Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 05:41 PM EDT

PDB ID	:	5KAG
Title	:	Crystal structure of a dioxygenase in the Crotonase superfamily in P21
Authors	:	Li, K.; Fielding, E.N.; Condurso, H.L.; Bruner, S.D.
Deposited on	:	2016-06-01
Resolution	:	2.46 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:

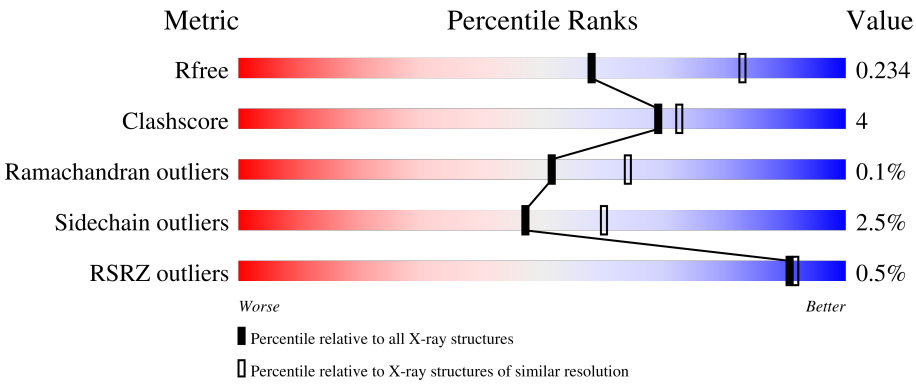
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	438	% 86% 10% •
1	B	438	87% 9% • •
1	C	438	87% 8% • •
1	D	438	86% 10% •
1	E	438	86% 9% • •

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Mol	Chain	Length	Quality of chain
1	F	438	86% 10%
1	G	438	87% 9%
1	H	438	85% 11%
1	I	438	85% 10%
1	J	438	3% 85% 11%
1	K	438	88% 8%
1	L	438	89% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 40937 atoms, of which 0 are hydrogens and 0 are deuteriums.

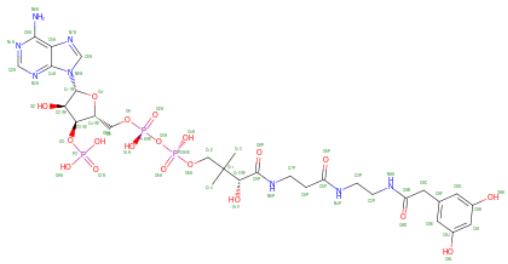
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3272	2056	611	595	10	0	0	0
1	B	422	3279	2060	612	597	10	0	0	0
1	C	421	3272	2056	611	595	10	0	0	0
1	D	423	3283	2062	613	598	10	0	0	0
1	E	421	3272	2056	611	595	10	0	0	0
1	F	421	3272	2056	611	595	10	0	0	0
1	G	422	3279	2060	612	597	10	0	0	0
1	H	422	3279	2060	612	597	10	0	0	0
1	I	421	3272	2056	611	595	10	0	0	0
1	J	422	3276	2058	612	596	10	0	0	0
1	K	422	3279	2060	612	597	10	0	0	0
1	L	421	3272	2056	611	595	10	0	0	0

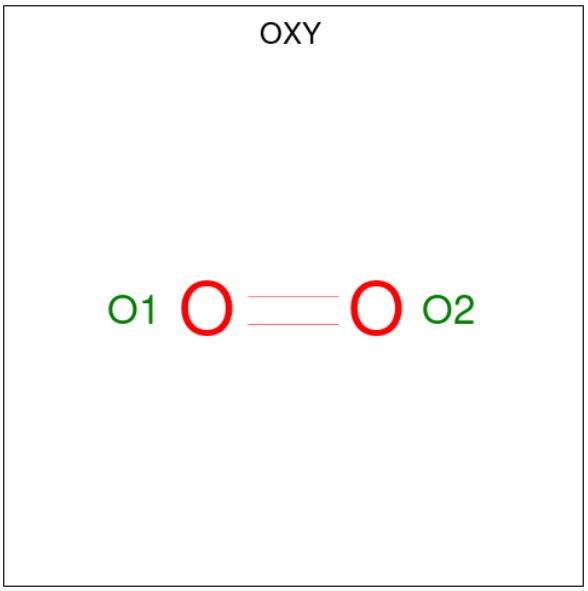
- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOOXY)TETRAHYDROFURAN-2-YL]METHYL (3R)-4-({3-[(2-{[(3,5-DIHYDROXYPHENYL)ACETYL]AMINO}ETHYL)AMINO]-3-OXOPROPYL}AMINO)-3-HYDROXY-2,2-DIMETHYL-4-OXOBUTYL DIHYDROGEN DIPHOSPHATE (three-letter code: YE1) (formula: $C_{29}H_{43}N_8O_{19}P_3$).

YE1



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	59	29	8	19	3	0	0
2	B	1	59	29	8	19	3	0	0
2	C	1	59	29	8	19	3	0	0
2	D	1	59	29	8	19	3	0	0
2	E	1	59	29	8	19	3	0	0
2	F	1	59	29	8	19	3	0	0
2	G	1	59	29	8	19	3	0	0
2	H	1	59	29	8	19	3	0	0
2	I	1	59	29	8	19	3	0	0
2	J	1	59	29	8	19	3	0	0
2	K	1	59	29	8	19	3	0	0
2	L	1	59	29	8	19	3	0	0

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0
3	E	1	Total O 2 2	0	0
3	F	1	Total O 2 2	0	0
3	G	1	Total O 2 2	0	0
3	H	1	Total O 2 2	0	0
3	I	1	Total O 2 2	0	0
3	J	1	Total O 2 2	0	0
3	K	1	Total O 2 2	0	0
3	L	1	Total O 2 2	0	0

- Molecule 4 is water.

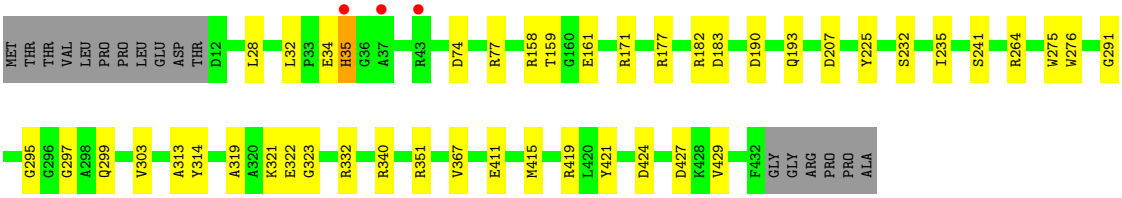
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	62	62	62	0	0
			Total	O		
4	B	76	76	76	0	0
			Total	O		
4	C	80	80	80	0	0
			Total	O		
4	D	102	102	102	0	0
			Total	O		
4	E	86	86	86	0	0
			Total	O		
4	F	73	73	73	0	0
			Total	O		
4	G	64	64	64	0	0
			Total	O		
4	H	62	62	62	0	0
			Total	O		
4	I	85	85	85	0	0
			Total	O		
4	J	51	51	51	0	0
			Total	O		
4	K	81	81	81	0	0
			Total	O		
4	L	76	76	76	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.

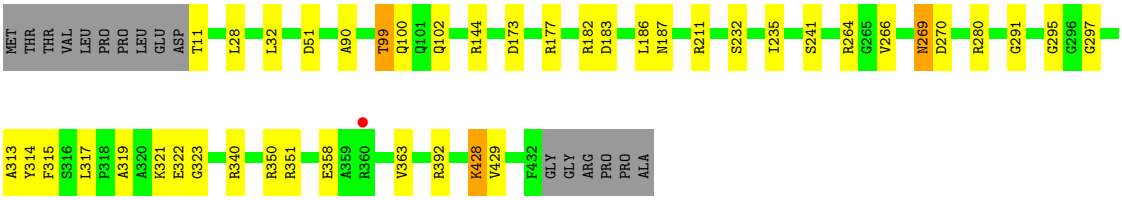
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain A:



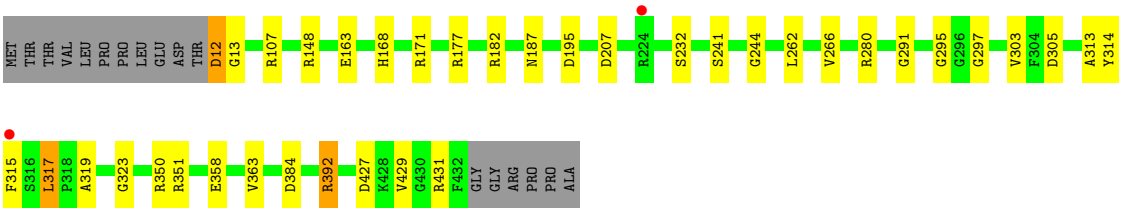
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain B:



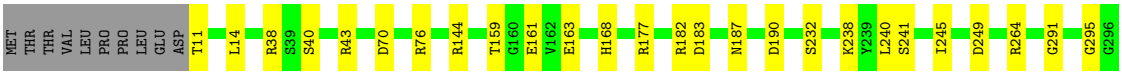
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain C:



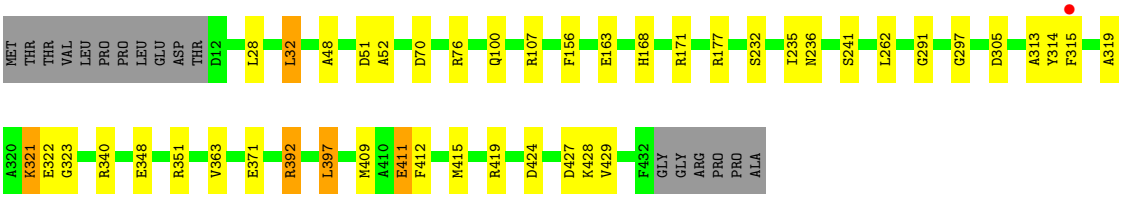
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain D:



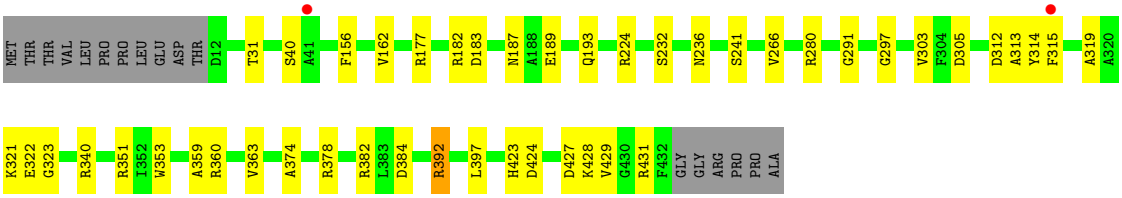
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain E:



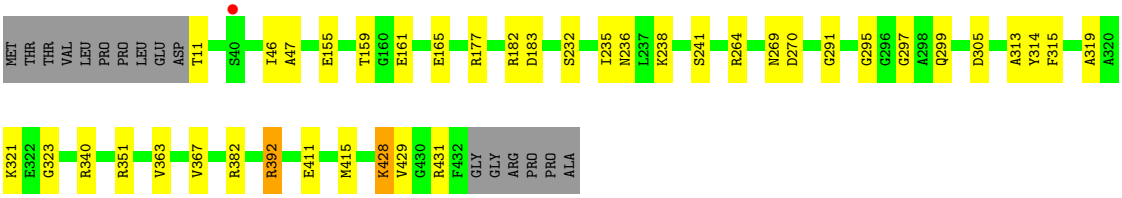
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain F:



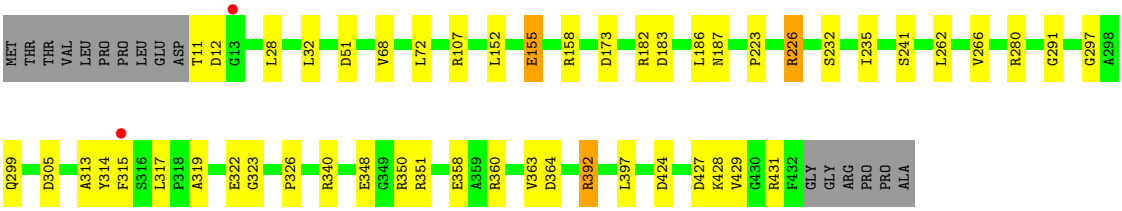
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain G:



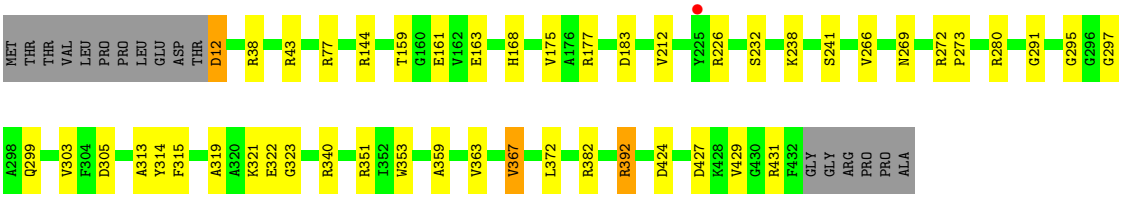
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain H:



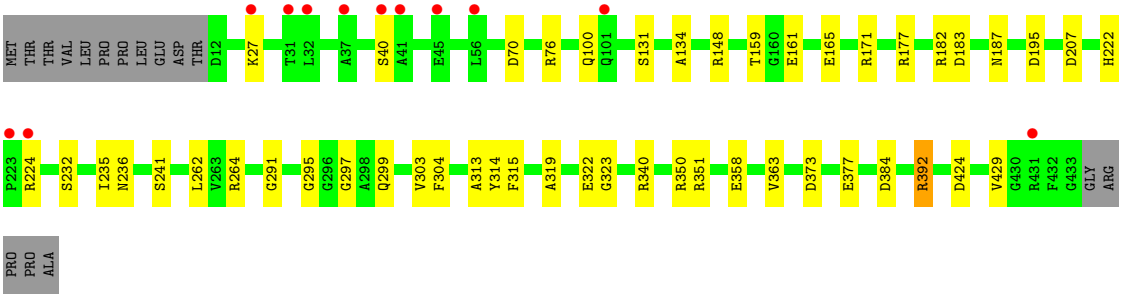
• Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain I:



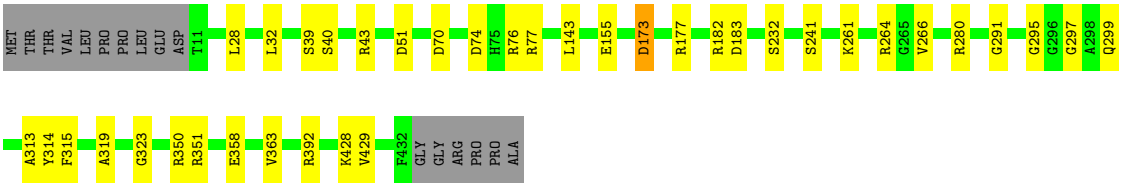
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain J:



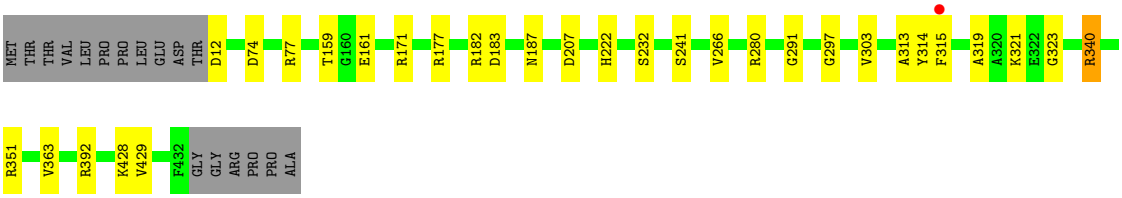
- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain K:



- Molecule 1: (3,5-dihydroxyphenyl)acetyl-CoA 1,2-dioxygenase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	138.96Å 170.45Å 156.28Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	43.64 – 2.46 43.64 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.64-2.46) 99.5 (43.64-2.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.212 , 0.238 0.209 , 0.234	Depositor DCC
R_{free} test set	13119 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 6.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	40937	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 27.13 % 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 2.3235e-03. 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: YE1, OXY

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	0.32	0/3333	0.56	0/4515
1	B	0.32	0/3340	0.54	0/4525
1	C	0.32	0/3333	0.54	0/4515
1	D	0.32	0/3344	0.56	0/4530
1	E	0.33	0/3333	0.55	0/4515
1	F	0.32	0/3333	0.56	0/4515
1	G	0.33	0/3340	0.55	0/4525
1	H	0.32	0/3340	0.56	0/4525
1	I	0.33	0/3333	0.56	0/4515
1	J	0.31	0/3337	0.55	0/4520
1	K	0.33	0/3340	0.55	0/4525
1	L	0.33	0/3333	0.55	0/4515
All	All	0.32	0/40039	0.55	0/54240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3272	0	3295	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3279	0	3302	28	0
1	C	3272	0	3295	21	0
1	D	3283	0	3305	24	0
1	E	3272	0	3295	29	0
1	F	3272	0	3295	31	0
1	G	3279	0	3302	23	0
1	H	3279	0	3302	28	0
1	I	3272	0	3295	28	0
1	J	3276	0	3298	28	0
1	K	3279	0	3302	16	0
1	L	3272	0	3295	14	0
2	A	59	0	37	2	0
2	B	59	0	39	1	0
2	C	59	0	38	1	0
2	D	59	0	39	2	0
2	E	59	0	38	3	0
2	F	59	0	38	6	0
2	G	59	0	38	4	0
2	H	59	0	38	3	0
2	I	59	0	39	2	0
2	J	59	0	38	5	0
2	K	59	0	39	1	0
2	L	59	0	38	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	62	0	0	6	0
4	B	76	0	0	5	0
4	C	80	0	0	1	0
4	D	102	0	0	8	0
4	E	86	0	0	4	0
4	F	73	0	0	6	0
4	G	64	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	62	0	0	4	0
4	I	85	0	0	5	0
4	J	51	0	0	2	0
4	K	81	0	0	1	0
4	L	76	0	0	0	0
All	All	40937	0	40040	297	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 4.

All (297) 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:428:LYS:HE3	1:B:428:LYS:HA	1.24	1.16
1:B:322:GLU:CD	1:B:428:LYS:HD2	1.98	0.84
1:E:397:LEU:HD22	1:E:397:LEU:O	1.78	0.83
1:B:428:LYS:HA	1:B:428:LYS:CE	2.09	0.79
1:F:428:LYS:HD2	1:F:431:ARG:HH21	1.46	0.79
1:I:226:ARG:HD2	4:I:623:HOH:O	1.84	0.78
1:D:241:SER:HB2	1:D:429:VAL:HG12	1.67	0.76
1:I:241:SER:HB2	1:I:429:VAL:HG12	1.69	0.74
1:E:415:MET:SD	4:F:666:HOH:O	2.45	0.74
1:A:295:GLY:HA2	4:A:660:HOH:O	1.88	0.73
1:G:241:SER:HB2	1:G:429:VAL:HG12	1.71	0.72
1:F:241:SER:HB2	1:F:429:VAL:HG12	1.71	0.72
1:E:241:SER:HB2	1:E:429:VAL:HG12	1.73	0.71
1:J:241:SER:HB2	1:J:429:VAL:HG12	1.73	0.70
1:C:241:SER:HB2	1:C:429:VAL:HG12	1.74	0.70
1:B:241:SER:HB2	1:B:429:VAL:HG12	1.73	0.70
1:K:241:SER:HB2	1:K:429:VAL:HG12	1.74	0.70
1:A:241:SER:HB2	1:A:429:VAL:HG12	1.74	0.69
1:L:241:SER:HB2	1:L:429:VAL:HG12	1.75	0.69
1:J:165:GLU:HG2	4:J:601:HOH:O	1.93	0.68
1:H:241:SER:HB2	1:H:429:VAL:HG12	1.76	0.67
1:H:223:PRO:HA	1:H:226:ARG:HG3	1.76	0.67
1:J:171:ARG:NH1	1:J:207:ASP:OD2	2.30	0.65
1:K:319:ALA:HB1	1:K:323:GLY:HA3	1.79	0.64
1:H:348:GLU:OE1	1:I:382:ARG:NE	2.31	0.63
1:A:171:ARG:NH1	1:A:207:ASP:OD2	2.32	0.62
1:G:165:GLU:HG2	1:G:182:ARG:NH1	2.15	0.62
1:G:165:GLU:HG2	1:G:182:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:319:ALA:HB1	1:H:323:GLY:HA3	1.82	0.60
1:B:428:LYS:HE3	1:B:428:LYS:CA	2.13	0.60
1:L:171:ARG:NH1	1:L:207:ASP:OD2	2.35	0.60
1:L:222:HIS:NE2	2:L:501:YE1:O8A	2.32	0.60
1:B:319:ALA:HB1	1:B:323:GLY:HA3	1.83	0.60
1:G:415:MET:SD	4:H:655:HOH:O	2.56	0.60
1:E:411:GLU:HG2	1:F:397:LEU:CD1	2.33	0.59
1:A:275:TRP:HE3	1:A:275:TRP:O	1.86	0.59
1:F:319:ALA:HB1	1:F:323:GLY:HA3	1.84	0.59
1:F:397:LEU:C	1:F:397:LEU:HD23	2.24	0.58
1:K:74:ASP:OD1	1:K:77:ARG:NH1	2.36	0.58
1:C:171:ARG:NH1	1:C:207:ASP:OD2	2.35	0.58
2:F:501:YE1:HN62	2:F:501:YE1:HC71	1.70	0.57
1:B:102:GLN:N	4:B:605:HOH:O	2.37	0.57
1:B:322:GLU:OE1	1:B:428:LYS:HD2	2.04	0.57
1:E:411:GLU:HG2	1:F:397:LEU:HD11	1.87	0.57
1:B:90:ALA:HB1	1:B:99:THR:HA	1.86	0.56
1:E:70:ASP:HA	4:E:601:HOH:O	2.04	0.56
1:C:314:TYR:CD1	1:C:351:ARG:HD2	2.41	0.55
1:G:382:ARG:HB3	4:G:611:HOH:O	2.05	0.55
1:H:186:LEU:HD22	2:H:501:YE1:HC8	1.89	0.55
1:L:314:TYR:CD1	1:L:351:ARG:HD2	2.41	0.55
1:A:415:MET:SD	4:A:661:HOH:O	2.57	0.55
1:J:236:ASN:HA	2:J:501:YE1:N1A	2.22	0.55
1:B:100:GLN:N	4:B:605:HOH:O	2.40	0.55
1:B:211:ARG:NH1	4:B:606:HOH:O	2.39	0.55
1:D:249:ASP:HA	4:D:630:HOH:O	2.06	0.55
1:A:74:ASP:O	1:A:77:ARG:HG2	2.06	0.55
1:I:314:TYR:CD1	1:I:351:ARG:HD2	2.42	0.55
1:K:70:ASP:OD1	1:K:76:ARG:NH1	2.41	0.54
1:E:232:SER:HB3	1:E:297:GLY:HA3	1.90	0.54
1:I:319:ALA:HB1	1:I:323:GLY:HA3	1.90	0.54
1:D:238:LYS:NZ	2:D:501:YE1:O9A	2.37	0.54
1:F:378:ARG:NE	4:F:612:HOH:O	2.41	0.54
1:H:427:ASP:OD2	1:H:431:ARG:NH1	2.41	0.54
1:H:299:GLN:NE2	4:H:606:HOH:O	2.36	0.53
1:C:12:ASP:HA	4:C:678:HOH:O	2.08	0.53
1:D:70:ASP:OD1	1:D:76:ARG:NH1	2.41	0.53
1:D:159:THR:HG22	1:D:161:GLU:N	2.24	0.53
1:A:411:GLU:HG2	4:A:626:HOH:O	2.09	0.53
1:A:319:ALA:HB1	1:A:323:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:ASP:OD1	1:J:183:ASP:N	2.38	0.53
1:J:319:ALA:HB1	1:J:323:GLY:HA3	1.89	0.53
2:I:501:YE1:OAD	2:I:501:YE1:HAE	2.09	0.53
1:G:238:LYS:NZ	2:G:501:YE1:O9A	2.40	0.53
1:D:314:TYR:CD1	1:D:351:ARG:HD2	2.45	0.52
1:I:367:VAL:HG21	1:I:372:LEU:HA	1.91	0.52
1:C:319:ALA:HB1	1:C:323:GLY:HA3	1.91	0.52
1:I:77:ARG:NE	4:I:604:HOH:O	2.43	0.52
1:D:159:THR:HG22	1:D:161:GLU:H	1.75	0.52
1:B:322:GLU:OE2	1:B:428:LYS:HD2	2.09	0.52
1:D:319:ALA:HB1	1:D:323:GLY:HA3	1.91	0.52
1:H:68:VAL:O	1:H:72:LEU:HG	2.10	0.52
1:C:427:ASP:OD2	1:C:431:ARG:NH1	2.44	0.51
1:D:394:MET:HA	1:D:397:LEU:HD23	1.91	0.51
1:E:409:MET:HA	1:E:412:PHE:HB3	1.93	0.51
1:J:314:TYR:CD1	1:J:351:ARG:HD2	2.46	0.51
1:G:319:ALA:HB1	1:G:323:GLY:HA3	1.91	0.51
2:J:501:YE1:OAD	2:J:501:YE1:HAE	2.10	0.51
1:B:144:ARG:NH2	1:B:269:ASN:OD1	2.34	0.51
1:A:159:THR:HG22	1:A:161:GLU:N	2.25	0.51
1:D:187:ASN:HB3	4:D:616:HOH:O	2.09	0.51
1:B:183:ASP:N	1:B:183:ASP:OD1	2.37	0.51
1:F:315:PHE:CZ	1:F:363:VAL:HG21	2.46	0.51
1:G:428:LYS:HE3	1:G:431:ARG:HH22	1.75	0.51
1:I:238:LYS:NZ	2:I:501:YE1:O7A	2.37	0.51
1:A:182:ARG:NH1	1:A:190:ASP:OD2	2.38	0.51
1:G:314:TYR:CD1	1:G:351:ARG:HD2	2.46	0.51
1:I:77:ARG:HB2	4:I:604:HOH:O	2.11	0.51
1:I:382:ARG:HD3	4:I:610:HOH:O	2.11	0.51
1:A:314:TYR:CD1	1:A:351:ARG:HD2	2.46	0.51
1:D:232:SER:HB3	1:D:297:GLY:HA3	1.93	0.50
1:F:236:ASN:HA	2:F:501:YE1:N1A	2.26	0.50
1:D:144:ARG:NE	4:D:614:HOH:O	2.44	0.50
1:E:348:GLU:OE1	1:F:382:ARG:NE	2.40	0.50
1:H:350:ARG:NH2	1:H:358:GLU:OE1	2.39	0.50
1:B:314:TYR:CD1	1:B:351:ARG:HD2	2.47	0.50
1:L:319:ALA:HB1	1:L:323:GLY:HA3	1.93	0.50
1:H:360:ARG:NH2	1:H:364:ASP:O	2.45	0.50
1:G:232:SER:HB3	1:G:297:GLY:HA3	1.94	0.50
1:J:70:ASP:OD1	1:J:76:ARG:NH1	2.44	0.50
1:I:427:ASP:OD2	1:I:431:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:HIS:CE1	4:F:621:HOH:O	2.65	0.49
1:J:222:HIS:NE2	2:J:501:YE1:O8A	2.39	0.49
1:F:314:TYR:CD1	1:F:351:ARG:HD2	2.48	0.49
1:A:332:ARG:HD2	4:A:615:HOH:O	2.12	0.49
1:D:240:LEU:HA	4:D:645:HOH:O	2.12	0.49
1:G:46:ILE:HG23	4:G:610:HOH:O	2.12	0.49
1:J:224:ARG:HD2	2:J:501:YE1:O2A	2.12	0.49
1:G:236:ASN:HA	2:G:501:YE1:N1A	2.28	0.49
1:J:291:GLY:O	1:J:313:ALA:HA	2.12	0.49
1:K:314:TYR:CD1	1:K:351:ARG:HD2	2.47	0.49
1:J:384:ASP:HB2	1:L:321:LYS:NZ	2.28	0.49
1:A:159:THR:HG22	1:A:161:GLU:H	1.78	0.49
1:A:291:GLY:O	1:A:313:ALA:HA	2.13	0.49
2:C:501:YE1:OAD	2:C:501:YE1:HAE	2.12	0.49
1:J:235:ILE:O	2:J:501:YE1:N6A	2.35	0.49
1:F:322:GLU:HG2	1:F:424:ASP:HB2	1.95	0.49
1:I:315:PHE:CZ	1:I:363:VAL:HG21	2.48	0.49
2:F:501:YE1:OAD	2:F:501:YE1:HAE	2.13	0.48
1:D:163:GLU:HG3	1:D:168:HIS:HD2	1.78	0.48
1:A:322:GLU:HG2	1:A:424:ASP:HB2	1.95	0.48
1:I:12:ASP:HB2	4:I:615:HOH:O	2.13	0.48
1:A:158:ARG:HB2	1:E:48:ALA:HB1	1.96	0.47
1:D:291:GLY:O	1:D:313:ALA:HA	2.13	0.47
1:A:34:GLU:HB3	1:A:35:HIS:CE1	2.48	0.47
1:D:295:GLY:O	1:D:299:GLN:HG3	2.14	0.47
1:F:291:GLY:O	1:F:313:ALA:HA	2.15	0.47
1:H:158:ARG:NH2	4:H:607:HOH:O	2.39	0.47
1:A:232:SER:HB3	1:A:297:GLY:HA3	1.97	0.47
1:B:295:GLY:HA2	4:B:673:HOH:O	2.14	0.47
1:J:159:THR:HG22	1:J:161:GLU:N	2.29	0.47
1:J:232:SER:HB3	1:J:297:GLY:HA3	1.97	0.47
1:L:315:PHE:CZ	1:L:363:VAL:HG21	2.50	0.47
1:E:76:ARG:N	4:E:601:HOH:O	2.46	0.47
1:B:182:ARG:HB2	1:B:187:ASN:HA	1.97	0.47
1:B:28:LEU:O	1:B:32:LEU:HB2	2.15	0.46
1:B:291:GLY:O	1:B:313:ALA:HA	2.15	0.46
1:G:159:THR:HG22	1:G:161:GLU:N	2.30	0.46
1:B:232:SER:HB3	1:B:297:GLY:HA3	1.97	0.46
1:E:314:TYR:CD1	1:E:351:ARG:HD2	2.50	0.46
1:H:315:PHE:CZ	1:H:363:VAL:HG21	2.51	0.46
1:I:305:ASP:OD2	1:I:392:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:SER:O	1:K:43:ARG:HG3	2.16	0.46
1:G:291:GLY:O	1:G:313:ALA:HA	2.16	0.46
1:E:315:PHE:CZ	1:E:363:VAL:HG21	2.51	0.46
1:E:319:ALA:HB1	1:E:323:GLY:HA3	1.97	0.46
1:I:144:ARG:NH2	1:I:269:ASN:OD1	2.33	0.46
1:J:295:GLY:O	1:J:299:GLN:HG3	2.16	0.46
1:K:28:LEU:O	1:K:32:LEU:HB2	2.15	0.46
1:C:295:GLY:HA2	1:C:317:LEU:HD12	1.97	0.46
1:F:305:ASP:OD2	1:F:392:ARG:HD2	2.16	0.46
1:J:182:ARG:HB2	1:J:187:ASN:HA	1.98	0.46
1:C:182:ARG:HB2	1:C:187:ASN:HA	1.99	0.45
1:H:314:TYR:CD1	1:H:351:ARG:HD2	2.52	0.45
1:I:291:GLY:O	1:I:313:ALA:HA	2.16	0.45
1:I:322:GLU:HG2	1:I:424:ASP:HB2	1.98	0.45
1:G:159:THR:HG22	1:G:161:GLU:H	1.82	0.45
1:H:11:THR:HG23	1:H:12:ASP:H	1.81	0.45
1:H:182:ARG:HB2	1:H:187:ASN:HA	1.99	0.45
1:C:232:SER:HB3	1:C:297:GLY:HA3	1.98	0.45
1:C:305:ASP:OD2	1:C:392:ARG:HD2	2.17	0.45
1:E:262:LEU:O	1:E:392:ARG:NH2	2.38	0.45
1:E:397:LEU:HD22	1:E:397:LEU:C	2.34	0.45
1:E:415:MET:O	1:E:419:ARG:HG2	2.16	0.45
1:J:148:ARG:NH1	1:J:195:ASP:OD2	2.49	0.45
1:B:322:GLU:OE2	1:B:428:LYS:CD	2.64	0.44
1:H:266:VAL:O	1:H:280:ARG:HA	2.17	0.44
1:G:235:ILE:HB	2:G:501:YE1:HAE	2.00	0.44
1:A:193:GLN:NE2	4:A:613:HOH:O	2.50	0.44
1:K:173:ASP:HB2	4:K:617:HOH:O	2.17	0.44
1:L:291:GLY:O	1:L:313:ALA:HA	2.17	0.44
1:B:315:PHE:CZ	1:B:363:VAL:HG21	2.53	0.44
1:F:189:GLU:OE1	2:F:501:YE1:OAL	2.34	0.44
1:E:236:ASN:HA	2:E:501:YE1:N1A	2.33	0.44
1:I:175:VAL:HA	1:I:212:VAL:O	2.17	0.44
1:B:321:LYS:NZ	1:C:384:ASP:HB2	2.32	0.44
1:A:235:ILE:HB	2:A:501:YE1:HAE	2.00	0.44
1:E:291:GLY:O	1:E:313:ALA:HA	2.18	0.44
1:F:305:ASP:OD1	1:F:392:ARG:NH1	2.51	0.44
2:H:501:YE1:HAE	2:H:501:YE1:OAD	2.17	0.44
1:C:291:GLY:O	1:C:313:ALA:HA	2.18	0.43
2:E:501:YE1:OAD	2:E:501:YE1:HAE	2.19	0.43
1:I:159:THR:HG22	1:I:161:GLU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:ARG:NH1	4:J:602:HOH:O	2.35	0.43
1:J:322:GLU:HG2	1:J:424:ASP:HB2	2.00	0.43
1:L:182:ARG:HB2	1:L:187:ASN:HA	1.99	0.43
1:C:163:GLU:HG3	1:C:168:HIS:HD2	1.82	0.43
1:J:262:LEU:O	1:J:392:ARG:NH2	2.42	0.43
1:F:374:ALA:HB1	4:F:612:HOH:O	2.19	0.43
1:H:291:GLY:O	1:H:313:ALA:HA	2.19	0.43
1:K:291:GLY:O	1:K:313:ALA:HA	2.19	0.43
1:L:232:SER:HB3	1:L:297:GLY:HA3	2.00	0.43
1:E:163:GLU:HG3	1:E:168:HIS:HD2	1.83	0.43
1:C:266:VAL:O	1:C:280:ARG:HA	2.19	0.43
1:D:76:ARG:NH2	4:D:609:HOH:O	2.39	0.43
1:E:305:ASP:OD2	1:E:392:ARG:HD2	2.17	0.43
1:G:305:ASP:OD1	1:G:392:ARG:NH1	2.52	0.43
1:F:378:ARG:NH2	4:F:612:HOH:O	2.51	0.43
1:K:264:ARG:HG2	1:K:264:ARG:HH11	1.84	0.43
1:A:158:ARG:HA	1:E:52:ALA:HB2	2.01	0.43
1:D:245:ILE:HB	4:D:645:HOH:O	2.19	0.43
1:E:156:PHE:O	1:E:171:ARG:NH2	2.52	0.43
1:H:305:ASP:OD1	1:H:392:ARG:NH1	2.52	0.43
1:J:131:SER:HB3	1:J:134:ALA:HB3	2.01	0.43
1:F:224:ARG:HD3	2:F:501:YE1:O2A	2.19	0.43
1:H:232:SER:HB3	1:H:297:GLY:HA3	2.01	0.43
1:J:159:THR:HG22	1:J:161:GLU:H	1.84	0.43
1:C:12:ASP:HB2	1:C:13:GLY:H	1.48	0.42
1:G:264:ARG:HG2	1:G:264:ARG:HH11	1.84	0.42
1:H:28:LEU:O	1:H:32:LEU:HB2	2.19	0.42
1:J:304:PHE:O	1:L:340:ARG:NH2	2.38	0.42
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.85	0.42
2:F:501:YE1:HC71	2:F:501:YE1:N6A	2.34	0.42
1:I:38:ARG:O	1:I:43:ARG:NH1	2.51	0.42
1:K:143:LEU:O	1:K:261:LYS:HE2	2.19	0.42
1:D:38:ARG:O	1:D:43:ARG:NH1	2.52	0.42
1:E:235:ILE:HB	2:E:501:YE1:HAE	2.00	0.42
1:I:12:ASP:OD1	1:I:12:ASP:N	2.51	0.42
1:I:163:GLU:HG3	1:I:168:HIS:HD2	1.83	0.42
1:F:305:ASP:CG	1:F:392:ARG:HH11	2.22	0.42
1:K:295:GLY:O	1:K:299:GLN:HG3	2.19	0.42
1:K:350:ARG:NH2	1:K:358:GLU:OE1	2.48	0.42
1:D:360:ARG:HD2	1:D:360:ARG:HA	1.87	0.42
1:E:76:ARG:HG3	4:E:601:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:SER:HB3	1:F:297:GLY:HA3	2.01	0.42
1:G:315:PHE:CZ	1:G:363:VAL:HG21	2.55	0.42
1:K:266:VAL:O	1:K:280:ARG:HA	2.19	0.42
1:F:314:TYR:HB3	1:F:353:TRP:CE3	2.55	0.42
2:K:501:YE1:OAD	2:K:501:YE1:HAE	2.18	0.42
1:L:74:ASP:OD1	1:L:77:ARG:NH2	2.52	0.42
1:C:315:PHE:CZ	1:C:363:VAL:HG21	2.54	0.42
1:C:350:ARG:NH2	1:C:358:GLU:OE1	2.48	0.42
1:D:264:ARG:HH11	1:D:264:ARG:HG2	1.84	0.42
1:F:428:LYS:HD2	1:F:431:ARG:NH2	2.23	0.42
1:H:152:LEU:O	1:H:155:GLU:HG2	2.20	0.42
1:J:264:ARG:HG2	1:J:264:ARG:HH11	1.84	0.42
1:J:315:PHE:CZ	1:J:363:VAL:HG21	2.55	0.42
1:G:295:GLY:O	1:G:299:GLN:HG3	2.19	0.42
1:H:183:ASP:OD1	1:H:183:ASP:N	2.47	0.42
1:K:315:PHE:CZ	1:K:363:VAL:HG21	2.54	0.42
1:C:305:ASP:CG	1:C:392:ARG:HH11	2.24	0.41
1:D:190:ASP:HB2	4:D:662:HOH:O	2.19	0.41
1:G:411:GLU:HG3	1:H:397:LEU:HD11	2.02	0.41
1:I:295:GLY:O	1:I:299:GLN:HG3	2.20	0.41
1:A:295:GLY:CA	4:A:660:HOH:O	2.58	0.41
1:L:159:THR:HG22	1:L:161:GLU:N	2.35	0.41
1:B:266:VAL:O	1:B:280:ARG:HA	2.20	0.41
1:B:350:ARG:NH2	1:B:358:GLU:OE1	2.49	0.41
1:E:321:LYS:NZ	1:F:384:ASP:H	2.19	0.41
1:I:266:VAL:O	1:I:280:ARG:HA	2.20	0.41
1:L:266:VAL:O	1:L:280:ARG:HA	2.20	0.41
1:E:322:GLU:HG2	1:E:424:ASP:HB2	2.02	0.41
1:F:156:PHE:CD1	1:F:162:VAL:HG23	2.55	0.41
1:C:107:ARG:CZ	1:C:244:GLY:HA2	2.51	0.41
1:F:353:TRP:O	1:F:359:ALA:HB2	2.20	0.41
1:I:353:TRP:O	1:I:359:ALA:HB2	2.20	0.41
1:A:295:GLY:O	1:A:299:GLN:HG3	2.20	0.41
1:D:322:GLU:HG2	1:D:424:ASP:HB2	2.03	0.41
1:K:232:SER:HB3	1:K:297:GLY:HA3	2.02	0.41
1:B:235:ILE:HB	2:B:501:YE1:HAE	2.02	0.41
1:H:262:LEU:O	1:H:392:ARG:NH2	2.39	0.41
1:H:322:GLU:HG2	1:H:424:ASP:HB2	2.02	0.41
1:A:419:ARG:C	1:A:421:TYR:H	2.24	0.41
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.86	0.41
1:B:317:LEU:N	4:B:601:HOH:O	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:501:YE1:HAE	2:G:501:YE1:OAD	2.21	0.41
1:H:235:ILE:HB	2:H:501:YE1:HAE	2.01	0.41
1:A:28:LEU:O	1:A:32:LEU:HB2	2.21	0.41
1:A:275:TRP:O	1:A:275:TRP:CE3	2.72	0.41
1:D:315:PHE:CZ	1:D:363:VAL:HG21	2.56	0.41
1:F:182:ARG:HB2	1:F:187:ASN:HA	2.03	0.41
1:F:266:VAL:O	1:F:280:ARG:HA	2.21	0.41
1:I:272:ARG:HD3	1:I:273:PRO:HD2	2.03	0.41
2:D:501:YE1:HAC2	4:D:674:HOH:O	2.20	0.40
1:G:47:ALA:HB2	4:G:610:HOH:O	2.21	0.40
1:G:155:GLU:O	1:G:159:THR:HB	2.22	0.40
1:A:225:TYR:OH	2:A:501:YE1:O5A	2.37	0.40
1:E:28:LEU:O	1:E:32:LEU:HB2	2.21	0.40
1:F:360:ARG:HB2	4:F:655:HOH:O	2.21	0.40
1:H:317:LEU:HD22	1:H:326:PRO:HB2	2.03	0.40
1:I:232:SER:HB3	1:I:297:GLY:HA3	2.02	0.40
1:J:373:ASP:O	1:J:377:GLU:HG2	2.20	0.40
1:E:371:GLU:HB3	4:E:607:HOH:O	2.21	0.40
1:H:280:ARG:NH1	4:H:611:HOH:O	2.44	0.40
1:C:148:ARG:NH1	1:C:195:ASP:OD2	2.53	0.40
1:C:262:LEU:O	1:C:392:ARG:NH2	2.46	0.40
1:F:312:ASP:HB3	1:I:353:TRP:CH2	2.57	0.40
1:J:350:ARG:NH2	1:J:358:GLU:OE1	2.47	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	419/438 (96%)	410 (98%)	7 (2%)	2 (0%)	29 34
1	B	420/438 (96%)	411 (98%)	6 (1%)	3 (1%)	22 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	419/438 (96%)	412 (98%)	7 (2%)	0	100	100
1	D	421/438 (96%)	416 (99%)	5 (1%)	0	100	100
1	E	419/438 (96%)	411 (98%)	8 (2%)	0	100	100
1	F	419/438 (96%)	414 (99%)	5 (1%)	0	100	100
1	G	420/438 (96%)	413 (98%)	5 (1%)	2 (0%)	29	34
1	H	420/438 (96%)	411 (98%)	9 (2%)	0	100	100
1	I	419/438 (96%)	413 (99%)	6 (1%)	0	100	100
1	J	420/438 (96%)	413 (98%)	7 (2%)	0	100	100
1	K	420/438 (96%)	414 (99%)	6 (1%)	0	100	100
1	L	419/438 (96%)	412 (98%)	7 (2%)	0	100	100
All	All	5035/5256 (96%)	4950 (98%)	78 (2%)	7 (0%)	51	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	B	99	THR
1	B	270	ASP
1	G	270	ASP
1	A	276	TRP
1	B	269	ASN
1	G	269	ASN

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	331/345 (96%)	324 (98%)	7 (2%)	53	66
1	B	332/345 (96%)	324 (98%)	8 (2%)	49	61
1	C	331/345 (96%)	326 (98%)	5 (2%)	65	76
1	D	332/345 (96%)	320 (96%)	12 (4%)	35	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	331/345 (96%)	319 (96%)	12 (4%)	35	46
1	F	331/345 (96%)	321 (97%)	10 (3%)	41	52
1	G	332/345 (96%)	324 (98%)	8 (2%)	49	61
1	H	332/345 (96%)	324 (98%)	8 (2%)	49	61
1	I	331/345 (96%)	323 (98%)	8 (2%)	49	61
1	J	331/345 (96%)	324 (98%)	7 (2%)	53	66
1	K	332/345 (96%)	323 (97%)	9 (3%)	44	57
1	L	331/345 (96%)	324 (98%)	7 (2%)	53	66
All	All	3977/4140 (96%)	3876 (98%)	101 (2%)	47	60

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ARG
1	A	183	ASP
1	A	303	VAL
1	A	321	LYS
1	A	340	ARG
1	A	367	VAL
1	A	427	ASP
1	B	11	THR
1	B	51	ASP
1	B	173	ASP
1	B	177	ARG
1	B	186	LEU
1	B	340	ARG
1	B	392	ARG
1	B	428	LYS
1	C	12	ASP
1	C	177	ARG
1	C	303	VAL
1	C	317	LEU
1	C	392	ARG
1	D	11	THR
1	D	14	LEU
1	D	40	SER
1	D	177	ARG
1	D	182	ARG
1	D	183	ASP

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Mol	Chain	Res	Type
1	D	303	VAL
1	D	321	LYS
1	D	340	ARG
1	D	397	LEU
1	D	427	ASP
1	D	428	LYS
1	E	32	LEU
1	E	51	ASP
1	E	100	GLN
1	E	107	ARG
1	E	177	ARG
1	E	321	LYS
1	E	340	ARG
1	E	392	ARG
1	E	397	LEU
1	E	411	GLU
1	E	427	ASP
1	E	428	LYS
1	F	31	THR
1	F	40	SER
1	F	177	ARG
1	F	183	ASP
1	F	193	GLN
1	F	303	VAL
1	F	321	LYS
1	F	340	ARG
1	F	392	ARG
1	F	427	ASP
1	G	11	THR
1	G	177	ARG
1	G	183	ASP
1	G	321	LYS
1	G	340	ARG
1	G	367	VAL
1	G	392	ARG
1	G	428	LYS
1	H	51	ASP
1	H	107	ARG
1	H	155	GLU
1	H	173	ASP
1	H	226	ARG
1	H	340	ARG

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Mol	Chain	Res	Type
1	H	392	ARG
1	H	428	LYS
1	I	12	ASP
1	I	177	ARG
1	I	183	ASP
1	I	303	VAL
1	I	321	LYS
1	I	340	ARG
1	I	367	VAL
1	I	392	ARG
1	J	27	LYS
1	J	40	SER
1	J	100	GLN
1	J	177	ARG
1	J	303	VAL
1	J	340	ARG
1	J	392	ARG
1	K	40	SER
1	K	51	ASP
1	K	155	GLU
1	K	173	ASP
1	K	177	ARG
1	K	182	ARG
1	K	183	ASP
1	K	392	ARG
1	K	428	LYS
1	L	12	ASP
1	L	177	ARG
1	L	183	ASP
1	L	303	VAL
1	L	340	ARG
1	L	392	ARG
1	L	428	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	168	HIS
1	F	193	GLN
1	I	168	HIS
1	L	299	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)

24 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	YE1	A	501	-	54,62,62	2.33	7 (12%)	70,92,92	1.38	10 (14%)
3	OXY	C	502	-	1,1,1	0.14	0	-		
2	YE1	K	501	-	54,62,62	1.76	9 (16%)	70,92,92	1.30	8 (11%)
3	OXY	F	502	-	1,1,1	0.13	0	-		
2	YE1	F	501	-	54,62,62	1.81	4 (7%)	70,92,92	1.33	8 (11%)
2	YE1	L	501	-	54,62,62	1.86	7 (12%)	70,92,92	1.42	10 (14%)
3	OXY	G	502	-	1,1,1	0.13	0	-		
2	YE1	G	501	-	54,62,62	2.10	6 (11%)	70,92,92	1.31	8 (11%)
3	OXY	L	502	-	1,1,1	0.13	0	-		
2	YE1	E	501	-	54,62,62	1.80	7 (12%)	70,92,92	1.29	9 (12%)
3	OXY	E	502	-	1,1,1	0.14	0	-		
3	OXY	I	502	-	1,1,1	0.14	0	-		
2	YE1	I	501	-	54,62,62	1.92	7 (12%)	70,92,92	1.29	8 (11%)
3	OXY	B	502	-	1,1,1	0.14	0	-		
2	YE1	B	501	-	54,62,62	1.80	8 (14%)	70,92,92	1.42	8 (11%)
2	YE1	D	501	-	54,62,62	2.08	6 (11%)	70,92,92	1.25	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OXY	D	502	-	1,1,1	0.13	0	-		
3	OXY	A	502	-	1,1,1	0.14	0	-		
2	YE1	C	501	-	54,62,62	1.80	6 (11%)	70,92,92	1.28	7 (10%)
3	OXY	H	502	-	1,1,1	0.13	0	-		
3	OXY	K	502	-	1,1,1	0.14	0	-		
3	OXY	J	502	-	1,1,1	0.13	0	-		
2	YE1	J	501	-	54,62,62	2.20	9 (16%)	70,92,92	1.26	9 (12%)
2	YE1	H	501	-	54,62,62	1.93	8 (14%)	70,92,92	1.29	7 (10%)

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	YE1	K	501	-	-	6/51/71/71	0/4/4/4
2	YE1	B	501	-	-	24/51/71/71	0/4/4/4
2	YE1	D	501	-	-	18/51/71/71	0/4/4/4
2	YE1	F	501	-	-	15/51/71/71	0/4/4/4
2	YE1	L	501	-	-	7/51/71/71	0/4/4/4
2	YE1	J	501	-	-	12/51/71/71	0/4/4/4
2	YE1	G	501	-	-	7/51/71/71	0/4/4/4
2	YE1	A	501	-	-	13/51/71/71	0/4/4/4
2	YE1	C	501	-	-	9/51/71/71	0/4/4/4
2	YE1	E	501	-	-	6/51/71/71	0/4/4/4
2	YE1	H	501	-	-	10/51/71/71	0/4/4/4
2	YE1	I	501	-	-	15/51/71/71	0/4/4/4

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	YE1	P3'-O3'	14.11	1.86	1.59
2	G	501	YE1	P3'-O3'	11.81	1.81	1.59
2	J	501	YE1	P3'-O3'	11.70	1.81	1.59
2	D	501	YE1	P3'-O3'	11.06	1.80	1.59
2	I	501	YE1	P3'-O3'	9.90	1.78	1.59
2	H	501	YE1	P3'-O3'	9.81	1.77	1.59
2	L	501	YE1	P3'-O3'	9.69	1.77	1.59
2	F	501	YE1	P3'-O3'	9.52	1.77	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	YE1	P3'-O3'	9.11	1.76	1.59
2	C	501	YE1	P3'-O3'	8.94	1.76	1.59
2	B	501	YE1	P3'-O3'	8.55	1.75	1.59
2	K	501	YE1	P3'-O3'	8.50	1.75	1.59
2	D	501	YE1	P2A-O6A	5.30	1.80	1.59
2	C	501	YE1	P2A-O6A	4.93	1.79	1.59
2	H	501	YE1	P2A-O6A	4.75	1.78	1.59
2	E	501	YE1	P2A-O6A	4.55	1.77	1.59
2	J	501	YE1	P2A-O6A	4.47	1.77	1.59
2	F	501	YE1	P2A-O6A	4.40	1.77	1.59
2	I	501	YE1	P2A-O6A	4.34	1.76	1.59
2	G	501	YE1	P2A-O6A	4.30	1.76	1.59
2	L	501	YE1	P2A-O6A	4.19	1.76	1.59
2	B	501	YE1	P2A-O6A	4.16	1.76	1.59
2	J	501	YE1	CAC-CAB	3.98	1.60	1.51
2	K	501	YE1	P2A-O6A	3.97	1.75	1.59
2	A	501	YE1	P2A-O6A	3.93	1.75	1.59
2	J	501	YE1	C5P-N4P	3.77	1.42	1.33
2	D	501	YE1	C5P-N4P	3.60	1.41	1.33
2	I	501	YE1	C5P-N4P	3.27	1.40	1.33
2	G	501	YE1	C5P-N4P	3.21	1.40	1.33
2	C	501	YE1	C5P-N4P	3.09	1.40	1.33
2	C	501	YE1	O3'-C3'	-3.02	1.33	1.44
2	E	501	YE1	C5P-N4P	2.90	1.40	1.33
2	H	501	YE1	C4A-N3A	2.90	1.39	1.35
2	B	501	YE1	C5P-N4P	2.88	1.39	1.33
2	A	501	YE1	C2'-C3'	2.79	1.59	1.52
2	L	501	YE1	C5P-N4P	2.75	1.39	1.33
2	K	501	YE1	C5P-N4P	2.74	1.39	1.33
2	A	501	YE1	C5P-N4P	2.73	1.39	1.33
2	B	501	YE1	O3'-C3'	-2.67	1.34	1.44
2	L	501	YE1	O3'-C3'	-2.60	1.34	1.44
2	H	501	YE1	C2A-N1A	2.59	1.38	1.33
2	K	501	YE1	O3'-C3'	-2.57	1.34	1.44
2	F	501	YE1	C5P-N4P	2.56	1.39	1.33
2	H	501	YE1	C5P-N4P	2.54	1.39	1.33
2	I	501	YE1	CAC-CAB	2.54	1.57	1.51
2	I	501	YE1	O3'-C3'	-2.51	1.35	1.44
2	E	501	YE1	O3'-C3'	-2.51	1.35	1.44
2	H	501	YE1	O3'-C3'	-2.50	1.35	1.44
2	D	501	YE1	C2A-N1A	2.48	1.38	1.33
2	K	501	YE1	P1A-O5'	2.46	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	501	YE1	P1A-O5'	2.45	1.69	1.59
2	E	501	YE1	C4A-N3A	2.45	1.39	1.35
2	A	501	YE1	O6A-C12	-2.40	1.36	1.43
2	D	501	YE1	O3'-C3'	-2.39	1.35	1.44
2	B	501	YE1	C4A-N3A	2.39	1.39	1.35
2	G	501	YE1	P1A-O5'	2.37	1.68	1.59
2	K	501	YE1	C2A-N3A	2.31	1.35	1.32
2	J	501	YE1	P1A-O5'	2.30	1.68	1.59
2	I	501	YE1	CAB-NAA	2.30	1.38	1.33
2	K	501	YE1	C2A-N1A	2.30	1.38	1.33
2	A	501	YE1	C2A-N1A	2.29	1.38	1.33
2	G	501	YE1	CAB-NAA	2.28	1.38	1.33
2	I	501	YE1	P1A-O5'	2.28	1.68	1.59
2	G	501	YE1	O3'-C3'	-2.26	1.35	1.44
2	F	501	YE1	O3'-C3'	-2.23	1.36	1.44
2	H	501	YE1	C2A-N3A	2.14	1.35	1.32
2	L	501	YE1	C3'-C4'	2.13	1.58	1.52
2	H	501	YE1	O5'-C5'	-2.13	1.36	1.44
2	E	501	YE1	C2A-N1A	2.11	1.37	1.33
2	B	501	YE1	C2A-N3A	2.11	1.35	1.32
2	J	501	YE1	O3'-C3'	-2.10	1.36	1.44
2	B	501	YE1	C2A-N1A	2.08	1.37	1.33
2	A	501	YE1	C6P-C5P	-2.06	1.47	1.51
2	L	501	YE1	O4'-C1'	-2.06	1.38	1.41
2	J	501	YE1	CAB-NAA	2.06	1.38	1.33
2	E	501	YE1	P1A-O5'	2.06	1.67	1.59
2	C	501	YE1	O5'-C5'	-2.05	1.36	1.44
2	B	501	YE1	O6A-C12	-2.04	1.37	1.43
2	J	501	YE1	C2A-N1A	2.03	1.37	1.33
2	K	501	YE1	C4A-N3A	2.03	1.38	1.35
2	J	501	YE1	O6A-C12	-2.03	1.37	1.43
2	C	501	YE1	CAC-CAB	2.03	1.56	1.51
2	K	501	YE1	O6A-C12	-2.02	1.37	1.43
2	D	501	YE1	CAC-CAB	2.02	1.56	1.51

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	YE1	CAC-CAB-NAA	-4.45	110.17	116.19
2	L	501	YE1	CAC-CAB-NAA	-4.09	110.66	116.19
2	B	501	YE1	O3'-P3'-O7A	-3.93	94.24	109.39
2	C	501	YE1	CAC-CAB-NAA	-3.86	110.97	116.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	501	YE1	O3'-P3'-O7A	-3.65	95.30	109.39
2	F	501	YE1	CAC-CAB-NAA	-3.64	111.27	116.19
2	I	501	YE1	O3'-P3'-O7A	-3.62	95.42	109.39
2	D	501	YE1	O3'-P3'-O7A	-3.62	95.43	109.39
2	E	501	YE1	O3'-P3'-O7A	-3.58	95.59	109.39
2	H	501	YE1	O3'-P3'-O7A	-3.56	95.66	109.39
2	C	501	YE1	O3'-P3'-O7A	-3.55	95.71	109.39
2	K	501	YE1	CAC-CAB-NAA	-3.52	111.43	116.19
2	A	501	YE1	CAC-CAB-NAA	-3.48	111.48	116.19
2	G	501	YE1	O3'-P3'-O7A	-3.47	95.98	109.39
2	B	501	YE1	C6P-C5P-N4P	-3.42	110.66	116.42
2	D	501	YE1	CAC-CAB-NAA	-3.39	111.61	116.19
2	K	501	YE1	O3'-P3'-O7A	-3.38	96.33	109.39
2	L	501	YE1	O3'-P3'-O7A	-3.37	96.40	109.39
2	L	501	YE1	O6A-C12-C11	-3.23	105.36	110.55
2	K	501	YE1	C6P-C5P-N4P	-3.13	111.15	116.42
2	L	501	YE1	C6P-C5P-N4P	-3.12	111.17	116.42
2	F	501	YE1	O3'-P3'-O7A	-3.11	97.38	109.39
2	H	501	YE1	C6P-C5P-N4P	-2.96	111.44	116.42
2	G	501	YE1	CAC-CAB-NAA	-2.81	112.39	116.19
2	E	501	YE1	CAC-CAB-NAA	-2.80	112.40	116.19
2	G	501	YE1	C6P-C5P-N4P	-2.79	111.73	116.42
2	I	501	YE1	C6P-C5P-N4P	-2.77	111.76	116.42
2	E	501	YE1	O6A-C12-C11	-2.77	106.10	110.55
2	B	501	YE1	O4A-P2A-O5A	2.75	125.85	112.24
2	H	501	YE1	CAC-CAB-NAA	-2.73	112.50	116.19
2	E	501	YE1	O4A-P2A-O5A	2.71	125.66	112.24
2	A	501	YE1	C1'-N9A-C4A	-2.70	121.89	126.64
2	G	501	YE1	O4A-P2A-O5A	2.69	125.54	112.24
2	I	501	YE1	CAC-CAB-NAA	-2.68	112.56	116.19
2	K	501	YE1	C7P-C6P-C5P	-2.68	107.89	112.36
2	A	501	YE1	O4A-P2A-O5A	2.67	125.45	112.24
2	J	501	YE1	CAC-CAB-NAA	-2.65	112.61	116.19
2	I	501	YE1	O4A-P2A-O5A	2.64	125.30	112.24
2	J	501	YE1	C6P-C5P-N4P	-2.63	111.99	116.42
2	D	501	YE1	C6P-C5P-N4P	-2.62	112.02	116.42
2	J	501	YE1	O4A-P2A-O5A	2.61	125.12	112.24
2	L	501	YE1	O4A-P2A-O5A	2.59	125.06	112.24
2	H	501	YE1	O4A-P2A-O5A	2.59	125.04	112.24
2	D	501	YE1	O4A-P2A-O5A	2.59	125.03	112.24
2	K	501	YE1	O4A-P2A-O5A	2.59	125.03	112.24
2	A	501	YE1	C6P-C5P-N4P	-2.58	112.07	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	YE1	O4A-P2A-O5A	2.58	125.00	112.24
2	L	501	YE1	O5P-C5P-C6P	2.56	126.70	122.02
2	F	501	YE1	C13-C11-C10	2.55	113.24	108.82
2	A	501	YE1	O3'-P3'-O7A	-2.55	99.56	109.39
2	A	501	YE1	C7P-C6P-C5P	-2.53	108.14	112.36
2	L	501	YE1	C1'-N9A-C4A	-2.51	122.23	126.64
2	F	501	YE1	C6P-C5P-N4P	-2.49	112.22	116.42
2	I	501	YE1	O6A-P2A-O5A	-2.47	99.41	109.07
2	C	501	YE1	O4A-P2A-O5A	2.45	124.37	112.24
2	B	501	YE1	O5P-C5P-C6P	2.44	126.48	122.02
2	B	501	YE1	CAF-CAC-CAB	2.43	119.78	112.57
2	G	501	YE1	C1'-N9A-C4A	-2.40	122.43	126.64
2	H	501	YE1	C6P-C7P-N8P	-2.40	107.06	111.90
2	F	501	YE1	O5P-C5P-C6P	2.40	126.40	122.02
2	H	501	YE1	O6A-C12-C11	-2.39	106.71	110.55
2	A	501	YE1	O4'-C1'-C2'	2.38	110.40	106.93
2	I	501	YE1	CAH-CAI-CAJ	-2.38	116.36	119.20
2	A	501	YE1	O6A-C12-C11	-2.35	106.77	110.55
2	I	501	YE1	C7P-C6P-C5P	-2.34	108.47	112.36
2	G	501	YE1	O5P-C5P-C6P	2.33	126.28	122.02
2	E	501	YE1	C7P-C6P-C5P	-2.32	108.49	112.36
2	F	501	YE1	O1A-P1A-O2A	2.32	123.69	112.24
2	J	501	YE1	O6A-C12-C11	-2.26	106.91	110.55
2	E	501	YE1	CAH-CAG-CAF	-2.26	118.68	120.35
2	L	501	YE1	CAH-CAI-CAJ	-2.25	116.51	119.20
2	C	501	YE1	C6P-C5P-N4P	-2.25	112.64	116.42
2	D	501	YE1	O5P-C5P-C6P	2.21	126.05	122.02
2	F	501	YE1	CAH-CAG-CAF	-2.20	118.72	120.35
2	D	501	YE1	CAF-CAC-CAB	2.20	119.08	112.57
2	J	501	YE1	C2'-C3'-C4'	-2.18	99.36	103.22
2	G	501	YE1	CAH-CAG-CAF	-2.18	118.74	120.35
2	L	501	YE1	CAF-CAC-CAB	2.18	119.02	112.57
2	C	501	YE1	O6A-C12-C11	-2.18	107.05	110.55
2	A	501	YE1	CAH-CAG-CAF	-2.17	118.75	120.35
2	C	501	YE1	O5P-C5P-C6P	2.16	125.97	122.02
2	D	501	YE1	C13-C11-C10	2.16	112.56	108.82
2	E	501	YE1	C6P-C5P-N4P	-2.16	112.79	116.42
2	H	501	YE1	O5P-C5P-C6P	2.15	125.95	122.02
2	G	501	YE1	O1A-P1A-O2A	2.13	122.78	112.24
2	I	501	YE1	O1A-P1A-O2A	2.13	122.76	112.24
2	J	501	YE1	CAH-CAG-CAF	-2.12	118.78	120.35
2	A	501	YE1	O1A-P1A-O2A	2.12	122.72	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	YE1	O5P-C5P-C6P	2.11	125.87	122.02
2	E	501	YE1	O1A-P1A-O2A	2.11	122.65	112.24
2	L	501	YE1	O1A-P1A-O2A	2.09	122.55	112.24
2	J	501	YE1	O1A-P1A-O2A	2.08	122.53	112.24
2	K	501	YE1	O1A-P1A-O2A	2.07	122.50	112.24
2	K	501	YE1	O5P-C5P-C6P	2.07	125.81	122.02
2	C	501	YE1	O1A-P1A-O2A	2.07	122.47	112.24
2	K	501	YE1	CAF-CAC-CAB	2.06	118.67	112.57
2	J	501	YE1	O6A-P2A-O5A	-2.05	101.06	109.07
2	D	501	YE1	O1A-P1A-O2A	2.04	122.34	112.24
2	B	501	YE1	C7P-N8P-C9P	2.02	126.19	122.59
2	B	501	YE1	C2'-C3'-C4'	-2.01	99.66	103.22

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	YE1	C5'-O5'-P1A-O1A
2	A	501	YE1	C5'-O5'-P1A-O2A
2	B	501	YE1	C5'-O5'-P1A-O2A
2	B	501	YE1	C12-O6A-P2A-O4A
2	B	501	YE1	C12-O6A-P2A-O5A
2	B	501	YE1	C10-C11-C12-O6A
2	B	501	YE1	O10-C10-C11-C12
2	B	501	YE1	O10-C10-C11-C13
2	C	501	YE1	C5'-O5'-P1A-O2A
2	D	501	YE1	C3'-O3'-P3'-O9A
2	D	501	YE1	C5'-O5'-P1A-O2A
2	D	501	YE1	C12-O6A-P2A-O4A
2	D	501	YE1	C12-O6A-P2A-O5A
2	D	501	YE1	C13-C11-C12-O6A
2	D	501	YE1	C10-C11-C12-O6A
2	E	501	YE1	C5'-O5'-P1A-O2A
2	F	501	YE1	C3'-O3'-P3'-O7A
2	F	501	YE1	C5'-O5'-P1A-O2A
2	F	501	YE1	O10-C10-C9P-N8P
2	G	501	YE1	C5'-O5'-P1A-O2A
2	H	501	YE1	C3'-O3'-P3'-O9A
2	H	501	YE1	C5'-O5'-P1A-O2A
2	I	501	YE1	C12-O6A-P2A-O5A
2	I	501	YE1	C10-C11-C12-O6A
2	J	501	YE1	C3'-O3'-P3'-O7A

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Mol	Chain	Res	Type	Atoms
2	J	501	YE1	C5'-O5'-P1A-O2A
2	K	501	YE1	C5'-O5'-P1A-O2A
2	L	501	YE1	C5'-O5'-P1A-O2A
2	B	501	YE1	C6P-C7P-N8P-C9P
2	A	501	YE1	C2'-C3'-O3'-P3'
2	A	501	YE1	C4'-C3'-O3'-P3'
2	B	501	YE1	C14-C11-C12-O6A
2	B	501	YE1	C13-C11-C12-O6A
2	D	501	YE1	C14-C11-C12-O6A
2	F	501	YE1	CAB-CAC-CAF-CAG
2	F	501	YE1	CAB-CAC-CAF-CAE
2	J	501	YE1	CAB-CAC-CAF-CAG
2	C	501	YE1	CAB-CAC-CAF-CAG
2	C	501	YE1	CAB-CAC-CAF-CAE
2	I	501	YE1	CAB-CAC-CAF-CAG
2	I	501	YE1	CAB-CAC-CAF-CAE
2	J	501	YE1	CAB-CAC-CAF-CAE
2	K	501	YE1	CAB-CAC-CAF-CAG
2	G	501	YE1	CAB-CAC-CAF-CAG
2	K	501	YE1	CAB-CAC-CAF-CAE
2	F	501	YE1	O10-C10-C9P-O9P
2	I	501	YE1	C14-C11-C12-O6A
2	I	501	YE1	C13-C11-C12-O6A
2	H	501	YE1	CAB-CAC-CAF-CAE
2	B	501	YE1	O10-C10-C11-C14
2	D	501	YE1	CAB-CAC-CAF-CAE
2	G	501	YE1	CAB-CAC-CAF-CAE
2	H	501	YE1	CAB-CAC-CAF-CAG
2	D	501	YE1	CAB-CAC-CAF-CAG
2	B	501	YE1	C11-C10-C9P-N8P
2	H	501	YE1	C4'-C5'-O5'-P1A
2	E	501	YE1	CAB-CAC-CAF-CAG
2	B	501	YE1	P1A-O3A-P2A-O6A
2	D	501	YE1	P1A-O3A-P2A-O6A
2	I	501	YE1	P1A-O3A-P2A-O6A
2	E	501	YE1	CAB-CAC-CAF-CAE
2	L	501	YE1	CAB-CAC-CAF-CAG
2	L	501	YE1	CAB-CAC-CAF-CAE
2	D	501	YE1	C3'-O3'-P3'-O7A
2	H	501	YE1	C3'-O3'-P3'-O7A
2	B	501	YE1	C2P-C3P-N4P-C5P
2	B	501	YE1	C3'-O3'-P3'-O9A

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Mol	Chain	Res	Type	Atoms
2	B	501	YE1	C12-O6A-P2A-O3A
2	C	501	YE1	C3'-O3'-P3'-O9A
2	D	501	YE1	C5'-O5'-P1A-O3A
2	E	501	YE1	C5'-O5'-P1A-O3A
2	F	501	YE1	C5'-O5'-P1A-O3A
2	G	501	YE1	C5'-O5'-P1A-O3A
2	I	501	YE1	C12-O6A-P2A-O3A
2	J	501	YE1	C3'-O3'-P3'-O9A
2	J	501	YE1	C5'-O5'-P1A-O3A
2	K	501	YE1	C5'-O5'-P1A-O3A
2	L	501	YE1	C5'-O5'-P1A-O3A
2	B	501	YE1	P2A-O3A-P1A-O2A
2	B	501	YE1	P1A-O3A-P2A-O5A
2	C	501	YE1	P1A-O3A-P2A-O4A
2	D	501	YE1	P2A-O3A-P1A-O1A
2	B	501	YE1	CAB-CAC-CAF-CAG
2	J	501	YE1	C6P-C7P-N8P-C9P
2	C	501	YE1	C4'-C5'-O5'-P1A
2	C	501	YE1	C5'-O5'-P1A-O1A
2	D	501	YE1	C5'-O5'-P1A-O1A
2	E	501	YE1	C5'-O5'-P1A-O1A
2	F	501	YE1	C5'-O5'-P1A-O1A
2	G	501	YE1	C5'-O5'-P1A-O1A
2	H	501	YE1	C5'-O5'-P1A-O1A
2	I	501	YE1	C12-O6A-P2A-O4A
2	J	501	YE1	C5'-O5'-P1A-O1A
2	K	501	YE1	C5'-O5'-P1A-O1A
2	L	501	YE1	C5'-O5'-P1A-O1A
2	A	501	YE1	C10-C11-C12-O6A
2	F	501	YE1	C10-C11-C12-O6A
2	H	501	YE1	C2P-C3P-N4P-C5P
2	D	501	YE1	C4'-C5'-O5'-P1A
2	J	501	YE1	C4'-C5'-O5'-P1A
2	L	501	YE1	C2P-C3P-N4P-C5P
2	A	501	YE1	C14-C11-C12-O6A
2	F	501	YE1	C14-C11-C12-O6A
2	B	501	YE1	CAB-CAC-CAF-CAE
2	B	501	YE1	C4'-C5'-O5'-P1A
2	G	501	YE1	C4'-C5'-O5'-P1A
2	B	501	YE1	P2A-O3A-P1A-O1A
2	D	501	YE1	P2A-O3A-P1A-O2A
2	A	501	YE1	C4'-C5'-O5'-P1A

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Mol	Chain	Res	Type	Atoms
2	F	501	YE1	C4'-C5'-O5'-P1A
2	J	501	YE1	O5P-C5P-C6P-C7P
2	B	501	YE1	C11-C10-C9P-O9P
2	E	501	YE1	C4'-C5'-O5'-P1A
2	K	501	YE1	C4'-C5'-O5'-P1A
2	C	501	YE1	P1A-O3A-P2A-O5A
2	D	501	YE1	P1A-O3A-P2A-O5A
2	J	501	YE1	N4P-C5P-C6P-C7P
2	I	501	YE1	O10-C10-C9P-O9P
2	A	501	YE1	C3'-O3'-P3'-O7A
2	I	501	YE1	C3'-O3'-P3'-O7A
2	I	501	YE1	O10-C10-C9P-N8P
2	F	501	YE1	C13-C11-C12-O6A
2	B	501	YE1	C9P-C10-C11-C13
2	A	501	YE1	C3'-O3'-P3'-O9A
2	A	501	YE1	C5'-O5'-P1A-O3A
2	B	501	YE1	C5'-O5'-P1A-O3A
2	C	501	YE1	C5'-O5'-P1A-O3A
2	D	501	YE1	C12-O6A-P2A-O3A
2	H	501	YE1	C5'-O5'-P1A-O3A
2	I	501	YE1	C3'-O3'-P3'-O8A
2	I	501	YE1	C3'-O3'-P3'-O9A
2	I	501	YE1	P2A-O3A-P1A-O1A
2	J	501	YE1	P1A-O3A-P2A-O4A
2	G	501	YE1	C12-O6A-P2A-O5A
2	A	501	YE1	C13-C11-C12-O6A
2	H	501	YE1	C14-C11-C12-O6A
2	F	501	YE1	C11-C10-C9P-O9P
2	F	501	YE1	C6P-C7P-N8P-C9P
2	L	501	YE1	C4'-C5'-O5'-P1A
2	F	501	YE1	O5P-C5P-C6P-C7P
2	A	501	YE1	CAB-CAC-CAF-CAG
2	A	501	YE1	CAB-CAC-CAF-CAE

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	YE1	2	0
2	K	501	YE1	1	0
2	F	501	YE1	6	0
2	L	501	YE1	1	0

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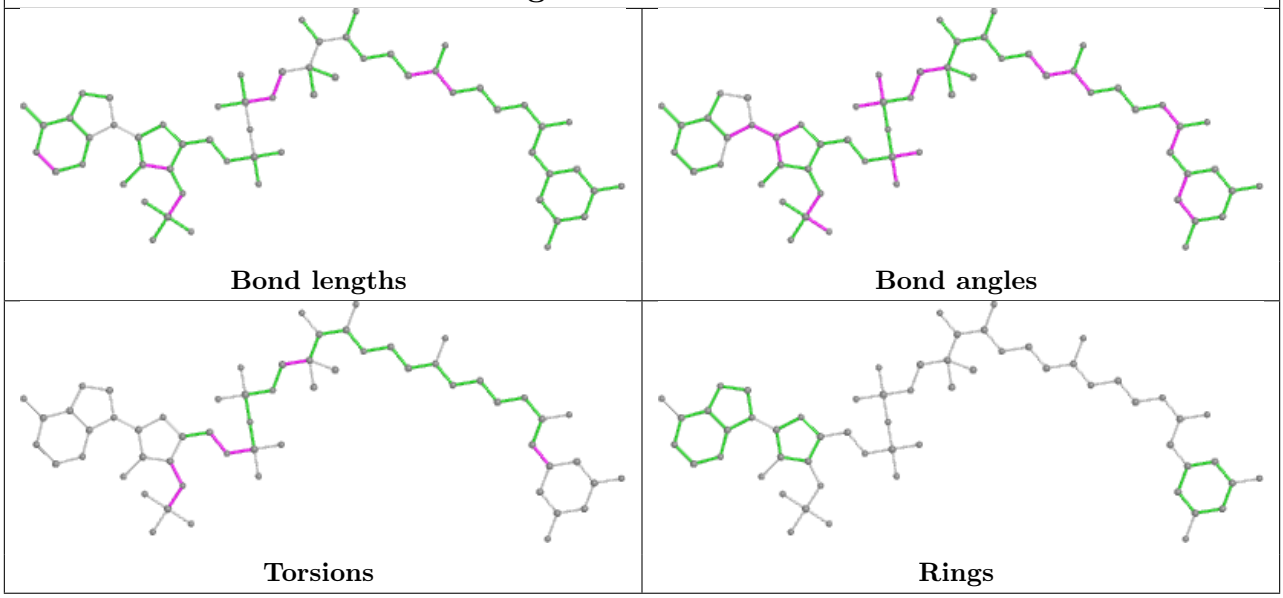
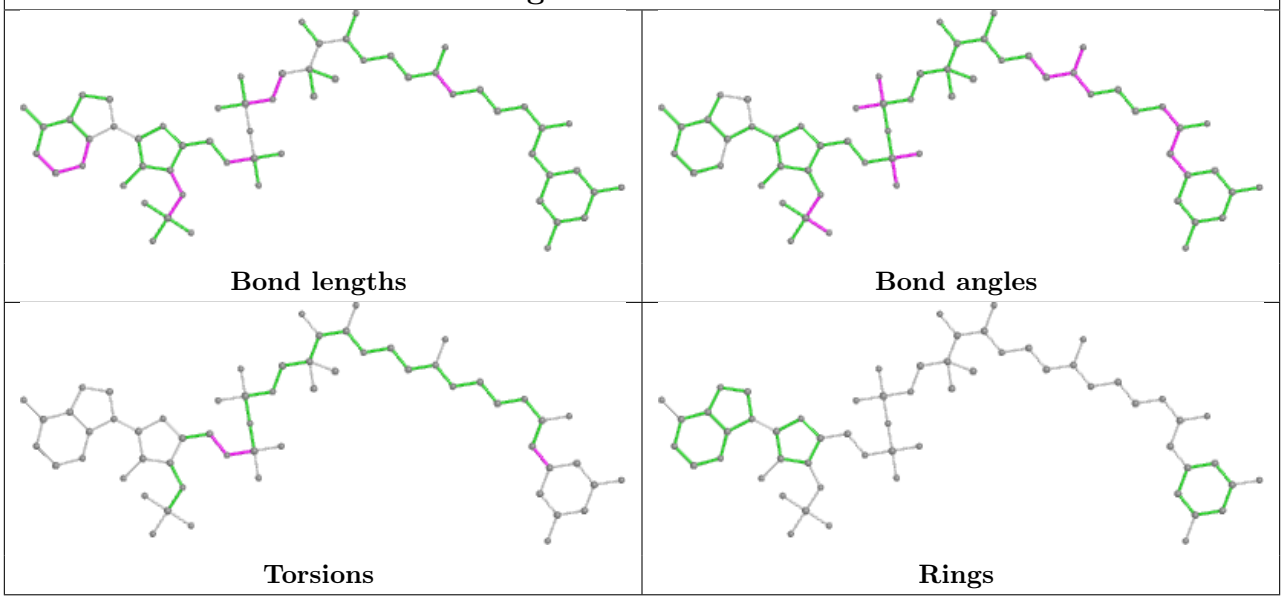
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	YE1	4	0
2	E	501	YE1	3	0
2	I	501	YE1	2	0
2	B	501	YE1	1	0
2	D	501	YE1	2	0
2	C	501	YE1	1	0
2	J	501	YE1	5	0
2	H	501	YE1	3	0

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.

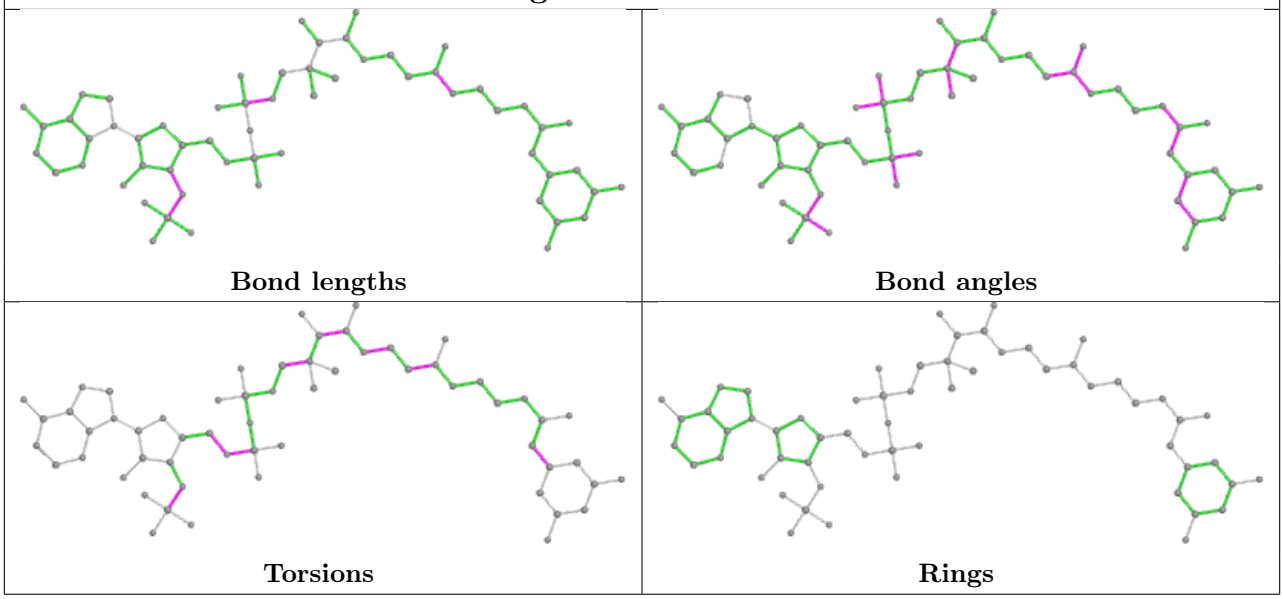
Ligand YE1 A 501



Ligand YE1 K 501



Ligand YE1 F 501



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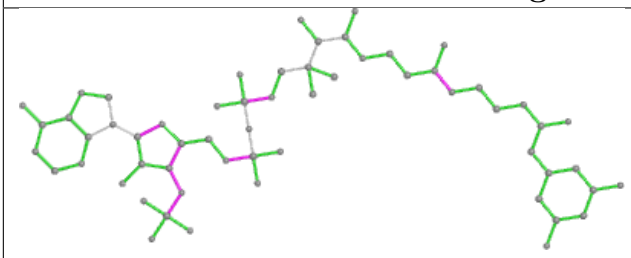
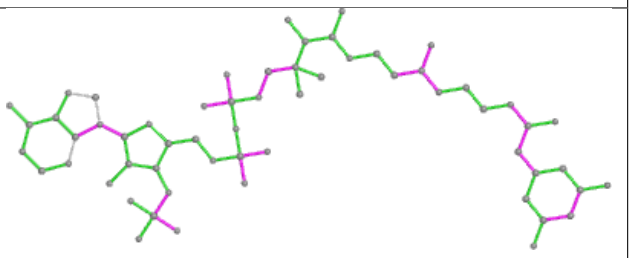
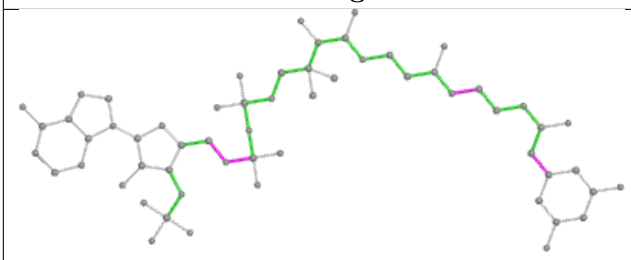
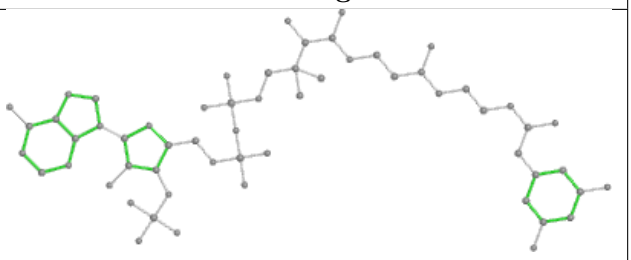
 Bond lengths	 Bond angles
 Torsions	 Rings

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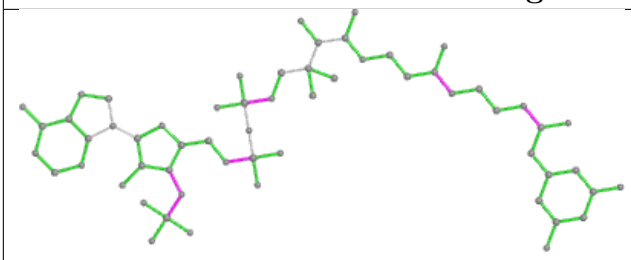
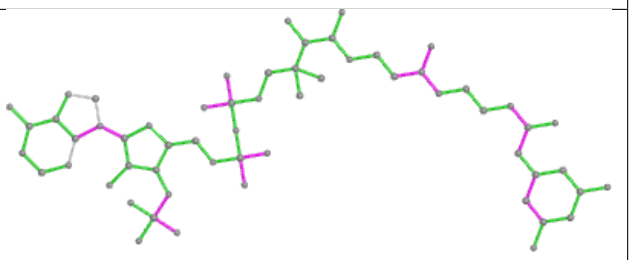
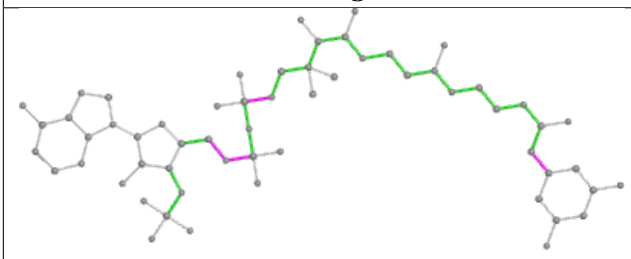
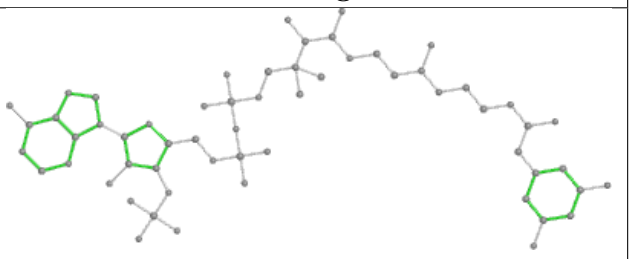
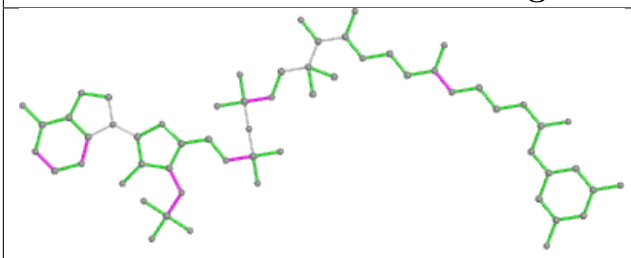
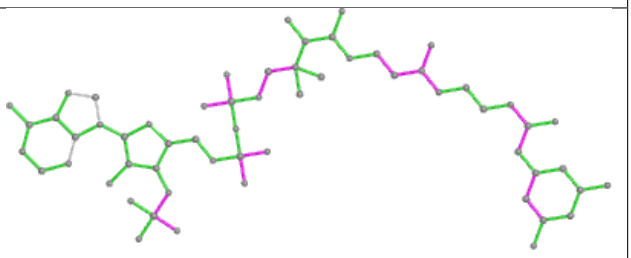
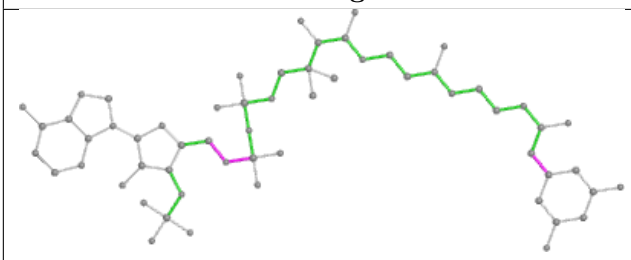
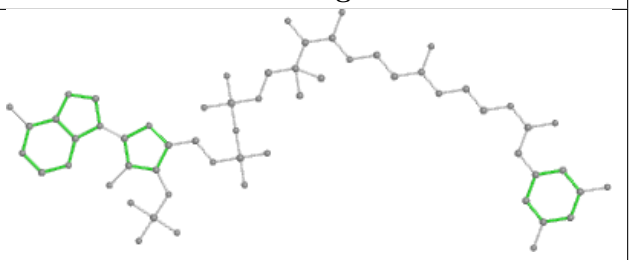
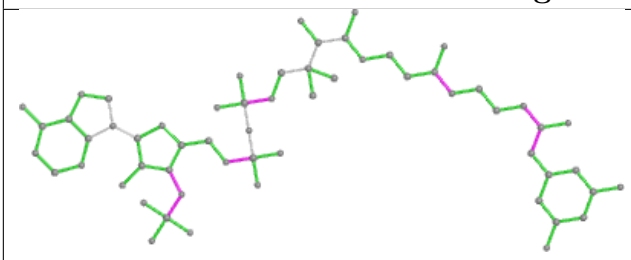
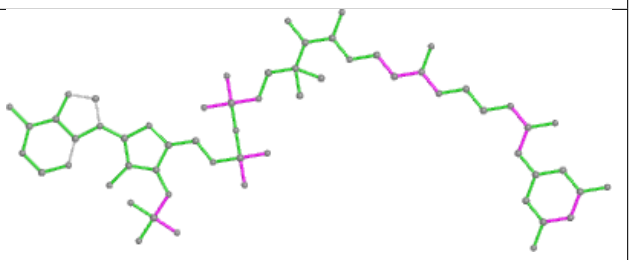
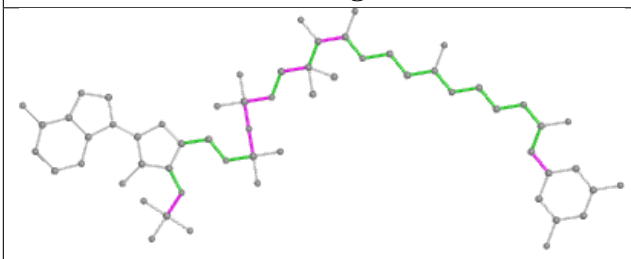
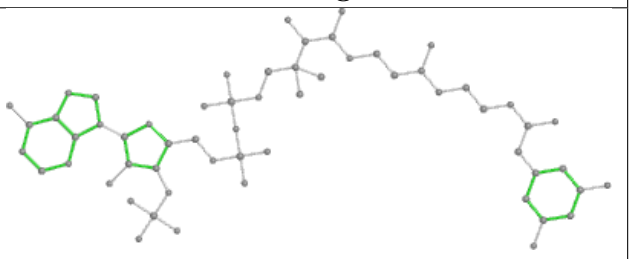
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand YE1 E 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand YE1 I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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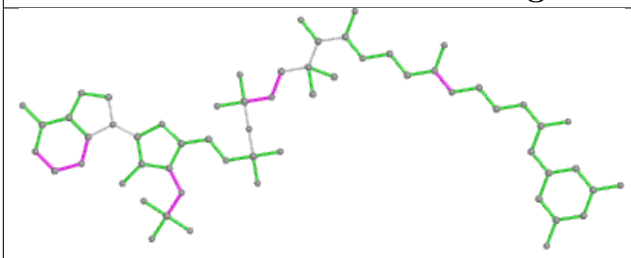
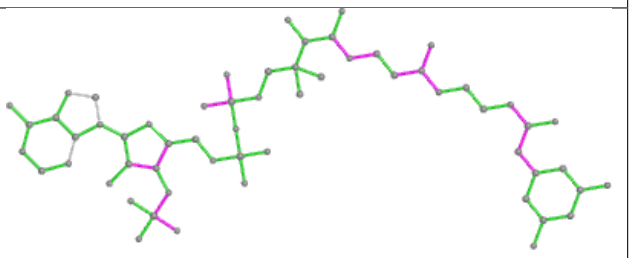
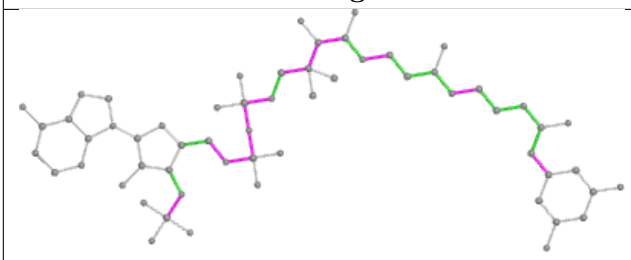
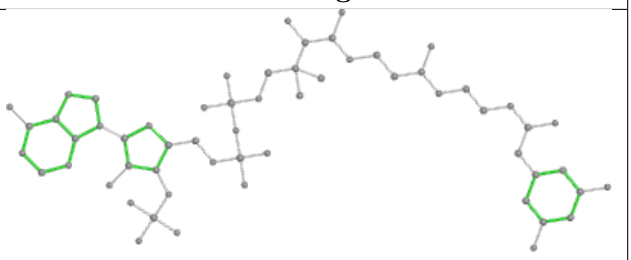
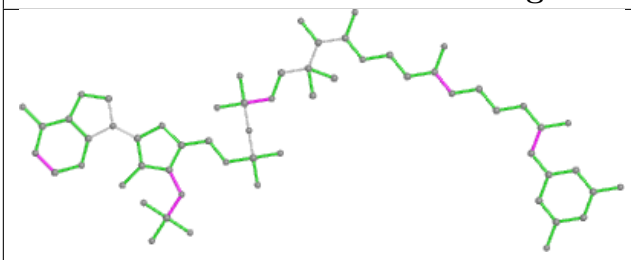
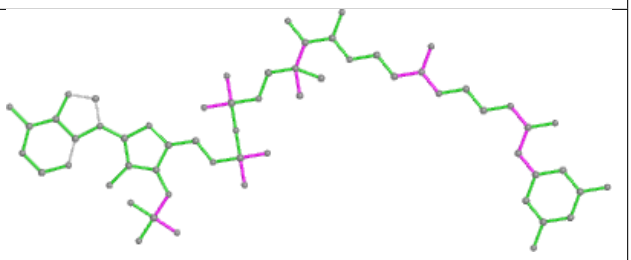
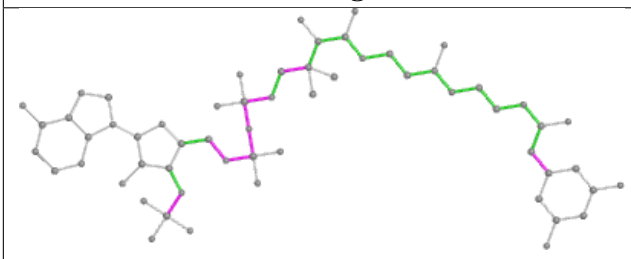
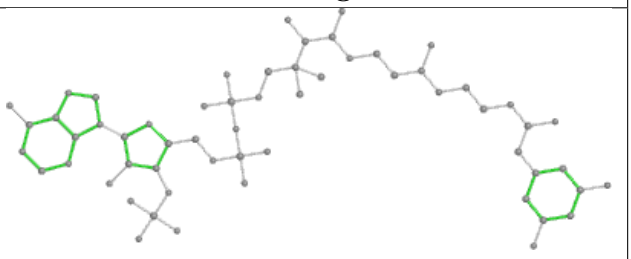
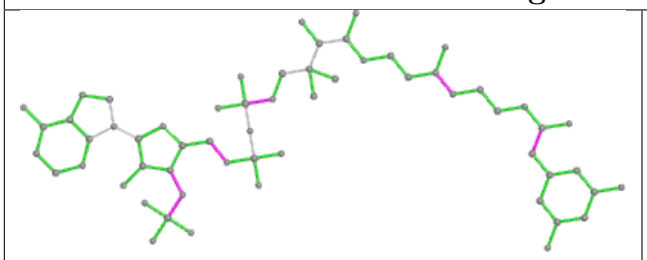
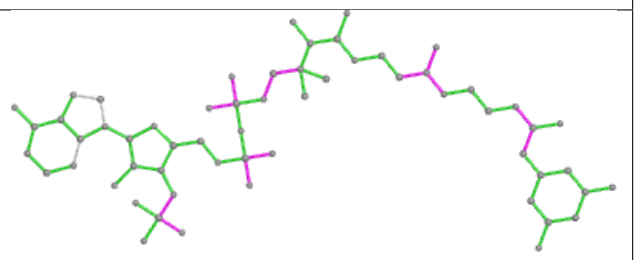
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand YE1 D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

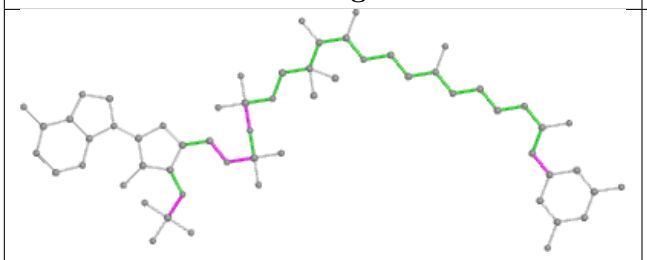
Ligand YE1 C 501



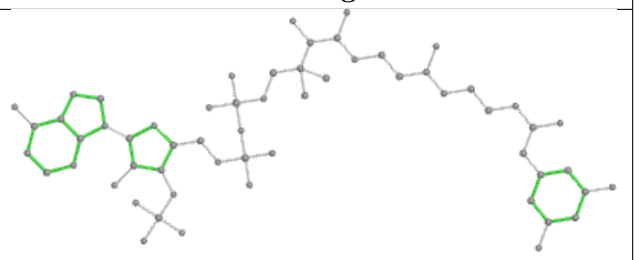
Bond lengths



Bond angles

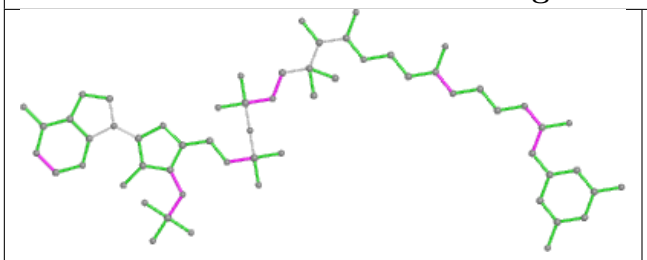


Torsions



Rings

Ligand YE1 J 501



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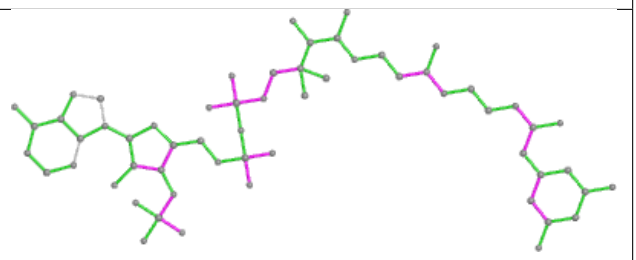

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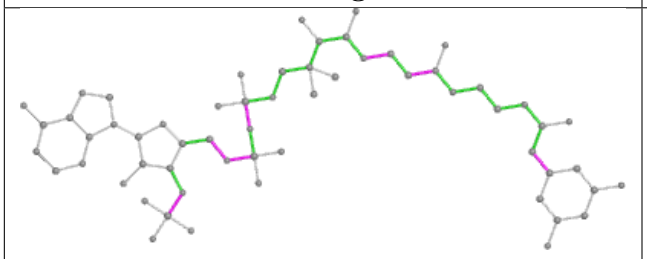
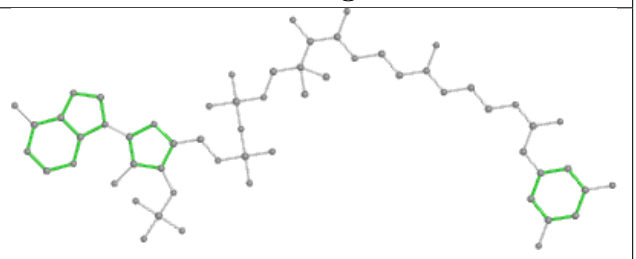
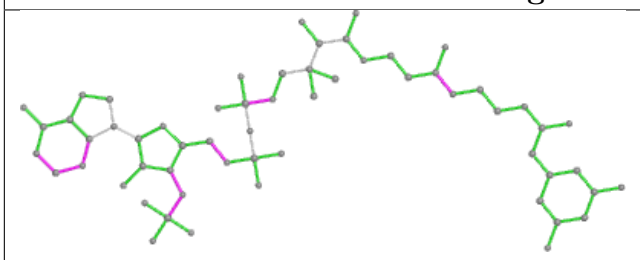
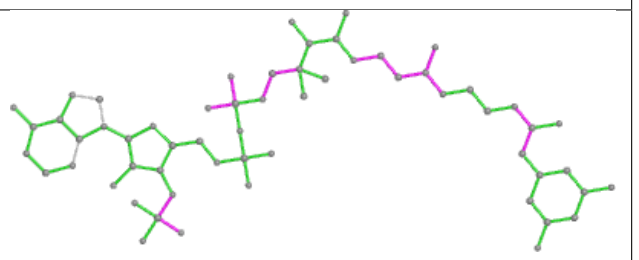
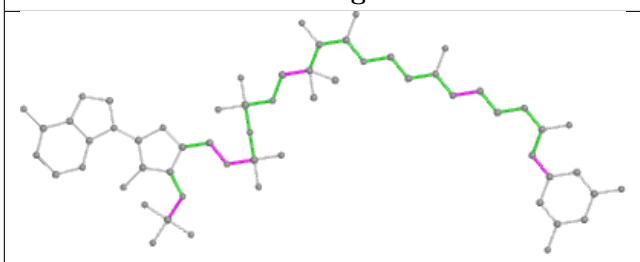
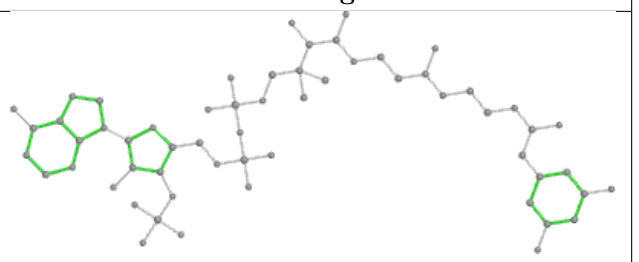


Torsions



Rings

Ligand YE1 H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	421/438 (96%)	-0.13	3 (0%)	87	88	17, 30, 60, 84	0
1	B	422/438 (96%)	-0.17	1 (0%)	95	95	20, 33, 51, 66	0
1	C	421/438 (96%)	-0.16	2 (0%)	91	92	16, 31, 53, 80	0
1	D	423/438 (96%)	-0.24	0	100	100	17, 26, 43, 56	0
1	E	421/438 (96%)	-0.28	1 (0%)	95	95	16, 28, 43, 59	0
1	F	421/438 (96%)	-0.22	2 (0%)	91	92	17, 28, 48, 63	0
1	G	422/438 (96%)	-0.17	1 (0%)	95	95	17, 30, 52, 68	0
1	H	422/438 (96%)	-0.00	2 (0%)	91	92	21, 38, 54, 65	0
1	I	421/438 (96%)	-0.14	1 (0%)	95	95	17, 31, 47, 61	0
1	J	422/438 (96%)	0.20	12 (2%)	53	49	24, 40, 73, 91	0
1	K	422/438 (96%)	-0.14	0	100	100	17, 29, 50, 64	0
1	L	421/438 (96%)	-0.08	1 (0%)	95	95	17, 32, 62, 73	0
All	All	5059/5256 (96%)	-0.13	26 (0%)	91	92	16, 31, 55, 91	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	224	ARG	3.4
1	A	35	HIS	3.3
1	J	31	THR	3.2
1	A	43	ARG	3.2
1	J	56	LEU	3.2
1	G	40	SER	3.1
1	C	315	PHE	3.0
1	F	315	PHE	2.8
1	J	41	ALA	2.8
1	J	223	PRO	2.7
1	C	224	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	431	ARG	2.6
1	J	45	GLU	2.6
1	A	37	ALA	2.6
1	J	32	LEU	2.5
1	L	315	PHE	2.4
1	J	101	GLN	2.4
1	E	315	PHE	2.4
1	J	40	SER	2.3
1	J	37	ALA	2.3
1	J	27	LYS	2.3
1	H	13	GLY	2.2
1	I	225	TYR	2.2
1	B	360	ARG	2.1
1	F	41	ALA	2.1
1	H	315	PHE	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
3	OXY	L	502	2/2	0.89	0.12	37,37,37,37	0
3	OXY	A	502	2/2	0.91	0.13	37,37,37,37	0
3	OXY	D	502	2/2	0.92	0.16	32,32,32,32	0
3	OXY	E	502	2/2	0.92	0.14	34,34,34,34	0
3	OXY	C	502	2/2	0.92	0.17	38,38,38,38	0
3	OXY	H	502	2/2	0.93	0.18	43,43,43,43	0
2	YE1	J	501	59/59	0.93	0.15	36,56,70,76	0
3	OXY	J	502	2/2	0.94	0.10	51,51,51,51	0

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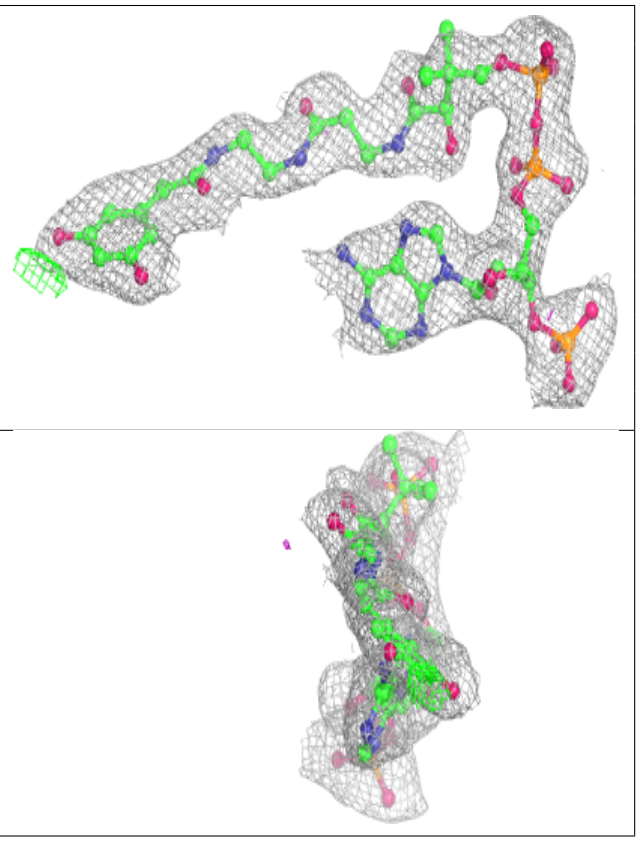
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OXY	I	502	2/2	0.94	0.12	31,31,31,31	0
2	YE1	H	501	59/59	0.95	0.16	24,38,45,52	0
2	YE1	I	501	59/59	0.95	0.14	16,28,36,42	0
3	OXY	B	502	2/2	0.95	0.10	30,30,30,30	0
3	OXY	F	502	2/2	0.95	0.10	24,24,24,24	0
2	YE1	E	501	59/59	0.96	0.14	15,32,37,46	0
2	YE1	F	501	59/59	0.96	0.14	16,32,41,44	0
2	YE1	G	501	59/59	0.96	0.14	23,32,47,53	0
2	YE1	A	501	59/59	0.96	0.14	23,32,43,50	0
2	YE1	B	501	59/59	0.96	0.15	19,41,48,55	0
3	OXY	G	502	2/2	0.96	0.11	33,33,33,33	0
2	YE1	C	501	59/59	0.96	0.12	16,32,38,41	0
2	YE1	K	501	59/59	0.96	0.13	16,29,35,44	0
2	YE1	L	501	59/59	0.96	0.14	23,35,43,46	0
3	OXY	K	502	2/2	0.96	0.15	30,30,30,30	0
2	YE1	D	501	59/59	0.96	0.13	18,25,32,35	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.

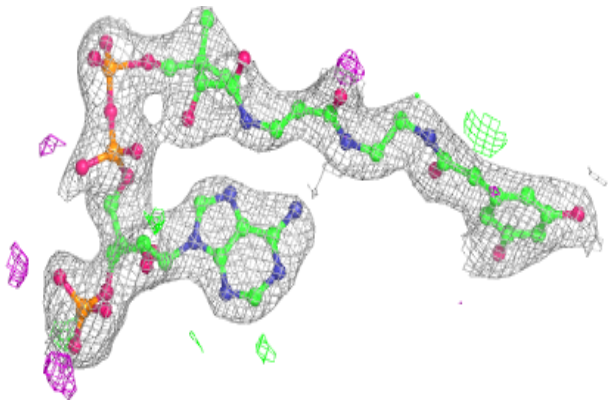
Electron density around YE1 J 501:

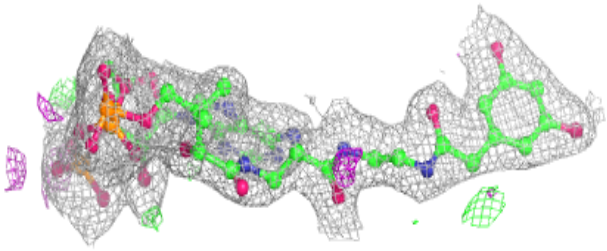
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

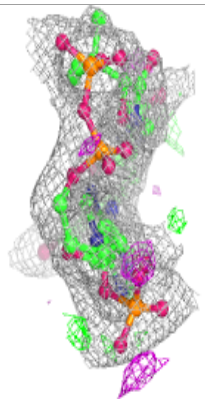


Electron density around YE1 H 501:

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

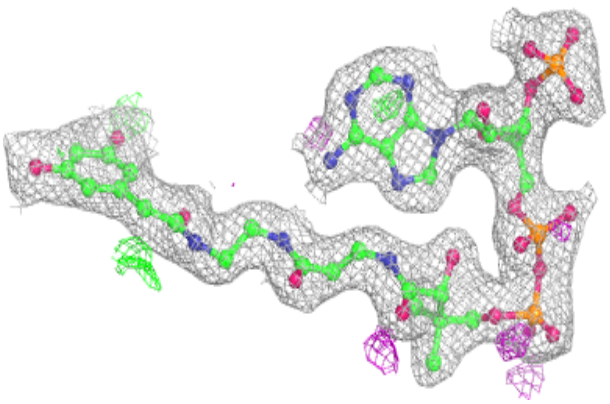


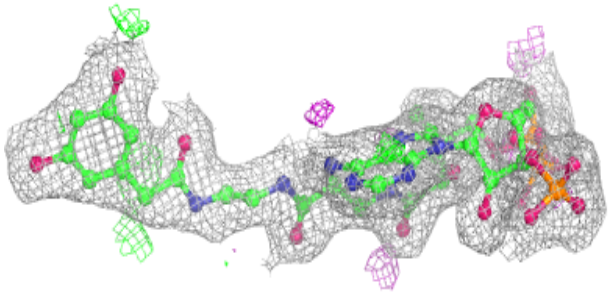


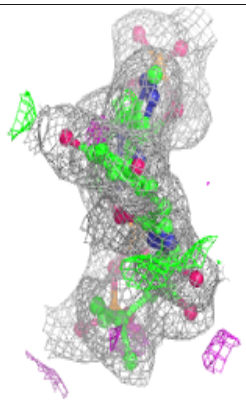


Electron density around YE1 I 501:

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

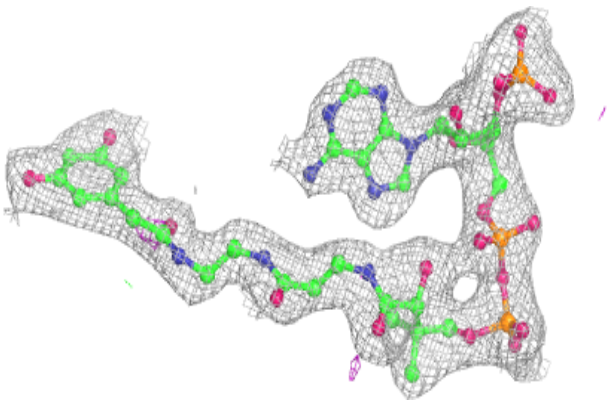


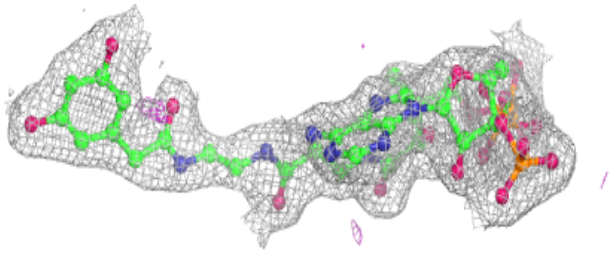


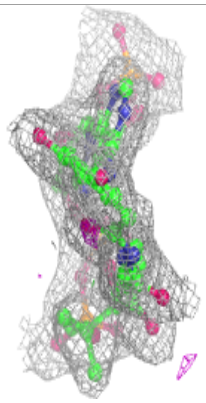


Electron density around YE1 E 501:

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

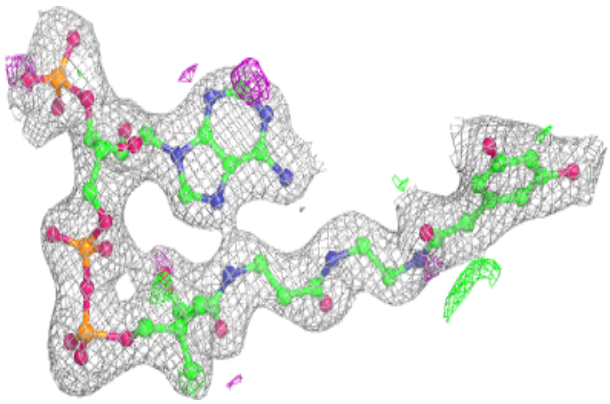


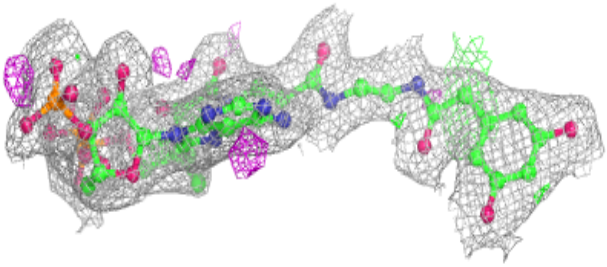


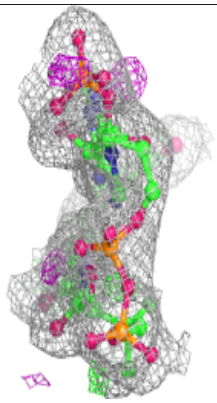


Electron density around YE1 F 501:

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

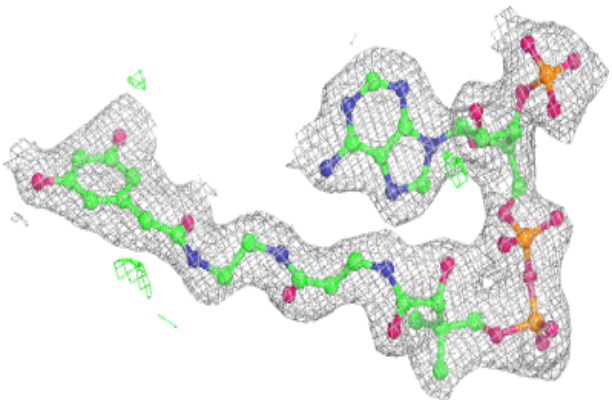


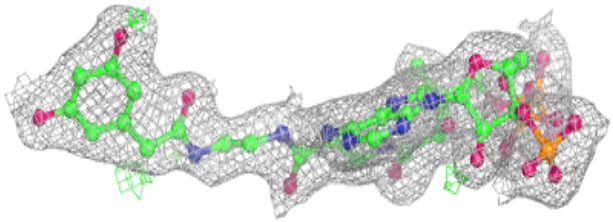


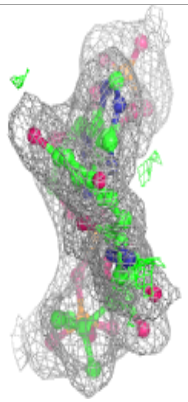


Electron density around YE1 G 501:

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

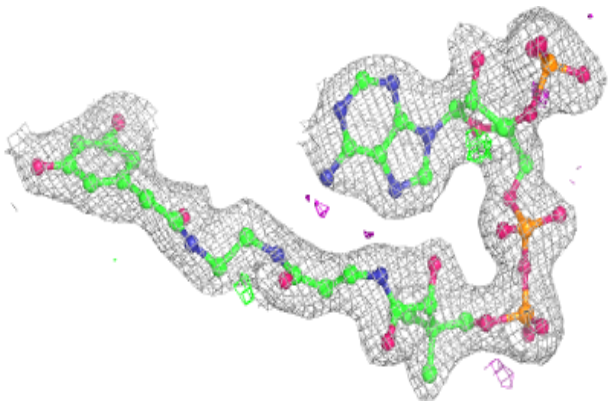


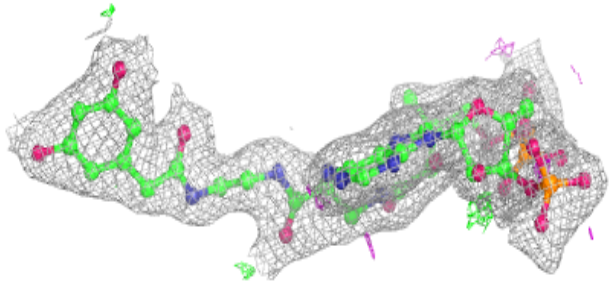


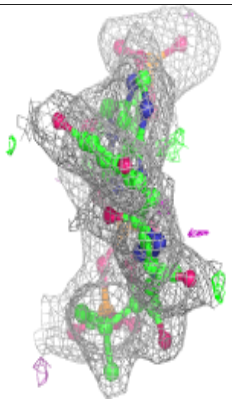


Electron density around YE1 A 501:

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

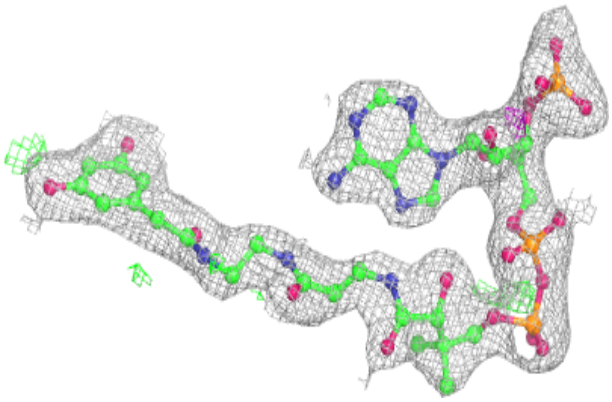


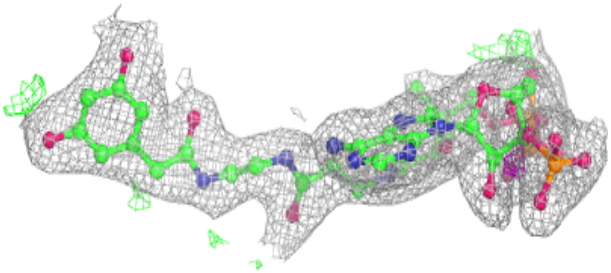


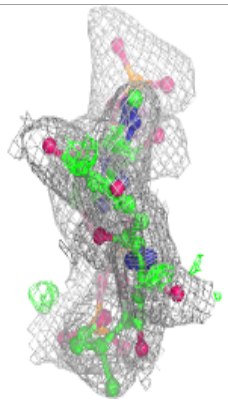


Electron density around YE1 B 501:

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

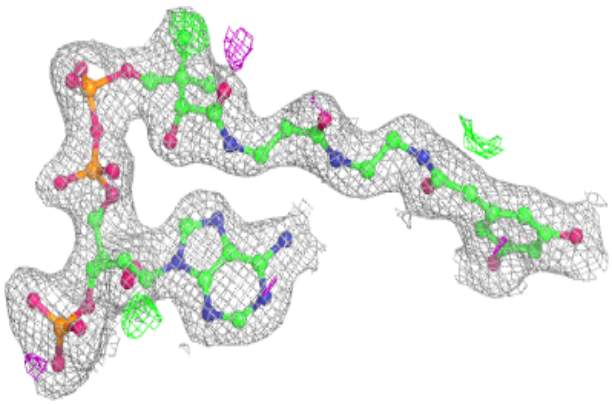


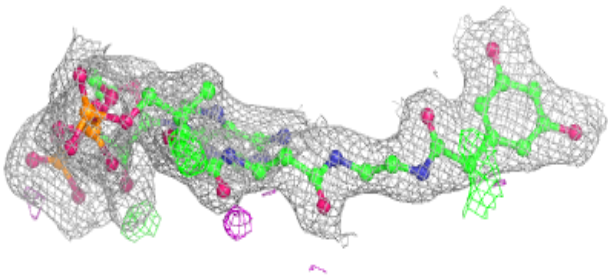


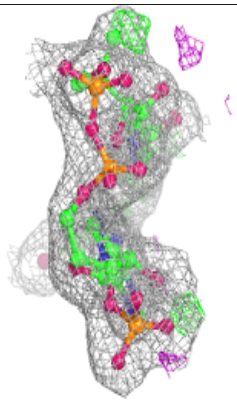


Electron density around YE1 C 501:

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

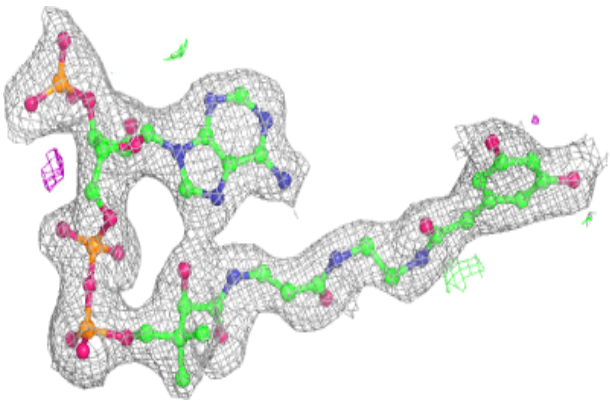


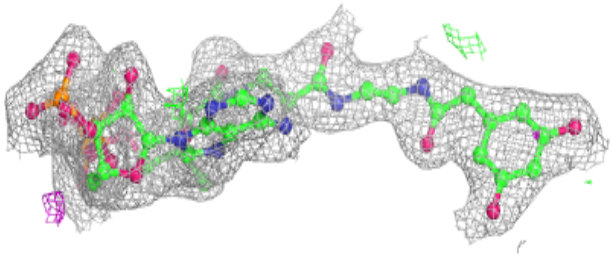


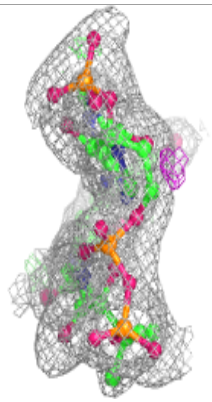


Electron density around YE1 K 501:

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

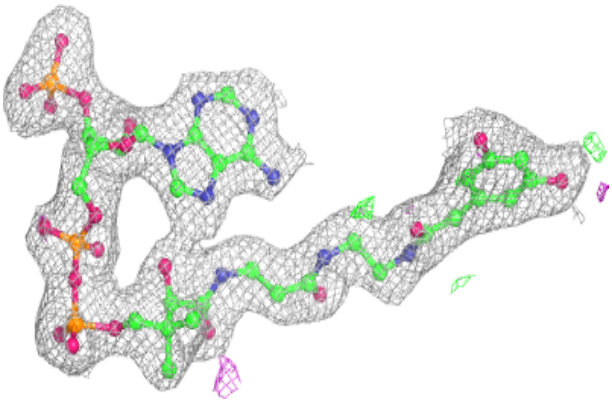


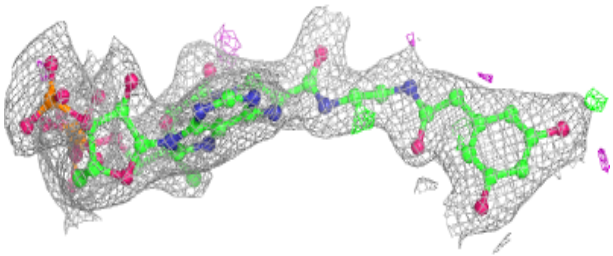


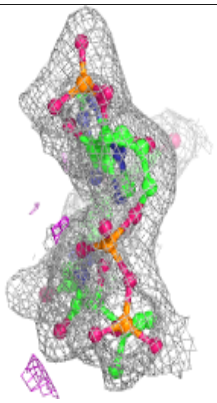


Electron density around YE1 L 501:

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

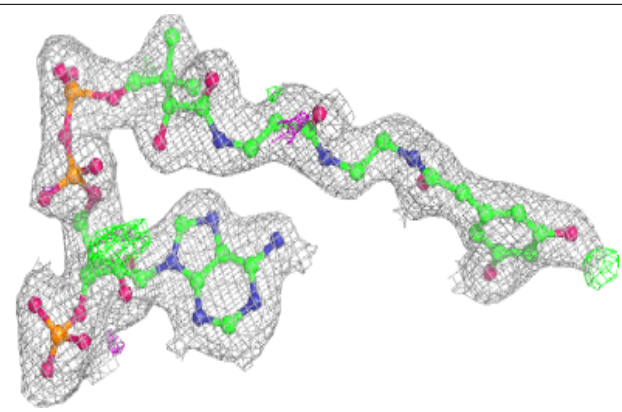


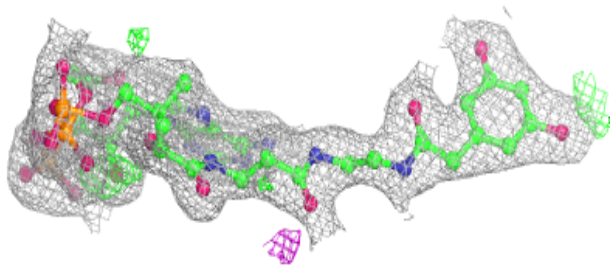


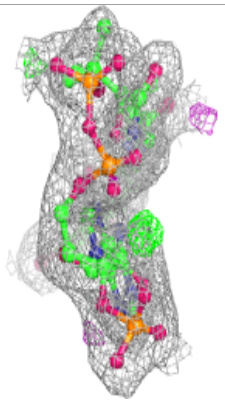


Electron density around YE1 D 501:

$2mF_o$-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.