-12.01	93.02	113.67
3	D	507	TRH	C1-O5-C5	-11.89	93.22	113.67
3	A	501	TRH	C1-O5-C5	-11.27	94.29	113.67
3	B	502	TRH	C1-O5-C5	-11.22	94.37	113.67
3	A	500	TRH	O5-C1-O1	10.77	125.44	111.36
3	D	506	TRH	C1-O5-C5	-9.72	96.96	113.67
3	B	503	TRH	O4'-C1'-C2'	-9.14	88.97	106.25
3	C	504	TRH	O4'-C1'-N11	9.00	123.94	107.86
3	D	507	TRH	O4'-C1'-C2'	-8.73	89.76	106.25
3	D	506	TRH	O4'-C1'-C2'	-8.61	89.98	106.25
3	B	502	TRH	O4'-C1'-C2'	-8.39	90.39	106.25
3	A	500	TRH	O41-C41-C51	-8.23	115.36	124.90
3	A	500	TRH	O5-C5-C4	-7.44	96.17	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	TRH	O4'-C1'-C2'	-7.01	93.00	106.25
3	D	507	TRH	C51-C41-N31	6.86	121.17	115.31
3	B	503	TRH	O41-C41-C51	-6.78	117.04	124.90
3	A	500	TRH	C41-N31-C21	-6.56	118.85	127.35
3	D	506	TRH	C41-N31-C21	-6.28	119.22	127.35
3	C	504	TRH	N31-C21-N11	6.19	123.10	114.89
3	D	506	TRH	O41-C41-C51	-6.18	117.74	124.90
3	C	505	TRH	C41-N31-C21	-6.10	119.45	127.35
3	C	505	TRH	O41-C41-C51	-6.02	117.92	124.90
3	A	500	TRH	C51-C41-N31	6.01	120.44	115.31
3	B	503	TRH	C41-N31-C21	-6.00	119.58	127.35
3	A	500	TRH	O4'-C1'-C2'	-5.88	95.13	106.25
3	C	504	TRH	C4'-O4'-C1'	5.87	123.64	109.45
3	A	501	TRH	C4'-O4'-C1'	5.87	123.64	109.45
3	C	505	TRH	C51-C41-N31	5.79	120.26	115.31
3	A	501	TRH	C41-N31-C21	-5.67	120.01	127.35
3	B	503	TRH	N31-C21-N11	5.64	122.38	114.89
3	C	505	TRH	O4'-C1'-C2'	-5.63	95.61	106.25
3	B	502	TRH	C41-N31-C21	-5.61	120.09	127.35
3	D	507	TRH	C41-N31-C21	-5.55	120.16	127.35
3	C	504	TRH	O4'-C1'-C2'	-5.53	95.81	106.25
3	B	502	TRH	O41-C41-C51	-5.48	118.55	124.90
3	B	503	TRH	C4'-O4'-C1'	5.47	122.67	109.45
3	B	503	TRH	C51-C41-N31	5.45	119.96	115.31
3	D	506	TRH	C51-C41-N31	5.40	119.92	115.31
3	A	501	TRH	N31-C21-N11	5.40	122.05	114.89
3	A	501	TRH	O41-C41-C51	-5.29	118.77	124.90
3	D	507	TRH	C51-C61-N11	-5.29	117.90	123.34
3	C	504	TRH	O21-C21-N11	-5.25	115.80	122.79
3	D	506	TRH	N31-C21-N11	5.23	121.83	114.89
3	C	505	TRH	O5-C5-C6	5.09	117.69	106.70
3	C	504	TRH	C41-N31-C21	-5.07	120.78	127.35
3	B	502	TRH	N31-C21-N11	5.07	121.62	114.89
3	A	501	TRH	C51-C41-N31	5.04	119.61	115.31
3	C	504	TRH	O1-C1-C2	4.98	117.50	108.38
3	B	503	TRH	C4-C3-C2	-4.90	102.26	110.82
3	A	500	TRH	C51-C61-N11	-4.86	118.33	123.34
3	A	501	TRH	C6-C5-C4	-4.82	104.17	113.07
3	B	503	TRH	C6-C5-C4	-4.75	104.30	113.07
3	D	506	TRH	O4'-C4'-C5'	-4.68	93.99	109.37
3	C	505	TRH	C6-C5-C4	-4.67	104.43	113.07
3	A	501	TRH	C51-C61-N11	-4.61	118.60	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	TRH	O4'-C1'-N11	4.55	115.99	107.86
3	A	500	TRH	N31-C21-N11	4.49	120.85	114.89
3	A	500	TRH	O5-C1-C2	-4.39	101.05	110.35
3	A	500	TRH	C4'-O4'-C1'	4.39	120.05	109.45
3	C	505	TRH	C4-C3-C2	-4.38	103.18	110.82
3	C	505	TRH	C4'-O4'-C1'	4.36	119.99	109.45
3	A	500	TRH	O21-C21-N11	-4.32	117.05	122.79
3	C	505	TRH	C51-C61-N11	-4.31	118.91	123.34
3	D	507	TRH	O41-C41-C51	-4.30	119.92	124.90
3	C	504	TRH	O5-C5-C6	4.27	115.92	106.70
3	A	500	TRH	C1-O5-C5	4.25	120.98	113.67
3	A	500	TRH	C6-C5-C4	4.22	120.86	113.07
3	C	504	TRH	C51-C41-N31	4.21	118.90	115.31
3	D	506	TRH	C51-C61-N11	-4.20	119.02	123.34
3	B	502	TRH	C1'-N11-C21	4.20	125.91	117.64
3	B	502	TRH	C51-C41-N31	4.19	118.89	115.31
3	B	502	TRH	C4'-O4'-C1'	4.00	119.12	109.45
3	D	507	TRH	O4'-C1'-N11	3.96	114.93	107.86
3	B	502	TRH	O5-C5-C6	3.95	115.22	106.70
3	A	500	TRH	O4'-C4'-C5'	-3.94	96.42	109.37
3	D	506	TRH	C1'-N11-C21	3.87	125.26	117.64
3	D	506	TRH	O4'-C1'-N11	3.83	114.72	107.86
3	C	504	TRH	C51-C61-N11	-3.82	119.41	123.34
3	D	507	TRH	C4'-O4'-C1'	3.82	118.67	109.45
3	C	504	TRH	P-OPP-P2	-3.80	119.78	132.83
3	B	503	TRH	O4'-C1'-N11	3.78	114.61	107.86
3	D	506	TRH	C4'-O4'-C1'	3.77	118.57	109.45
3	C	504	TRH	C6-C5-C4	-3.73	106.19	113.07
3	C	505	TRH	N31-C21-N11	3.73	119.84	114.89
3	D	507	TRH	N31-C21-N11	3.72	119.83	114.89
3	C	504	TRH	O4'-C4'-C3'	-3.63	97.21	105.67
3	D	507	TRH	O4'-C4'-C3'	-3.59	97.29	105.67
3	D	506	TRH	C1'-N11-C61	-3.56	114.64	120.77
3	B	502	TRH	C5A-C51-C61	-3.53	118.13	122.85
3	D	507	TRH	O4'-C4'-C5'	-3.47	97.94	109.37
3	A	500	TRH	P2-O1-C1	3.41	132.93	119.74
3	D	506	TRH	O4-C4-C5	3.40	117.21	109.67
3	D	507	TRH	O5-C5-C6	3.38	114.00	106.70
3	B	502	TRH	C1'-N11-C61	-3.38	114.95	120.77
3	B	503	TRH	O5-C5-C6	3.33	113.88	106.70
3	A	500	TRH	C1'-N11-C61	-3.31	115.07	120.77
3	A	500	TRH	O4-C4-C5	-3.28	102.39	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	507	TRH	O4-C4-C3	-3.24	102.87	110.35
3	C	504	TRH	O41-C41-C51	-3.23	121.16	124.90
3	A	501	TRH	O21-C21-N31	-3.17	115.60	121.50
3	C	505	TRH	P-OPP-P2	-3.16	121.97	132.83
3	C	505	TRH	O5'-C5'-C4'	-3.16	98.11	108.99
3	A	501	TRH	C61-C51-C41	3.05	120.58	118.03
3	C	505	TRH	O3-C3-C4	-3.03	103.33	110.35
3	B	502	TRH	P-OPP-P2	-3.02	122.47	132.83
3	C	504	TRH	C4-C3-C2	-3.02	105.56	110.82
3	D	506	TRH	O21-C21-N31	-3.01	115.89	121.50
3	C	505	TRH	O4'-C4'-C5'	-2.99	99.55	109.37
3	B	503	TRH	O4'-C4'-C5'	-2.97	99.61	109.37
3	C	504	TRH	C61-N11-C21	-2.96	118.30	121.30
3	C	504	TRH	C3'-C2'-C1'	2.95	109.93	102.54
3	C	505	TRH	C5A-C51-C61	-2.93	118.94	122.85
3	B	502	TRH	C5A-C51-C41	2.93	121.99	118.77
3	B	503	TRH	P-OPP-P2	-2.89	122.92	132.83
3	C	505	TRH	O1P-P-O2P	2.87	126.42	112.24
3	B	503	TRH	O5'-P-O2P	-2.85	97.93	109.07
3	A	501	TRH	O5-C5-C6	2.83	112.82	106.70
3	D	507	TRH	P-OPP-P2	-2.81	123.19	132.83
3	C	505	TRH	C1'-N11-C61	-2.78	115.99	120.77
3	C	504	TRH	O5-C1-C2	2.76	116.20	110.35
3	C	504	TRH	C1'-N11-C61	2.73	125.48	120.77
3	B	502	TRH	C51-C61-N11	-2.73	120.53	123.34
3	D	506	TRH	P-OPP-P2	-2.71	123.53	132.83
3	B	503	TRH	C61-N11-C21	-2.70	118.56	121.30
3	B	503	TRH	C51-C61-N11	-2.68	120.58	123.34
3	D	506	TRH	O5-C5-C6	2.66	112.44	106.70
3	B	502	TRH	O1-C1-C2	2.66	113.25	108.38
3	B	503	TRH	C1'-N11-C21	2.66	122.87	117.64
3	D	506	TRH	C2'-C1'-N11	-2.63	107.71	113.77
3	C	505	TRH	C5A-C51-C41	2.62	121.65	118.77
3	D	506	TRH	O4'-C4'-C3'	-2.59	99.63	105.67
3	A	500	TRH	O4'-C4'-C3'	-2.55	99.72	105.67
3	B	502	TRH	O4'-C4'-C5'	-2.54	101.01	109.37
3	D	506	TRH	C5A-C51-C61	-2.53	119.46	122.85
3	B	502	TRH	C3'-C2'-C1'	2.53	108.88	102.54
3	B	502	TRH	O1P-P-O2P	2.52	124.72	112.24
3	A	500	TRH	C1'-N11-C21	2.52	122.61	117.64
3	B	503	TRH	O4'-C4'-C3'	-2.50	99.84	105.67
3	B	503	TRH	O5-C5-C4	2.48	113.97	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	505	TRH	O4'-C4'-C3'	-2.47	99.92	105.67
3	C	505	TRH	O4-C4-C5	2.43	115.05	109.67
3	C	504	TRH	C2'-C3'-C4'	2.43	107.82	102.76
3	D	507	TRH	O2-C2-C1	-2.41	104.20	110.05
3	A	500	TRH	O1P-P-O2P	2.39	124.05	112.24
3	A	501	TRH	P-OPP-P2	-2.39	124.64	132.83
3	B	502	TRH	O4'-C4'-C3'	-2.38	100.11	105.67
3	D	507	TRH	O4-C4-C5	2.37	114.91	109.67
3	B	502	TRH	O3-C3-C4	-2.34	104.93	110.35
3	A	501	TRH	O4'-C4'-C3'	-2.32	100.26	105.67
3	B	502	TRH	C61-N11-C21	-2.30	118.97	121.30
3	C	505	TRH	O2-C2-C3	-2.29	105.06	110.35
3	A	501	TRH	C3'-C2'-C1'	2.24	108.16	102.54
3	D	506	TRH	C61-C51-C41	2.24	119.90	118.03
3	A	500	TRH	O5-C5-C6	-2.23	101.89	106.70
3	B	503	TRH	O21-C21-N31	-2.23	117.36	121.50
3	B	502	TRH	C61-C51-C41	2.21	119.88	118.03
3	B	503	TRH	O2-C2-C3	-2.21	105.25	110.35
3	C	504	TRH	P-O5'-C5'	-2.20	108.79	121.68
3	A	501	TRH	C61-N11-C21	-2.17	119.10	121.30
3	C	505	TRH	O5'-P-O2P	-2.15	100.67	109.07
3	A	500	TRH	C4-C3-C2	2.15	114.58	110.82
3	B	502	TRH	O21-C21-N11	-2.15	119.93	122.79
3	A	501	TRH	O5-C5-C4	2.14	113.36	109.52
3	C	504	TRH	O3-C3-C4	-2.13	105.42	110.35
3	A	500	TRH	O41-C41-N31	2.12	124.19	120.12
3	A	501	TRH	O4'-C4'-C5'	-2.11	102.43	109.37
3	B	503	TRH	O1P-P-O2P	2.10	122.63	112.24
3	C	504	TRH	OPP-P2-O1	-2.10	98.26	102.48
3	C	505	TRH	C1'-N11-C21	2.06	121.70	117.64
3	C	504	TRH	O3-C3-C2	2.06	115.10	110.35
3	A	500	TRH	P-OPP-P2	-2.05	125.78	132.83
3	B	502	TRH	O4P-P2-O3P	2.05	122.35	112.24
3	D	507	TRH	O4P-P2-O3P	2.00	122.15	112.24

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	TRH	C1-O1-P2-O4P
3	A	500	TRH	C2-C1-O1-P2
3	A	500	TRH	O5-C1-O1-P2

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Mol	Chain	Res	Type	Atoms
3	A	501	TRH	C5'-O5'-P-OPP
3	B	502	TRH	C1-O1-P2-O4P
3	B	502	TRH	O5-C1-O1-P2
3	B	503	TRH	C5'-O5'-P-OPP
3	C	504	TRH	C1-O1-P2-O4P
3	C	504	TRH	O5-C1-O1-P2
3	C	505	TRH	O4'-C4'-C5'-O5'
3	D	506	TRH	O5-C1-O1-P2
3	D	507	TRH	P2-OPP-P-O5'
3	C	505	TRH	C3'-C4'-C5'-O5'
3	A	500	TRH	C1-O1-P2-OPP
3	C	504	TRH	C1-O1-P2-OPP
3	C	504	TRH	C3'-C4'-C5'-O5'
3	D	506	TRH	C1-O1-P2-O4P
3	B	502	TRH	C1-O1-P2-OPP
3	B	503	TRH	P2-OPP-P-O5'
3	A	501	TRH	C1-O1-P2-OPP
3	B	503	TRH	C1-O1-P2-OPP
3	D	507	TRH	C1-O1-P2-OPP
3	C	504	TRH	C2-C1-O1-P2
3	A	500	TRH	C3'-C4'-C5'-O5'
3	B	502	TRH	C1-O1-P2-O3P
3	A	501	TRH	C5'-O5'-P-O1P
3	A	501	TRH	C5'-O5'-P-O2P
3	A	501	TRH	O5-C1-O1-P2
3	C	505	TRH	O5-C1-O1-P2
3	D	507	TRH	O5-C1-O1-P2
3	D	507	TRH	O4'-C4'-C5'-O5'
3	C	505	TRH	C1-O1-P2-OPP
3	C	504	TRH	O4'-C4'-C5'-O5'
3	B	502	TRH	P-OPP-P2-O3P
3	B	503	TRH	C5'-O5'-P-O2P

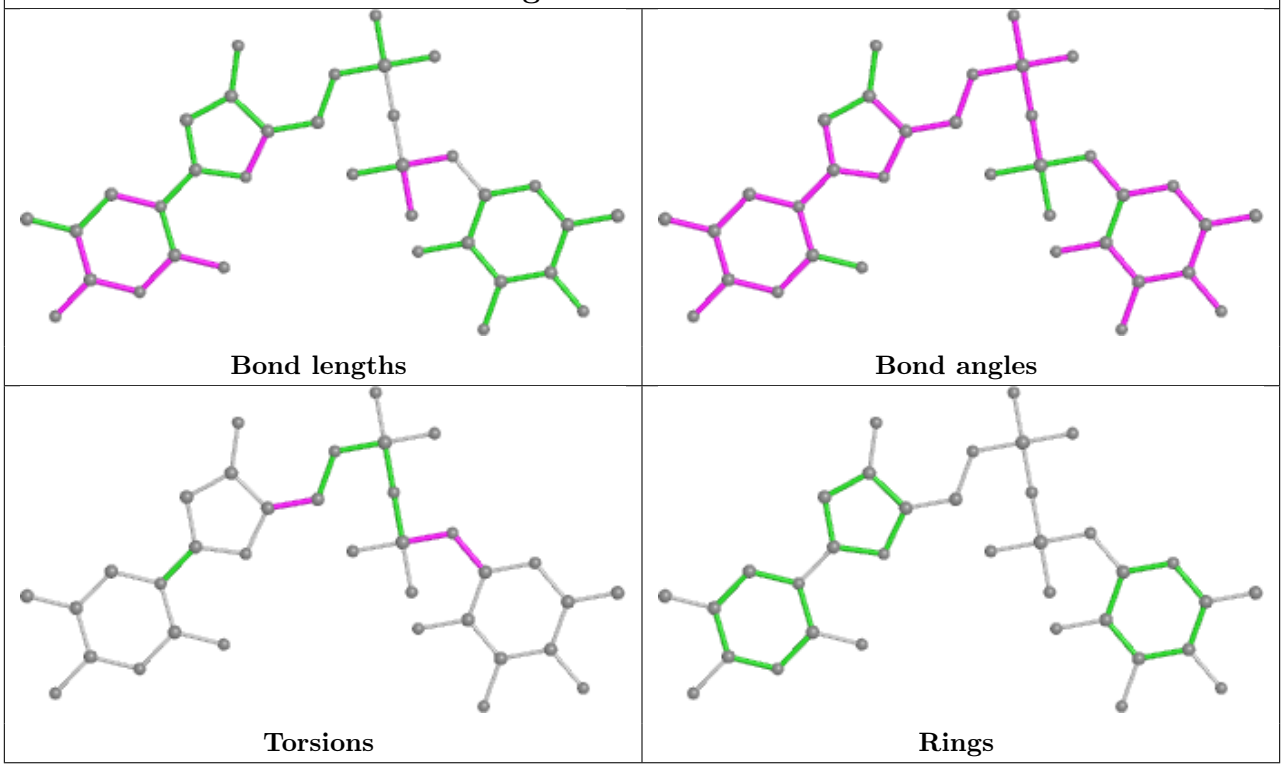
There are no ring outliers.

5 monomers are involved in 7 short contacts:

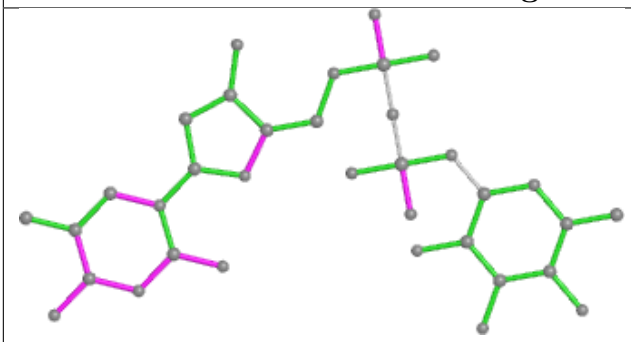
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	703	SO4	1	0
3	A	500	TRH	1	0
3	C	504	TRH	3	0
2	D	704	SO4	1	0
3	D	506	TRH	1	0

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 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.

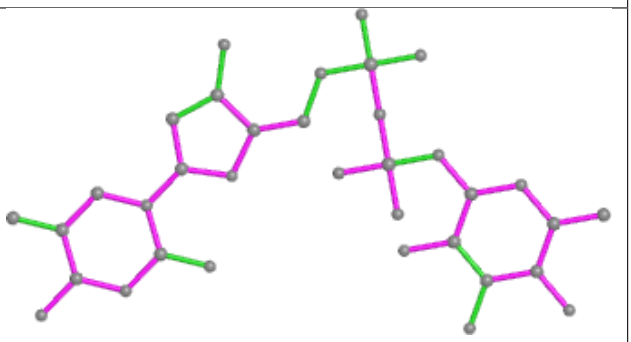
Ligand TRH C 505



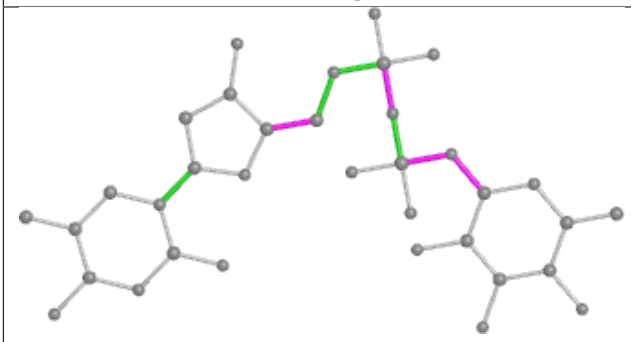
Ligand TRH D 507



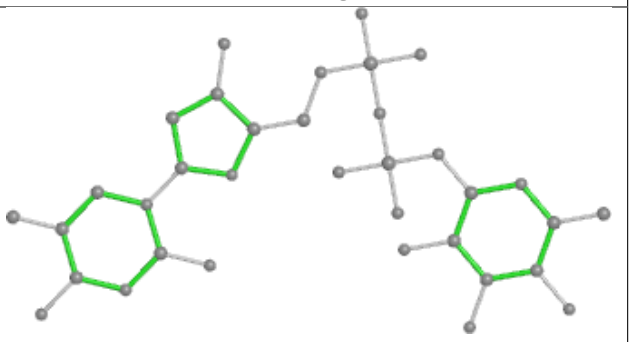
Bond lengths



Bond angles

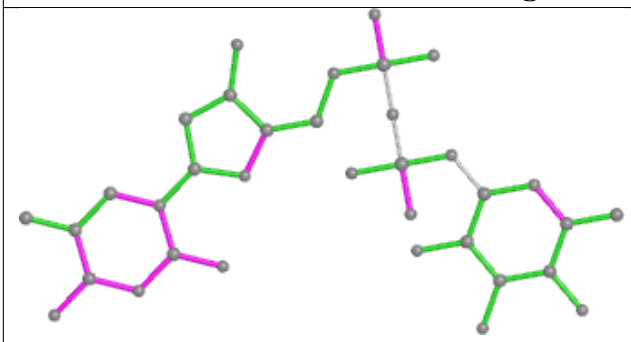


Torsions

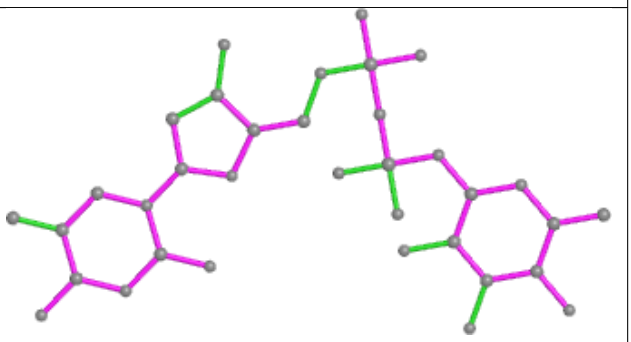


Rings

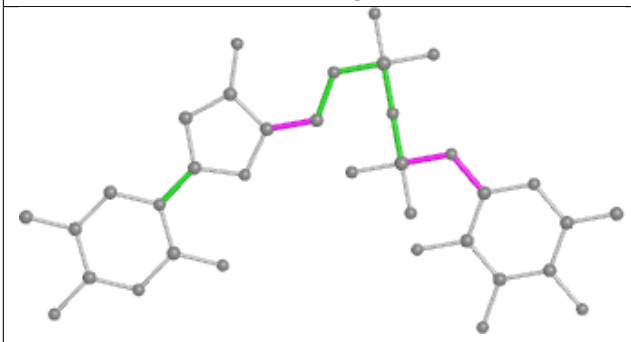
Ligand TRH A 500



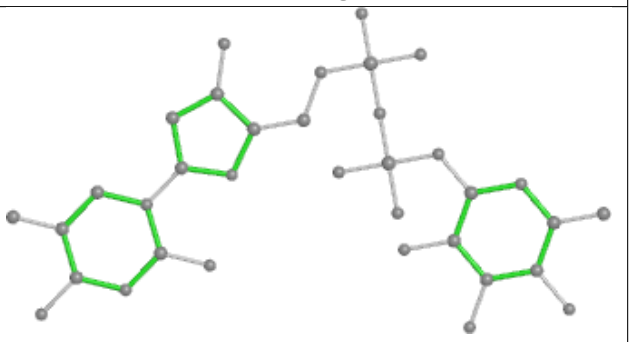
Bond lengths



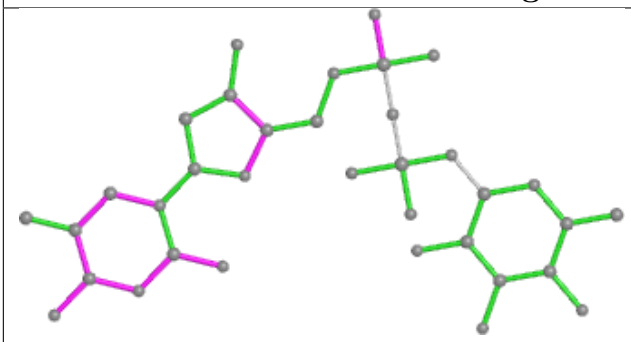
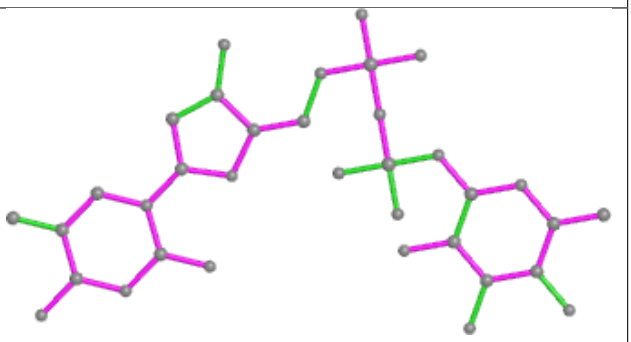
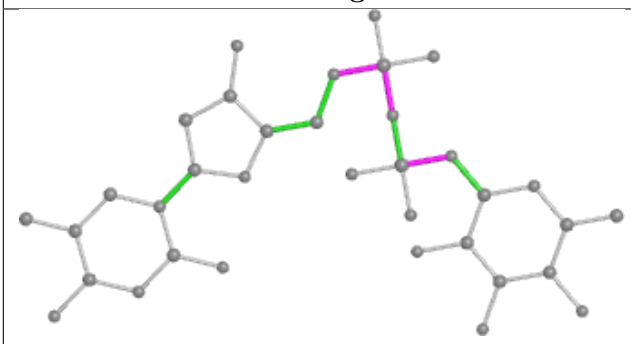
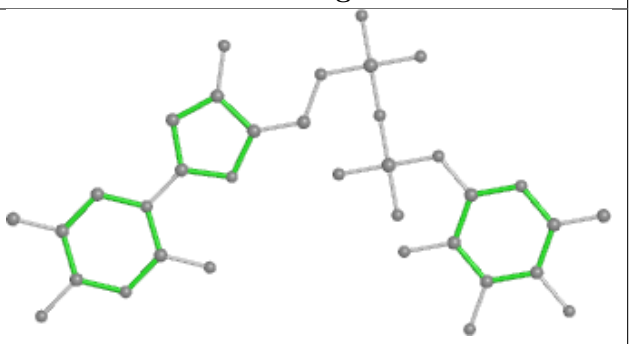
Bond angles

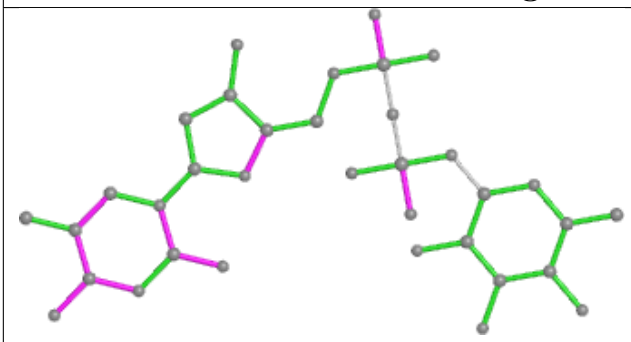
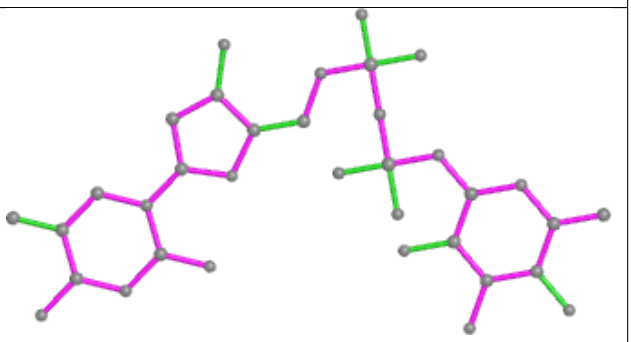
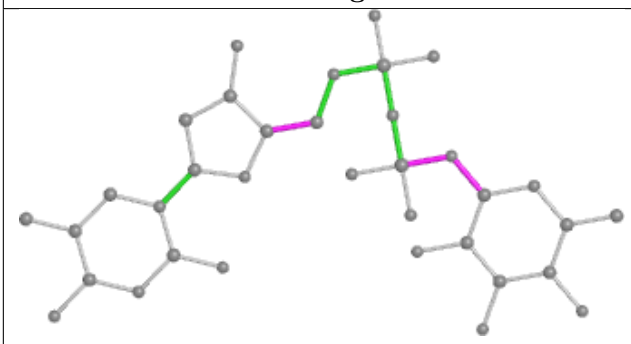
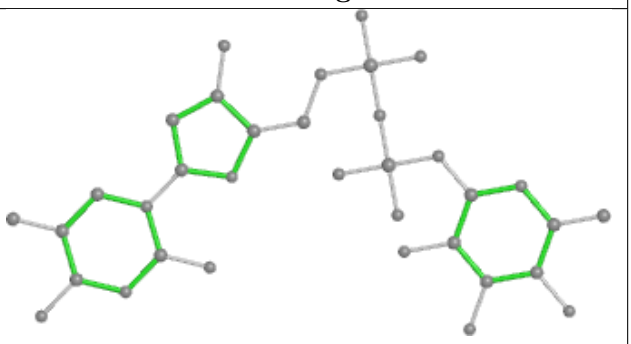


Torsions

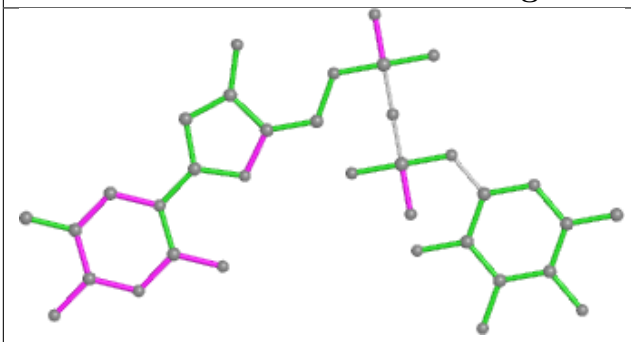


Rings

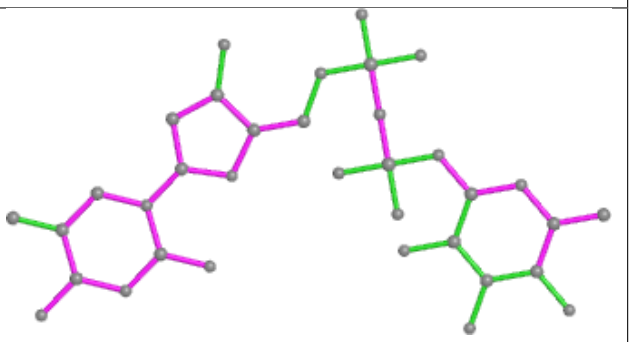
Ligand TRH B 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TRH C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

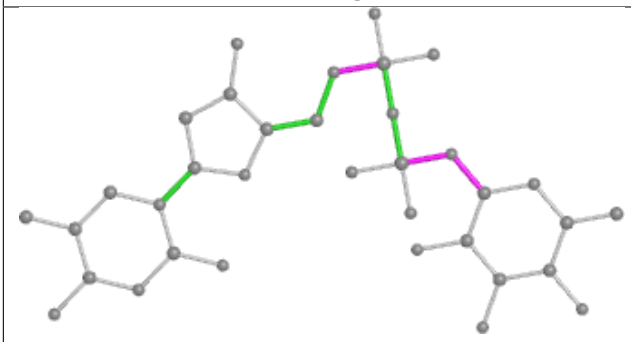
Ligand TRH A 501



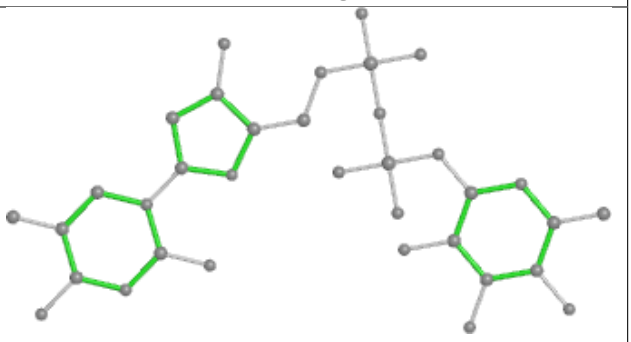
Bond lengths



Bond angles

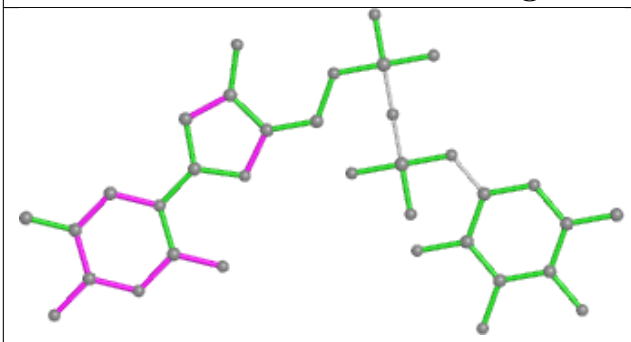


Torsions

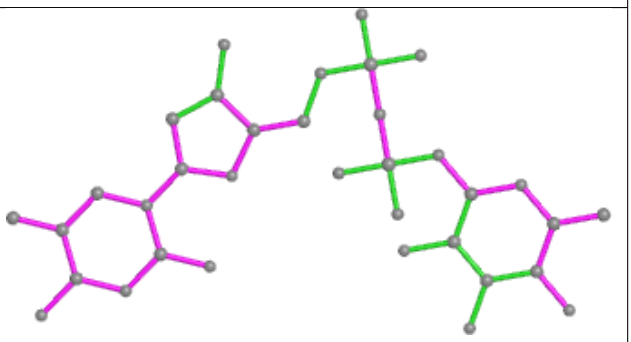


Rings

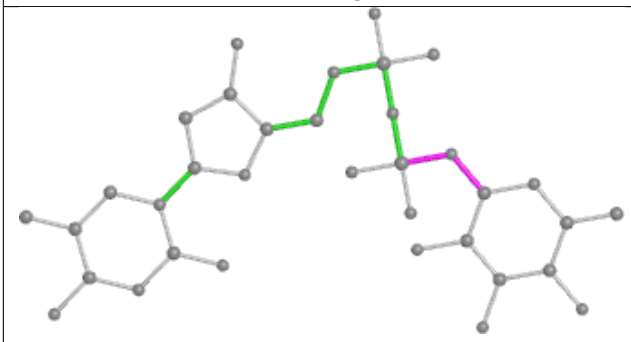
Ligand TRH D 506



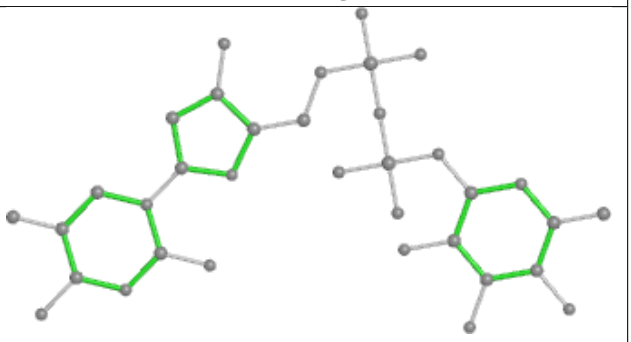
Bond lengths



Bond angles

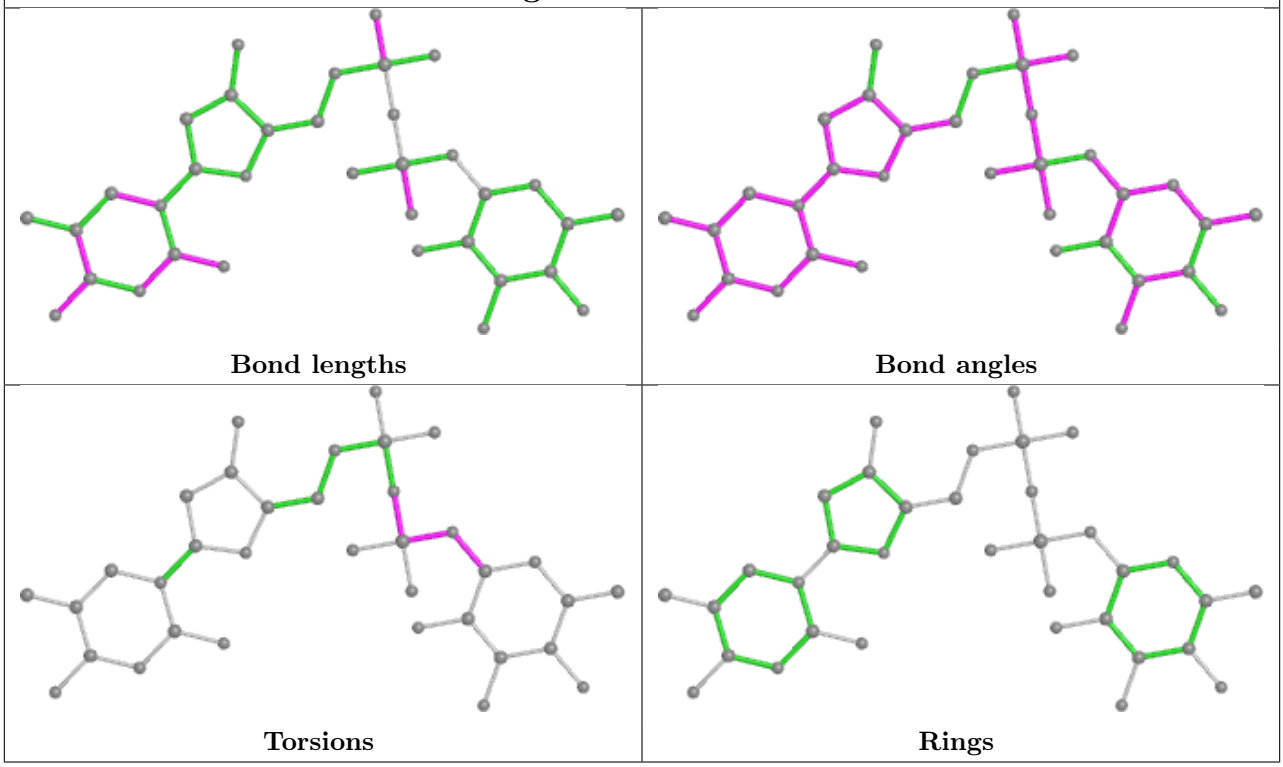


Torsions



Rings

Ligand TRH B 502



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	292/293 (99%)	-0.30	1 (0%)	94	95	6, 11, 21, 34	0
1	B	292/293 (99%)	-0.27	2 (0%)	87	89	7, 12, 22, 33	0
1	C	292/293 (99%)	-0.20	1 (0%)	94	95	6, 13, 23, 35	0
1	D	293/293 (100%)	-0.23	1 (0%)	94	95	7, 11, 22, 36	0
All	All	1169/1172 (99%)	-0.25	5 (0%)	92	93	6, 11, 22, 36	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.9
1	C	152	GLN	2.6
1	A	13	GLY	2.3
1	B	15	ARG	2.3
1	B	152	GLN	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,

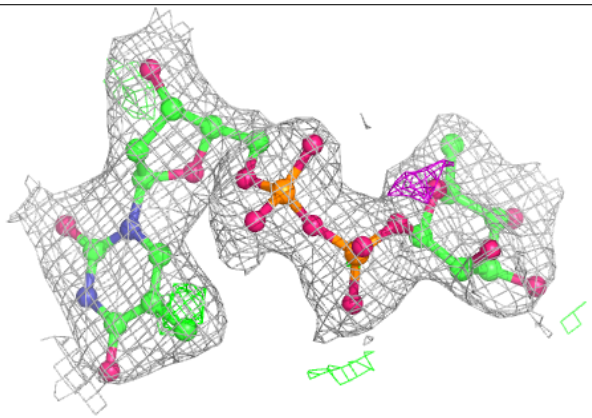
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

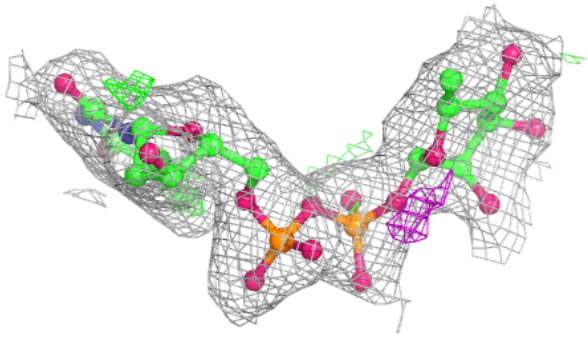
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	702	5/5	0.83	0.30	41,42,46,47	0
2	SO4	D	704	5/5	0.87	0.45	43,44,45,46	0
2	SO4	B	700	5/5	0.91	0.21	42,42,45,46	0
2	SO4	C	703	5/5	0.93	0.47	41,44,46,46	0
2	SO4	A	701	5/5	0.94	0.20	38,40,41,42	0
3	TRH	B	502	35/35	0.95	0.16	8,12,16,20	0
3	TRH	C	504	35/35	0.95	0.16	9,13,18,21	0
3	TRH	D	507	35/35	0.95	0.16	7,14,20,22	0
3	TRH	D	506	35/35	0.96	0.15	8,14,18,18	0
3	TRH	C	505	35/35	0.96	0.15	8,12,15,17	0
3	TRH	A	500	35/35	0.97	0.15	6,11,14,19	0
3	TRH	B	503	35/35	0.97	0.16	8,13,16,19	0
3	TRH	A	501	35/35	0.97	0.16	7,10,17,19	0

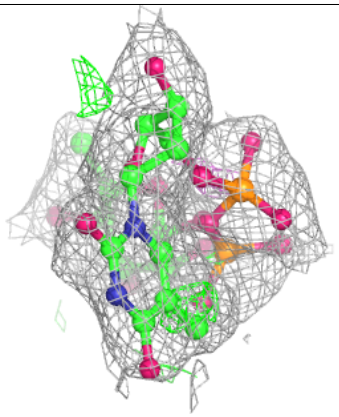
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRH B 502:

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

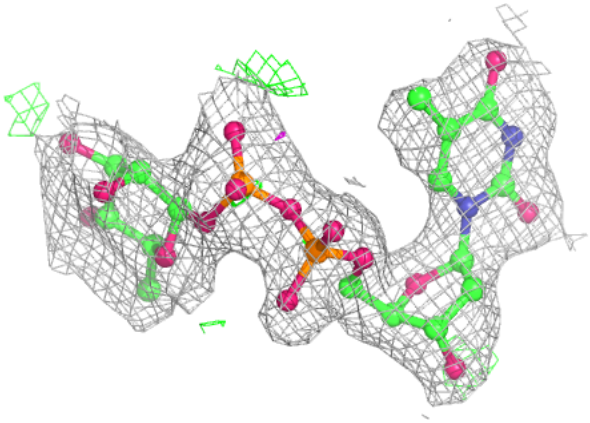


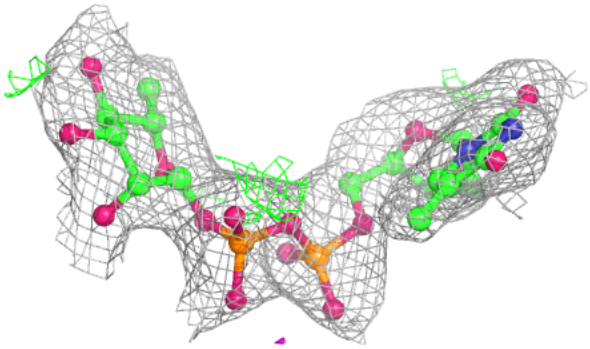


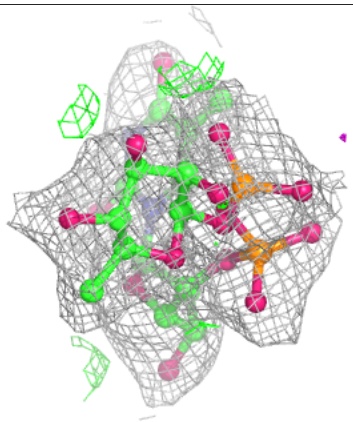


Electron density around TRH C 504:

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

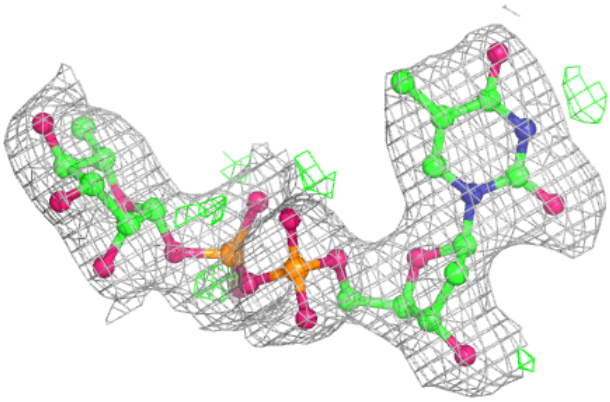


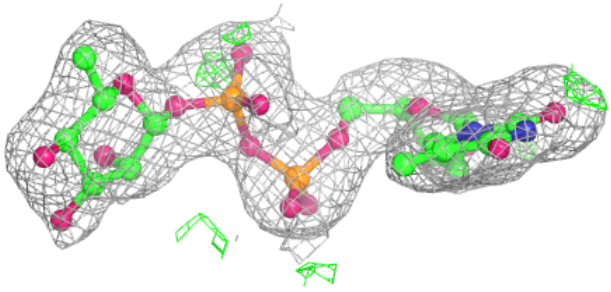


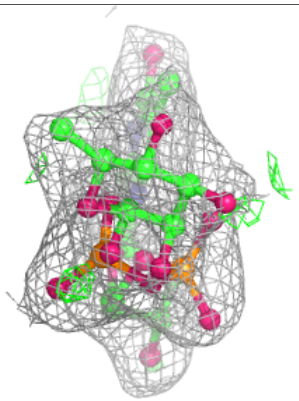


Electron density around TRH D 507:

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

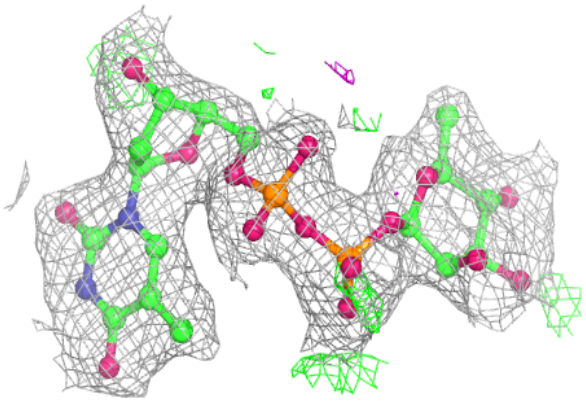


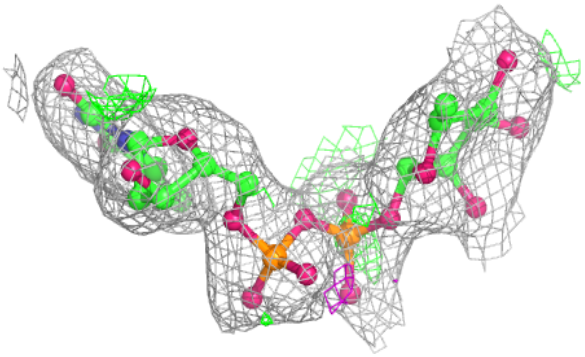


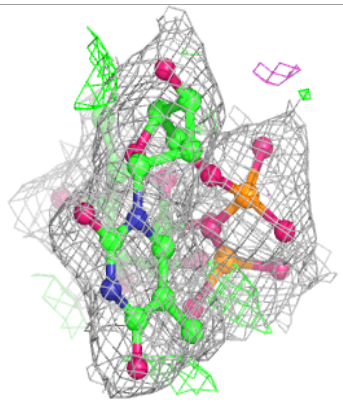


Electron density around TRH D 506:

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

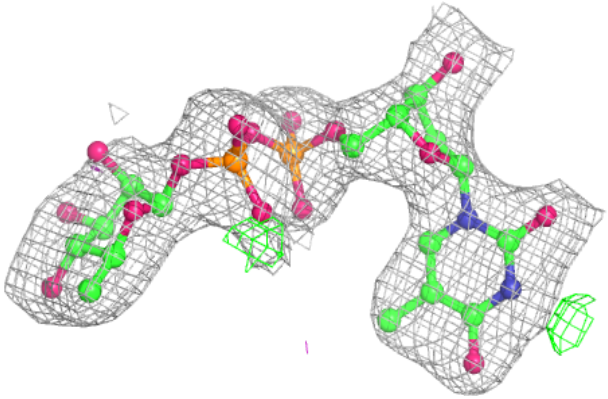


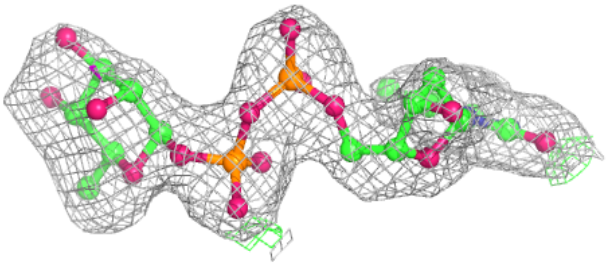


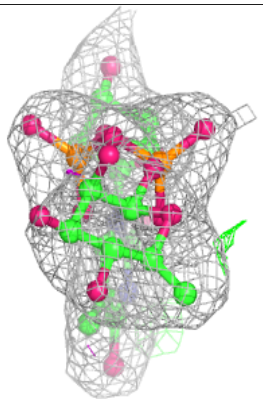


Electron density around TRH C 505:

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

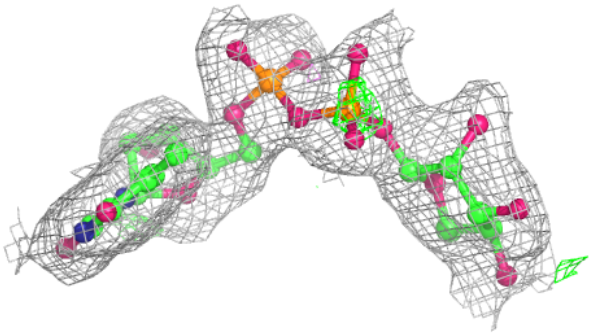


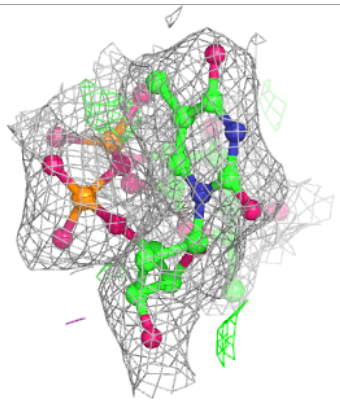




Electron density around TRH A 500:

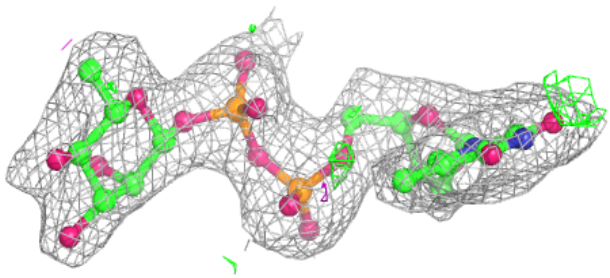
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

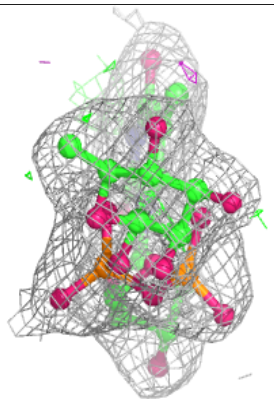




Electron density around TRH B 503:

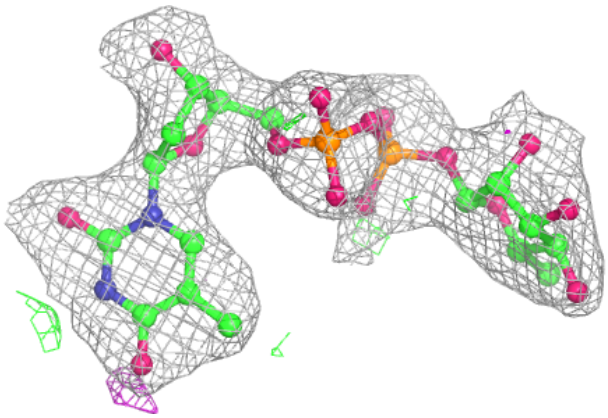
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

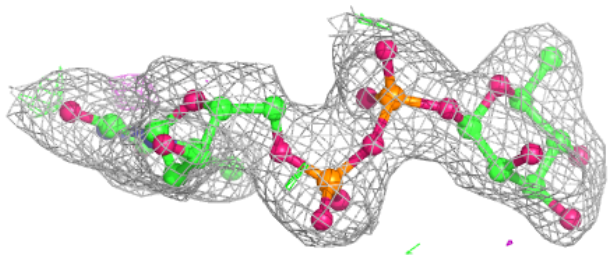


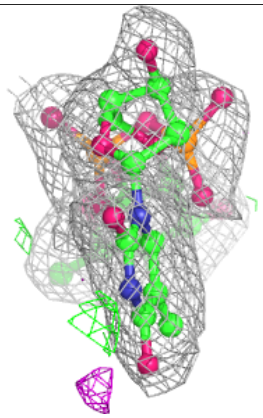


Electron density around TRH A 501:

$2mF_o$-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.