Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 01:25 AM EST

PDB ID	:	3W54
Title	:	Crystal structure of cyanide-insensitive alternative oxidase from Trypanosoma brucei with colletochlorin B
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Deposited on	:	2013-01-21
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

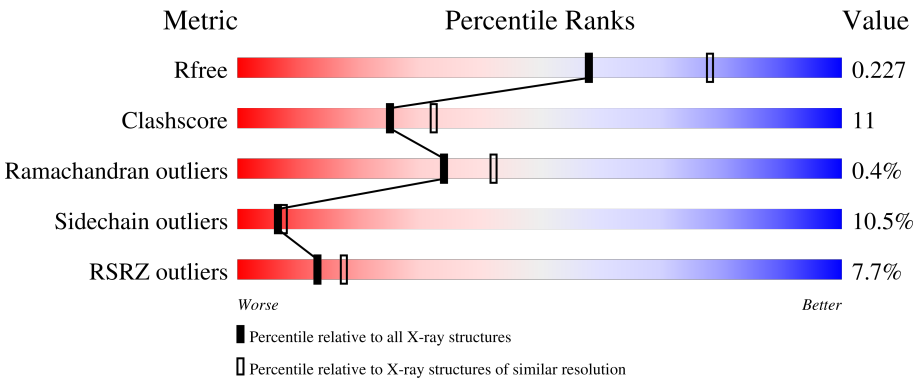
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	329	2%, 61%, 16%, •, 20%
1	B	329	10%, 57%, 20%, • •, 19%
1	C	329	10%, 58%, 20%, •, 19%
1	D	329	2%, 57%, 21%, •, 20%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9022 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.

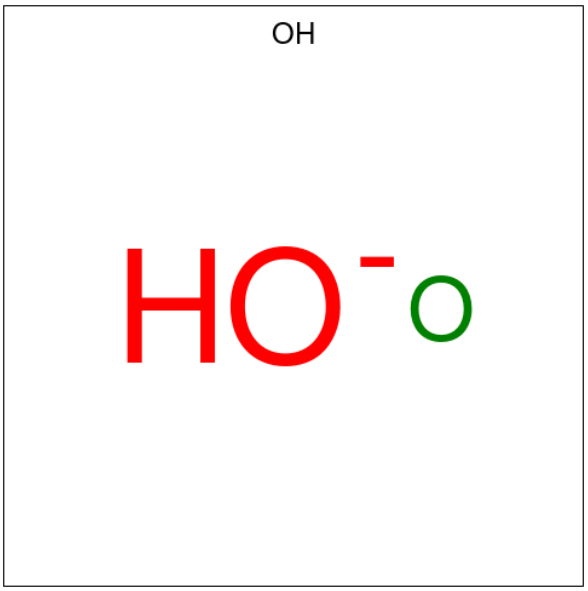
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2146	1375	381	380	10	0	0	0
1	B	266	2162	1386	384	382	10	0	0	0
1	C	266	2163	1385	385	383	10	0	0	0
1	D	263	2146	1374	380	382	10	0	1	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

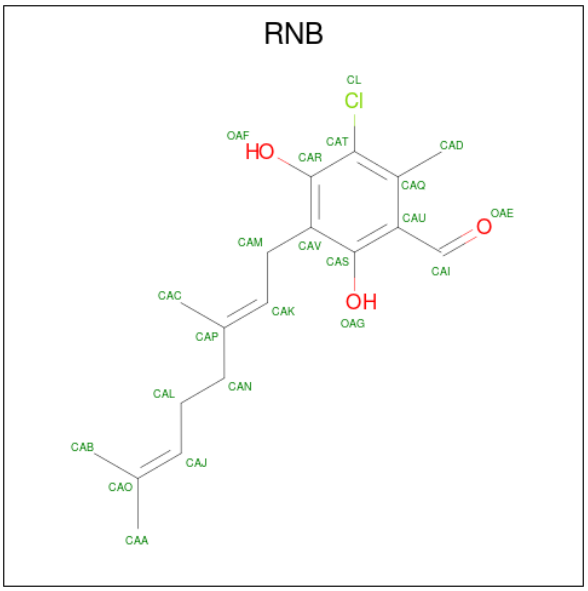
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



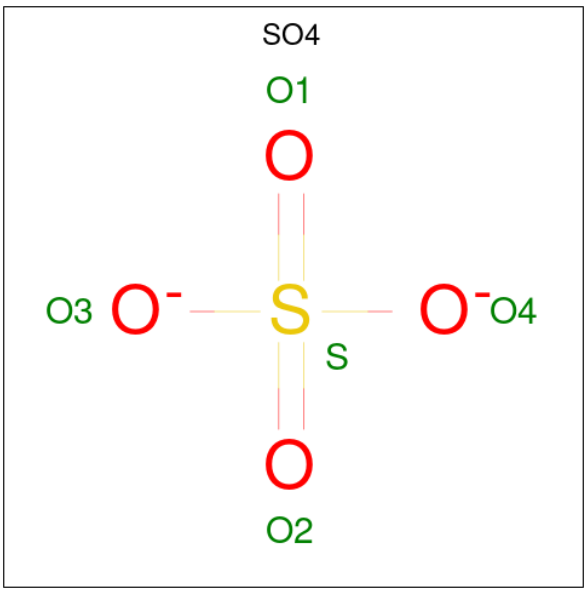
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

- Molecule 4 is 3-chloro-5-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-4,6-dihydroxy-2-methylbenzal dehyde (three-letter code: RNB) (formula: $C_{18}H_{23}ClO_3$).



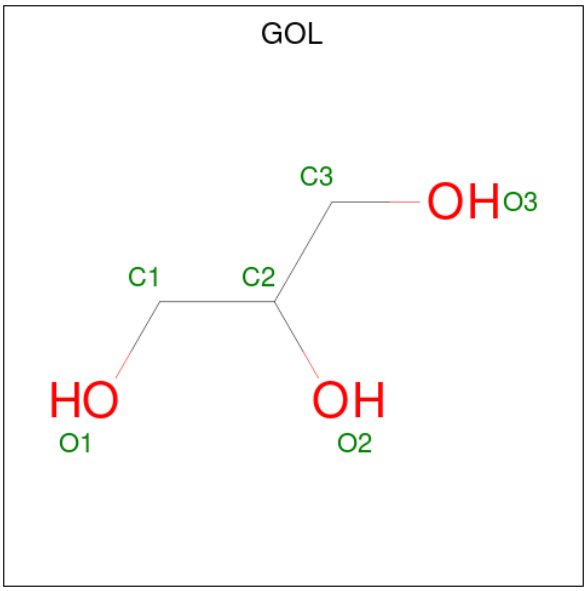
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
4	A	1	22	18	1	3	0	0
4	B	1	22	18	1	3	0	0
4	C	1	22	18	1	3	0	0
4	D	1	22	18	1	3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	D	1	6	3	3	0	0

- Molecule 7 is water.

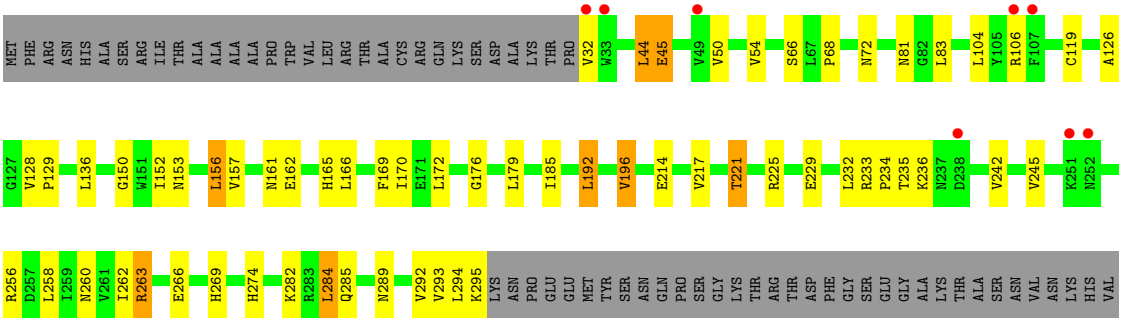
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	90	90	90	0	0
			Total	O		
7	B	65	65	65	0	0
			Total	O		
7	C	54	54	54	0	0
			Total	O		
7	D	80	80	80	0	0

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.

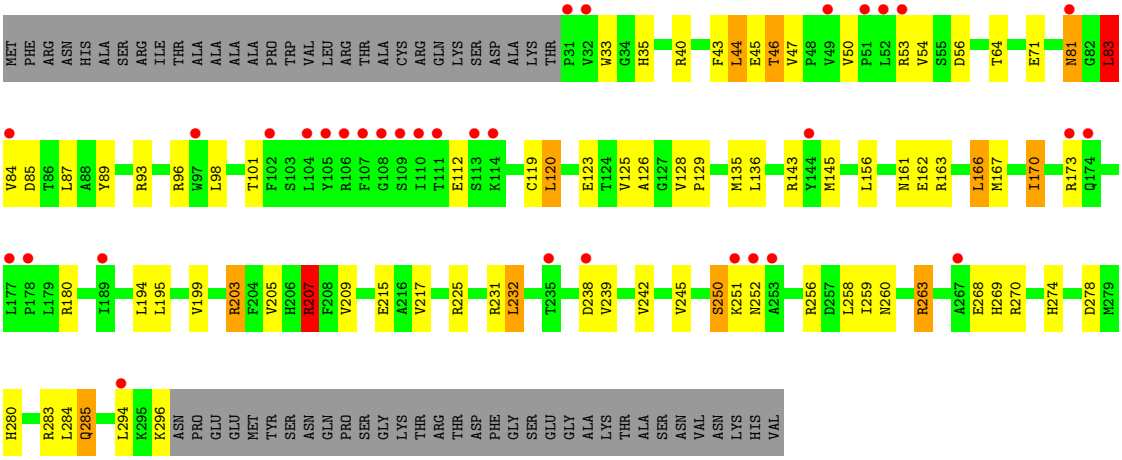
• Molecule 1: Alternative oxidase, mitochondrial

Chain A:



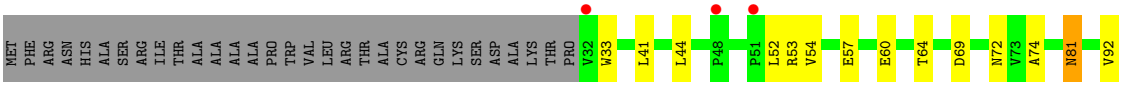
• Molecule 1: Alternative oxidase, mitochondrial

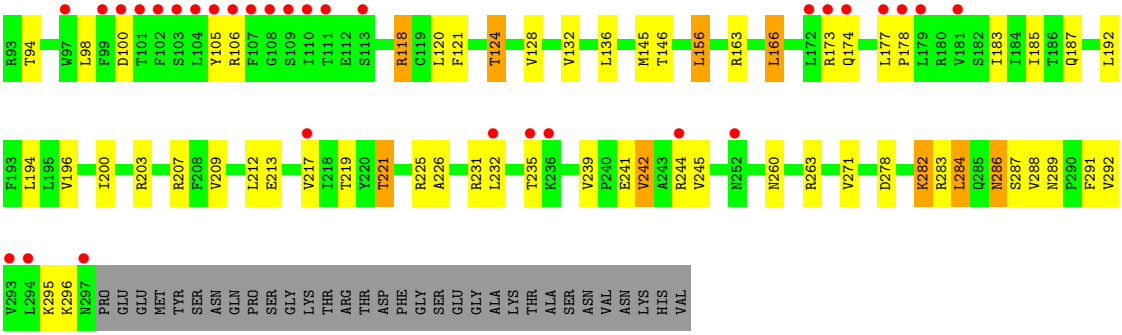
Chain B:



• Molecule 1: Alternative oxidase, mitochondrial

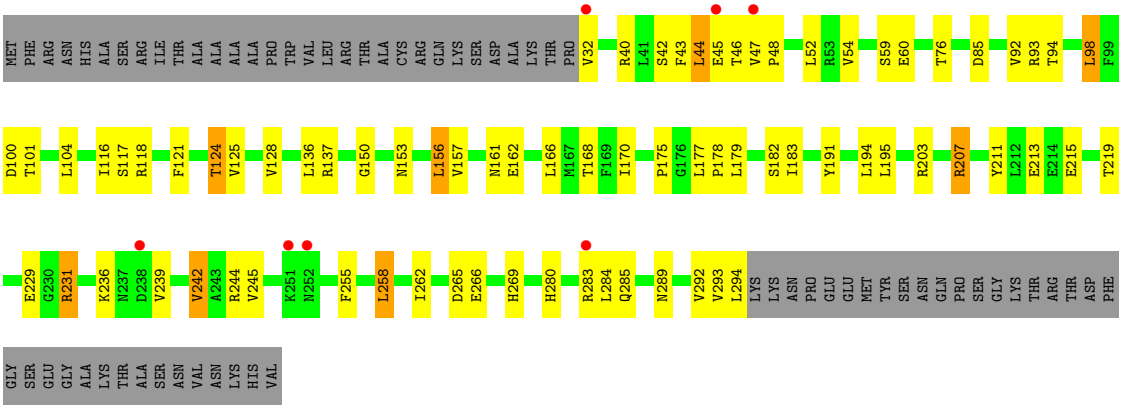
Chain C:





- Molecule 1: Alternative oxidase, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	228.02Å 137.92Å 63.06Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	42.89 – 2.30 42.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (42.89-2.30) 99.6 (42.89-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.185 , 0.227 0.193 , 0.227	Depositor DCC
R_{free} test set	4089 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 65.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.219 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.473 for H, K, L 0.527 for H+4/2L, -K, -L	Depositor
Outliers	0 of 82820 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9022	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OH, GOL, RNB, FE, 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	0.50	0/2195	0.75	0/2982
1	B	0.49	0/2212	0.71	4/3004 (0.1%)
1	C	0.50	0/2212	0.70	0/3004
1	D	0.53	0/2195	0.76	1/2983 (0.0%)
All	All	0.51	0/8814	0.73	5/11973 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	83	LEU	N-CA-CB	-5.74	98.92	110.40
1	B	225	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	B	225	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	B	207	ARG	CG-CD-NE	5.22	122.77	111.80
1	D	156	LEU	CA-CB-CG	5.16	127.16	115.30

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	2146	0	2175	39	0
1	B	2162	0	2196	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2163	0	2194	51	0
1	D	2146	0	2167	51	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	22	0	21	1	0
4	B	22	0	21	1	0
4	C	22	0	22	2	0
4	D	22	0	21	4	0
5	A	5	0	0	1	0
5	D	5	0	0	0	0
6	D	6	0	8	0	0
7	A	90	0	0	4	0
7	B	65	0	0	4	0
7	C	54	0	0	5	0
7	D	80	0	0	1	0
All	All	9022	0	8825	187	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 11.

All (187) 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:83:LEU:HD12	1:B:84:VAL:H	1.25	0.97
1:A:217:VAL:O	1:A:221:THR:HG22	1.73	0.89
1:B:81:ASN:HD22	1:B:81:ASN:C	1.77	0.86
1:D:125:VAL:O	1:D:128:VAL:HG22	1.77	0.85
1:D:54:VAL:HG13	1:D:242:VAL:HA	1.65	0.77
1:D:219:THR:HG21	4:D:504:RNB:H19	1.65	0.77
1:A:217:VAL:O	1:A:221:THR:CG2	2.33	0.76
1:C:217:VAL:O	1:C:221:THR:HG23	1.86	0.76
1:B:83:LEU:CD1	1:B:84:VAL:H	1.99	0.75
1:D:124:THR:HG21	1:D:183:ILE:HG23	1.70	0.73
1:B:83:LEU:HD13	1:B:84:VAL:HG23	1.71	0.72
1:D:85:ASP:OD1	1:D:207:ARG:HD2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:HD11	1:C:145:MET:SD	2.30	0.72
1:C:207:ARG:CZ	7:C:601:HOH:O	2.39	0.71
1:C:286:ASN:HB2	7:C:638:HOH:O	1.89	0.71
1:C:221:THR:HG22	1:C:263:ARG:HD2	1.72	0.70
1:B:268:GLU:OE2	1:C:33:TRP:NE1	2.22	0.69
1:A:292:VAL:HG23	1:A:293:VAL:HG23	1.78	0.65
1:D:175:PRO:HB3	1:D:179:LEU:HD23	1.79	0.64
1:B:40:ARG:O	1:C:271:VAL:HG12	1.98	0.63
1:D:239:VAL:HA	7:D:661:HOH:O	1.96	0.63
1:A:214:GLU:OE1	1:A:274:HIS:HE1	1.83	0.61
1:D:153:ASN:O	1:D:157:VAL:HG13	2.00	0.61
1:C:291:PHE:O	1:C:295:LYS:HB2	2.00	0.61
1:B:53:ARG:NH1	1:B:56:ASP:OD2	2.33	0.61
1:A:293:VAL:O	1:A:295:LYS:N	2.33	0.61
1:D:161:ASN:HD22	1:D:269:HIS:CE1	2.19	0.61
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.66	0.60
1:A:152:ILE:HG22	1:A:156:LEU:HD22	1.83	0.60
1:D:283:ARG:HA	1:D:285:GLN:HE22	1.65	0.60
1:D:54:VAL:CG1	1:D:242:VAL:HA	2.31	0.60
1:B:166:LEU:HD11	1:C:145:MET:HG2	1.83	0.60
1:D:289:ASN:O	1:D:292:VAL:HG22	2.02	0.60
1:C:54:VAL:CG2	1:C:242:VAL:HG13	2.32	0.60
1:D:128:VAL:HG23	1:D:194:LEU:CD1	2.33	0.58
1:A:263:ARG:HD2	7:A:684:HOH:O	2.03	0.58
1:C:118:ARG:NH2	4:C:504:RNB:OAG	2.36	0.58
1:D:191:TYR:CE1	1:D:195:LEU:HD22	2.38	0.58
1:A:54:VAL:CG2	1:A:242:VAL:HA	2.34	0.58
1:B:85:ASP:OD1	1:B:207:ARG:NH1	2.37	0.57
1:A:221:THR:HB	1:A:263:ARG:HH21	1.69	0.57
1:B:84:VAL:HG21	1:B:203:ARG:NH2	2.20	0.57
1:D:283:ARG:HA	1:D:285:GLN:NE2	2.19	0.57
1:A:54:VAL:CG2	1:A:242:VAL:HG12	2.35	0.56
1:B:207:ARG:NH2	1:B:278:ASP:OD1	2.38	0.56
1:A:258:LEU:C	1:A:258:LEU:HD23	2.26	0.56
1:B:83:LEU:HD12	7:B:663:HOH:O	2.05	0.56
1:B:128:VAL:HG13	1:B:194:LEU:CD1	2.35	0.56
1:B:54:VAL:HG12	1:B:245:VAL:HG11	1.88	0.55
1:B:84:VAL:CG2	1:B:203:ARG:NH2	2.69	0.55
1:B:81:ASN:C	1:B:81:ASN:ND2	2.51	0.54
1:B:54:VAL:HG22	1:B:242:VAL:HG12	1.89	0.54
1:C:241:GLU:O	1:C:245:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LEU:O	1:D:47:VAL:HG12	2.08	0.54
3:A:503:OH:O	4:A:504:RNB:H20	2.08	0.54
1:A:176:GLY:N	5:A:505:SO4:O4	2.32	0.53
1:D:40:ARG:NH2	1:D:42:SER:O	2.41	0.53
1:B:54:VAL:HG13	1:B:242:VAL:HA	1.90	0.53
1:A:32:VAL:O	1:A:32:VAL:HG13	2.08	0.53
1:C:92:VAL:HG22	1:C:212:LEU:CD2	2.38	0.53
1:C:219:THR:HG21	4:C:504:RNB:H19	1.91	0.53
1:A:45:GLU:H	1:A:45:GLU:CD	2.11	0.53
1:D:293:VAL:O	1:D:294:LEU:HG	2.09	0.52
1:B:126:ALA:HB1	1:B:162:GLU:OE2	2.10	0.52
1:C:209:VAL:O	1:C:213:GLU:HG2	2.10	0.51
1:C:239:VAL:O	1:C:239:VAL:HG13	2.11	0.51
1:B:120:LEU:C	1:B:120:LEU:HD12	2.31	0.51
1:D:150:GLY:HA3	1:D:292:VAL:HG11	1.92	0.51
4:D:504:RNB:OAF	4:D:504:RNB:CAK	2.59	0.50
1:B:96:ARG:NH2	1:B:215:GLU:OE2	2.44	0.50
1:A:192:LEU:O	1:A:196:VAL:HG13	2.12	0.50
1:A:54:VAL:HG22	1:A:242:VAL:HA	1.92	0.50
1:B:205:VAL:O	1:B:209:VAL:HG23	2.11	0.50
1:B:256:ARG:NH2	7:B:642:HOH:O	2.44	0.49
1:D:219:THR:CG2	4:D:504:RNB:H19	2.39	0.49
1:A:289:ASN:O	1:A:292:VAL:HG22	2.12	0.49
1:A:229:GLU:OE2	1:B:89:TYR:OH	2.20	0.49
1:B:207:ARG:HH11	1:B:207:ARG:CG	2.26	0.49
1:D:229:GLU:OE1	1:D:231:ARG:HD2	2.13	0.49
1:B:83:LEU:CD1	1:B:84:VAL:HG23	2.41	0.48
1:D:121:PHE:O	1:D:124:THR:HB	2.14	0.48
1:B:43:PHE:O	1:B:46:THR:HG22	2.14	0.48
1:C:120:LEU:HD12	1:C:166:LEU:HD23	1.94	0.48
1:D:293:VAL:O	1:D:294:LEU:CG	2.61	0.48
1:B:128:VAL:HG12	1:B:129:PRO:HD3	1.95	0.48
1:C:57:GLU:O	1:C:163:ARG:NH1	2.47	0.48
1:D:43:PHE:O	1:D:46:THR:HG22	2.13	0.48
1:A:150:GLY:HA3	1:A:292:VAL:HG11	1.96	0.47
1:A:54:VAL:HG13	1:A:245:VAL:HG21	1.95	0.47
1:B:119:CYS:O	1:B:123:GLU:HG2	2.14	0.47
1:D:32:VAL:O	1:D:32:VAL:HG13	2.14	0.47
1:A:232:LEU:O	1:A:234:PRO:HD3	2.14	0.47
1:A:289:ASN:HB3	1:A:292:VAL:HG13	1.97	0.47
1:C:121:PHE:O	1:C:124:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:HA	1:B:285:GLN:HE21	1.78	0.47
1:A:263:ARG:NH2	7:A:651:HOH:O	2.40	0.47
1:D:215:GLU:HB3	4:D:504:RNB:H17	1.96	0.47
1:B:207:ARG:HD3	1:B:274:HIS:HD2	1.79	0.47
1:B:217:VAL:HG11	1:B:270:ARG:NH2	2.29	0.47
1:B:263:ARG:HD2	7:B:626:HOH:O	2.14	0.47
1:B:125:VAL:O	1:B:128:VAL:HG12	2.15	0.46
1:A:162:GLU:O	1:A:165:HIS:HB2	2.15	0.46
1:B:35:HIS:ND1	1:C:69:ASP:OD1	2.39	0.46
1:D:161:ASN:HD21	1:D:265:ASP:HB3	1.80	0.46
1:A:242:VAL:HG13	7:A:662:HOH:O	2.15	0.46
1:B:170:ILE:HD12	1:C:145:MET:HB3	1.98	0.46
1:C:296:LYS:NZ	7:C:642:HOH:O	2.49	0.46
1:A:262:ILE:O	1:A:266:GLU:HG2	2.15	0.46
1:B:89:TYR:O	1:B:93:ARG:HG2	2.16	0.46
1:C:292:VAL:O	1:C:296:LYS:HG2	2.16	0.46
1:D:128:VAL:HG23	1:D:194:LEU:HD13	1.98	0.46
1:B:207:ARG:HD3	1:B:274:HIS:CD2	2.51	0.46
1:B:163:ARG:O	1:B:167:MET:HG2	2.16	0.46
1:A:54:VAL:HG21	1:A:242:VAL:HA	1.98	0.45
1:D:244:ARG:HB3	1:D:244:ARG:NH1	2.31	0.45
1:D:162:GLU:HA	1:D:162:GLU:OE1	2.17	0.45
1:D:213:GLU:HA	1:D:213:GLU:OE1	2.16	0.45
1:D:177:LEU:N	1:D:178:PRO:HD2	2.32	0.45
1:D:258:LEU:HD22	1:D:262:ILE:CD1	2.46	0.45
1:C:284:LEU:HA	1:C:284:LEU:HD12	1.69	0.45
1:A:153:ASN:O	1:A:157:VAL:HG22	2.17	0.44
1:A:172:LEU:O	1:A:236:LYS:NZ	2.49	0.44
1:A:119:CYS:HB3	1:A:169:PHE:CE2	2.53	0.44
1:B:64:THR:HG22	1:B:64:THR:O	2.17	0.44
1:D:116:ILE:HD11	1:D:255:PHE:CZ	2.53	0.44
1:C:100:ASP:OD1	1:C:118:ARG:NH1	2.49	0.44
1:C:196:VAL:O	1:C:200:ILE:HG12	2.18	0.44
1:C:124:THR:HG21	1:C:183:ILE:HB	1.99	0.43
1:B:143:ARG:NH1	1:C:187:GLN:OE1	2.51	0.43
1:C:225:ARG:NH2	1:D:93:ARG:NH2	2.65	0.43
1:D:168:THR:HG21	1:D:258:LEU:HD11	2.00	0.43
1:A:44:LEU:HD22	1:A:44:LEU:O	2.18	0.43
1:B:280:HIS:HA	1:B:285:GLN:HG3	2.00	0.43
1:C:128:VAL:HG22	1:C:194:LEU:CD1	2.49	0.43
1:D:293:VAL:O	1:D:294:LEU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HG	1:C:278:ASP:HB3	2.00	0.43
1:B:47:VAL:HA	1:B:50:VAL:HG22	2.01	0.43
1:D:85:ASP:OD1	1:D:207:ARG:CD	2.61	0.43
1:B:56:ASP:HB3	1:C:292:VAL:HG21	2.01	0.43
1:C:245:VAL:HG22	7:C:609:HOH:O	2.17	0.43
1:B:156:LEU:HD13	1:C:156:LEU:HG	1.99	0.43
1:A:128:VAL:HB	1:A:129:PRO:HD3	2.00	0.43
1:A:72:ASN:ND2	1:C:41:LEU:HD11	2.34	0.43
1:C:74:ALA:HB2	1:D:76:THR:HG22	2.01	0.43
1:C:289:ASN:O	1:C:292:VAL:HG22	2.18	0.43
1:D:161:ASN:HD22	1:D:269:HIS:HE1	1.67	0.43
1:D:94:THR:HG22	1:D:98:LEU:HD22	1.99	0.42
1:D:40:ARG:NH2	1:D:45[B]:GLU:OE1	2.52	0.42
1:C:226:ALA:HB3	1:C:232:LEU:HD23	2.01	0.42
1:B:239:VAL:HA	7:B:659:HOH:O	2.19	0.42
1:C:283:ARG:O	1:C:284:LEU:HD12	2.20	0.42
1:D:45[B]:GLU:O	1:D:48:PRO:HD2	2.19	0.42
1:B:112:GLU:HB3	1:B:232:LEU:HD12	2.01	0.42
1:A:165:HIS:CE1	1:A:266:GLU:OE1	2.73	0.42
1:A:256:ARG:NE	7:A:682:HOH:O	2.53	0.42
1:B:35:HIS:CG	1:C:72:ASN:HB3	2.54	0.42
1:B:135:MET:SD	1:B:136:LEU:HD12	2.59	0.42
1:D:100:ASP:OD1	1:D:118:ARG:NH1	2.43	0.42
1:D:191:TYR:O	1:D:195:LEU:HB2	2.20	0.42
1:D:280:HIS:CD2	1:D:285:GLN:HG3	2.55	0.42
3:B:503:OH:O	4:B:504:RNB:H20	2.20	0.42
1:A:128:VAL:N	1:A:129:PRO:CD	2.83	0.41
1:C:282:LYS:O	1:C:284:LEU:HD13	2.20	0.41
1:D:92:VAL:HG21	1:D:211:TYR:HB2	2.01	0.41
1:B:54:VAL:CG1	1:B:245:VAL:HG11	2.49	0.41
1:B:84:VAL:HG21	1:B:203:ARG:CZ	2.50	0.41
1:C:207:ARG:NH2	7:C:601:HOH:O	2.48	0.41
1:D:124:THR:CG2	1:D:183:ILE:HG23	2.47	0.41
1:B:195:LEU:O	1:B:199:VAL:HG23	2.21	0.41
1:C:177:LEU:N	1:C:178:PRO:HD2	2.34	0.41
1:C:192:LEU:O	1:C:196:VAL:HG12	2.21	0.41
1:C:225:ARG:CZ	1:D:93:ARG:NH2	2.83	0.41
1:B:161:ASN:OD1	1:B:269:HIS:CE1	2.74	0.41
1:C:81:ASN:O	1:C:81:ASN:CG	2.58	0.41
1:B:252:ASN:N	1:B:252:ASN:HD22	2.17	0.41
1:C:60:GLU:HA	1:C:60:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:THR:HG22	1:C:98:LEU:HD13	2.02	0.41
1:C:284:LEU:N	1:C:284:LEU:CD1	2.81	0.41
1:D:262:ILE:O	1:D:266:GLU:HG2	2.20	0.41
1:B:250:SER:OG	1:B:251:LYS:N	2.54	0.40
1:C:288:VAL:CG2	1:C:289:ASN:N	2.84	0.40
1:A:66:SER:OG	1:A:68:PRO:HD2	2.21	0.40
1:A:161:ASN:OD1	1:A:269:HIS:CE1	2.75	0.40
1:B:283:ARG:HA	1:B:285:GLN:NE2	2.36	0.40
1:C:81:ASN:O	1:C:81:ASN:ND2	2.54	0.40
1:A:282:LYS:HB2	1:A:284:LEU:HD22	2.04	0.40
1:D:137:ARG:NH2	1:D:285:GLN:O	2.41	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	262/329 (80%)	254 (97%)	6 (2%)	2 (1%)	19 23
1	B	264/329 (80%)	249 (94%)	15 (6%)	0	100 100
1	C	264/329 (80%)	251 (95%)	12 (4%)	1 (0%)	34 42
1	D	262/329 (80%)	252 (96%)	9 (3%)	1 (0%)	34 42
All	All	1052/1316 (80%)	1006 (96%)	42 (4%)	4 (0%)	34 42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	LEU
1	C	235	THR
1	D	59	SER
1	A	126	ALA

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	239/292 (82%)	216 (90%)	23 (10%)	8 10
1	B	241/292 (82%)	211 (88%)	30 (12%)	4 5
1	C	241/292 (82%)	214 (89%)	27 (11%)	6 6
1	D	239/292 (82%)	218 (91%)	21 (9%)	10 12
All	All	960/1168 (82%)	859 (90%)	101 (10%)	7 8

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

Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	GLU
1	A	50	VAL
1	A	81	ASN
1	A	83	LEU
1	A	104	LEU
1	A	106	ARG
1	A	136	LEU
1	A	156	LEU
1	A	166	LEU
1	A	170	ILE
1	A	179	LEU
1	A	185	ILE
1	A	192	LEU
1	A	196	VAL
1	A	221	THR
1	A	225	ARG
1	A	233	ARG
1	A	235	THR
1	A	260	ASN
1	A	263	ARG
1	A	284	LEU
1	A	285	GLN
1	B	33	TRP

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Mol	Chain	Res	Type
1	B	44	LEU
1	B	45	GLU
1	B	46	THR
1	B	71	GLU
1	B	81	ASN
1	B	83	LEU
1	B	87	LEU
1	B	98	LEU
1	B	101	THR
1	B	120	LEU
1	B	145	MET
1	B	166	LEU
1	B	170	ILE
1	B	173	ARG
1	B	180	ARG
1	B	203	ARG
1	B	207	ARG
1	B	231	ARG
1	B	232	LEU
1	B	238	ASP
1	B	250	SER
1	B	258	LEU
1	B	259	ILE
1	B	260	ASN
1	B	263	ARG
1	B	284	LEU
1	B	285	GLN
1	B	294	LEU
1	B	296	LYS
1	C	44	LEU
1	C	52	LEU
1	C	53	ARG
1	C	64	THR
1	C	81	ASN
1	C	105	TYR
1	C	106	ARG
1	C	118	ARG
1	C	124	THR
1	C	132	VAL
1	C	136	LEU
1	C	146	THR
1	C	156	LEU

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Mol	Chain	Res	Type
1	C	166	LEU
1	C	173	ARG
1	C	174	GLN
1	C	185	ILE
1	C	203	ARG
1	C	221	THR
1	C	231	ARG
1	C	242	VAL
1	C	244	ARG
1	C	260	ASN
1	C	282	LYS
1	C	284	LEU
1	C	286	ASN
1	C	287	SER
1	D	44	LEU
1	D	52	LEU
1	D	60	GLU
1	D	98	LEU
1	D	101	THR
1	D	104	LEU
1	D	117	SER
1	D	124	THR
1	D	136	LEU
1	D	156	LEU
1	D	166	LEU
1	D	170	ILE
1	D	182	SER
1	D	203	ARG
1	D	207	ARG
1	D	231	ARG
1	D	236	LYS
1	D	242	VAL
1	D	245	VAL
1	D	258	LEU
1	D	284	LEU

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

Mol	Chain	Res	Type
1	A	72	ASN
1	A	248	ASN
1	A	260	ASN

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Mol	Chain	Res	Type
1	A	269	HIS
1	A	274	HIS
1	B	72	ASN
1	B	81	ASN
1	B	187	GLN
1	B	248	ASN
1	B	252	ASN
1	B	260	ASN
1	B	269	HIS
1	B	273	ASN
1	B	274	HIS
1	B	285	GLN
1	C	72	ASN
1	C	81	ASN
1	C	237	ASN
1	C	252	ASN
1	C	260	ASN
1	C	269	HIS
1	D	72	ASN
1	D	161	ASN
1	D	260	ASN
1	D	269	HIS
1	D	273	ASN
1	D	274	HIS
1	D	280	HIS
1	D	285	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)

Of 19 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	A	505	-	4,4,4	0.46	0	6,6,6	0.18	0
5	SO4	D	505	-	4,4,4	0.35	0	6,6,6	0.18	0
4	RNB	A	504	-	22,22,22	3.72	7 (31%)	29,30,30	2.29	8 (27%)
4	RNB	C	504	-	22,22,22	3.80	6 (27%)	29,30,30	1.66	6 (20%)
4	RNB	B	504	-	22,22,22	3.62	6 (27%)	29,30,30	1.96	8 (27%)
6	GOL	D	506	-	5,5,5	0.59	0	5,5,5	0.51	0
4	RNB	D	504	-	22,22,22	3.50	5 (22%)	29,30,30	1.71	9 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RNB	A	504	-	-	2/13/13/13	0/1/1/1
4	RNB	C	504	-	-	2/13/13/13	0/1/1/1
4	RNB	B	504	-	-	3/13/13/13	0/1/1/1
6	GOL	D	506	-	-	2/4/4/4	-
4	RNB	D	504	-	-	5/13/13/13	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	RNB	CAM-CAV	-10.98	1.39	1.51
4	D	504	RNB	CAM-CAV	-9.81	1.41	1.51
4	A	504	RNB	CAM-CAV	-9.47	1.41	1.51
4	B	504	RNB	CAM-CAV	-9.27	1.41	1.51
4	C	504	RNB	CAK-CAP	8.99	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	RNB	CAK-CAP	8.65	1.53	1.33
4	D	504	RNB	CAK-CAP	8.02	1.52	1.33
4	A	504	RNB	CAJ-CAO	7.99	1.55	1.32
4	C	504	RNB	CAJ-CAO	7.76	1.54	1.32
4	D	504	RNB	CAJ-CAO	7.71	1.54	1.32
4	A	504	RNB	CAK-CAP	7.65	1.51	1.33
4	B	504	RNB	CAJ-CAO	7.63	1.54	1.32
4	A	504	RNB	CAT-CL	6.67	1.87	1.72
4	C	504	RNB	CAD-CAQ	-5.40	1.40	1.51
4	B	504	RNB	CAD-CAQ	-5.36	1.40	1.51
4	A	504	RNB	CAD-CAQ	-5.06	1.41	1.51
4	B	504	RNB	CAT-CL	4.48	1.82	1.72
4	D	504	RNB	CAD-CAQ	-4.09	1.43	1.51
4	D	504	RNB	CAU-CAI	-3.71	1.37	1.46
4	C	504	RNB	CAU-CAI	-3.05	1.39	1.46
4	B	504	RNB	CAU-CAI	-2.80	1.39	1.46
4	A	504	RNB	CAC-CAP	2.49	1.57	1.50
4	A	504	RNB	CAU-CAI	-2.46	1.40	1.46
4	C	504	RNB	CAT-CL	2.17	1.77	1.72

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	RNB	CAR-CAT-CAQ	-7.53	118.01	122.79
4	B	504	RNB	CAR-CAT-CAQ	-5.60	119.24	122.79
4	C	504	RNB	CAR-CAT-CAQ	-5.08	119.57	122.79
4	A	504	RNB	CAQ-CAT-CL	4.99	126.15	118.58
4	B	504	RNB	CAV-CAM-CAK	-4.36	105.27	112.17
4	B	504	RNB	CAQ-CAT-CL	3.98	124.61	118.58
4	D	504	RNB	CAM-CAV-CAR	3.93	125.99	120.82
4	D	504	RNB	CAM-CAK-CAP	-3.87	121.24	127.24
4	A	504	RNB	CAV-CAM-CAK	-3.47	106.67	112.17
4	D	504	RNB	CAR-CAV-CAS	-3.31	114.58	118.60
4	C	504	RNB	CAV-CAM-CAK	-3.17	107.14	112.17
4	A	504	RNB	CAM-CAK-CAP	-3.08	122.46	127.24
4	C	504	RNB	CAM-CAK-CAP	-2.95	122.67	127.24
4	A	504	RNB	CAC-CAP-CAN	2.70	119.81	115.27
4	C	504	RNB	CAQ-CAT-CL	2.50	122.38	118.58
4	D	504	RNB	CAR-CAT-CAQ	-2.45	121.23	122.79
4	C	504	RNB	CAC-CAP-CAN	2.45	119.40	115.27
4	B	504	RNB	CAM-CAK-CAP	-2.41	123.50	127.24
4	D	504	RNB	CAU-CAS-CAV	2.38	124.40	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	RNB	CAL-CAJ-CAO	-2.38	119.63	127.75
4	B	504	RNB	CAB-CAO-CAA	2.35	119.79	114.60
4	A	504	RNB	CAL-CAJ-CAO	-2.34	119.77	127.75
4	D	504	RNB	CAC-CAP-CAN	2.27	119.10	115.27
4	B	504	RNB	CAR-CAV-CAS	-2.24	115.88	118.60
4	A	504	RNB	CAB-CAO-CAA	2.23	119.54	114.60
4	C	504	RNB	CAB-CAO-CAA	2.20	119.46	114.60
4	D	504	RNB	CAS-CAU-CAI	-2.13	116.88	119.90
4	D	504	RNB	CAB-CAO-CAA	2.05	119.12	114.60
4	B	504	RNB	CAC-CAP-CAN	2.01	118.65	115.27
4	D	504	RNB	CAL-CAJ-CAO	-2.00	120.90	127.75
4	A	504	RNB	CAR-CAT-CL	-2.00	115.84	118.08

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	504	RNB	OAE-CAI-CAU-CAQ
4	C	504	RNB	OAE-CAI-CAU-CAS
4	C	504	RNB	OAE-CAI-CAU-CAQ
4	D	504	RNB	CAK-CAM-CAV-CAR
6	D	506	GOL	C1-C2-C3-O3
4	B	504	RNB	OAE-CAI-CAU-CAS
4	D	504	RNB	CAK-CAM-CAV-CAS
4	A	504	RNB	OAE-CAI-CAU-CAS
4	D	504	RNB	OAE-CAI-CAU-CAS
6	D	506	GOL	O2-C2-C3-O3
4	D	504	RNB	CAP-CAK-CAM-CAV
4	D	504	RNB	CAJ-CAL-CAN-CAP
4	A	504	RNB	OAE-CAI-CAU-CAQ
4	B	504	RNB	CAJ-CAL-CAN-CAP

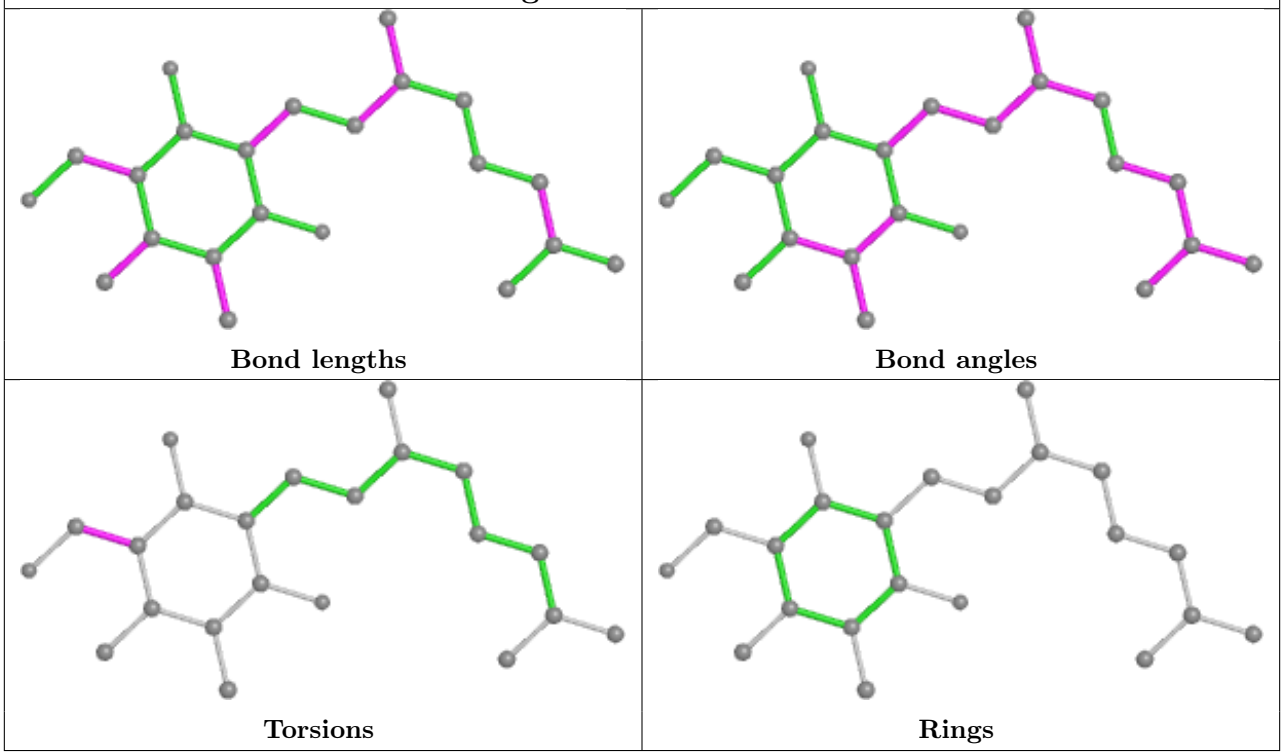
There are no ring outliers.

5 monomers are involved in 9 short contacts:

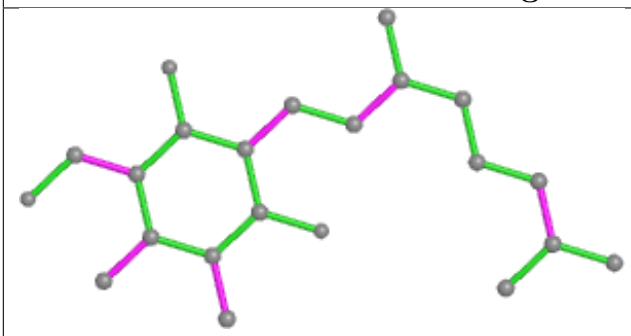
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	SO4	1	0
4	A	504	RNB	1	0
4	C	504	RNB	2	0
4	B	504	RNB	1	0
4	D	504	RNB	4	0

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.

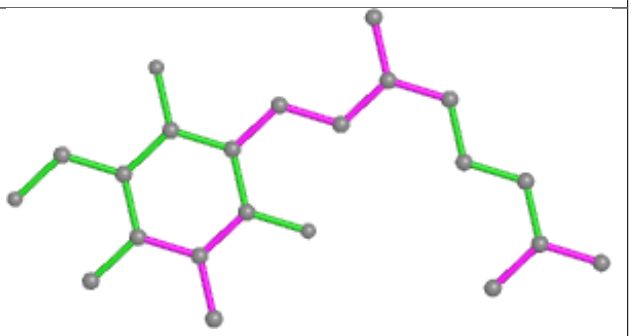
Ligand RNB A 504



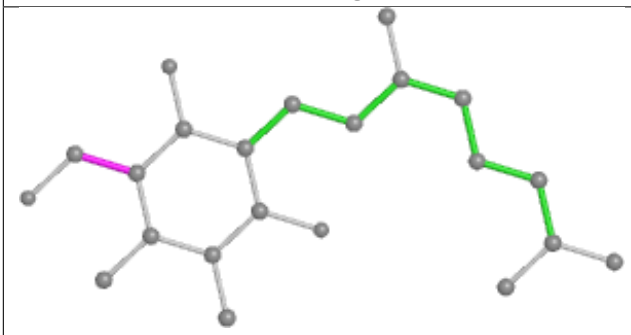
Ligand RNB C 504



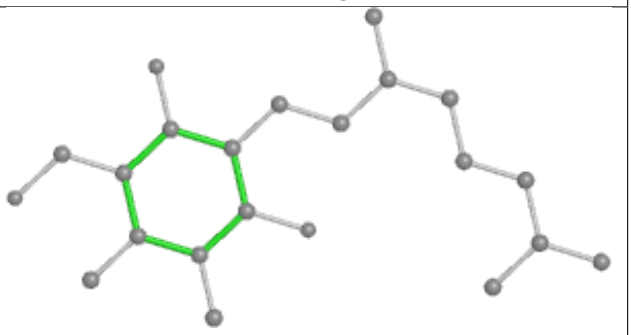
Bond lengths



Bond angles

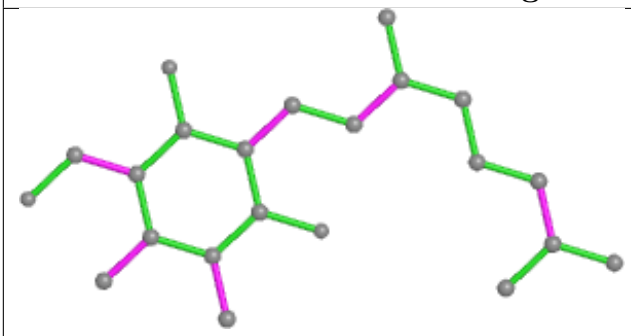


Torsions

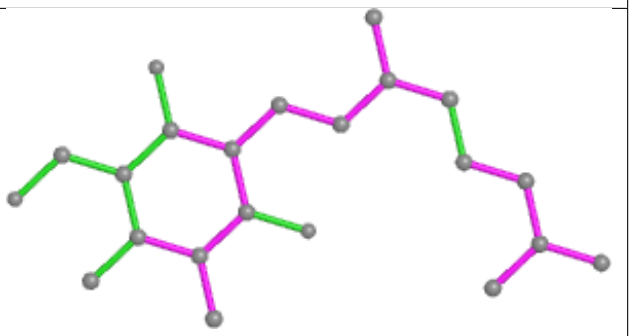


Rings

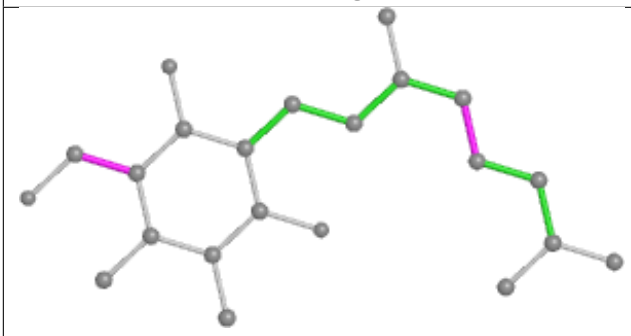
Ligand RNB B 504



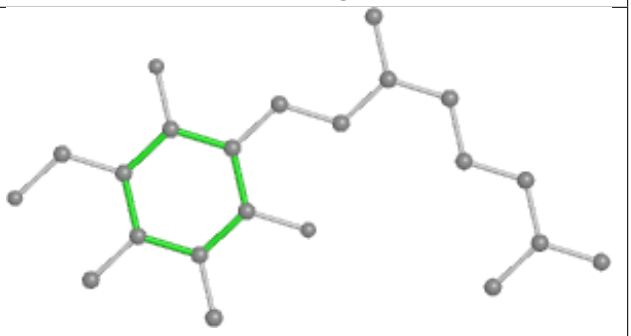
Bond lengths



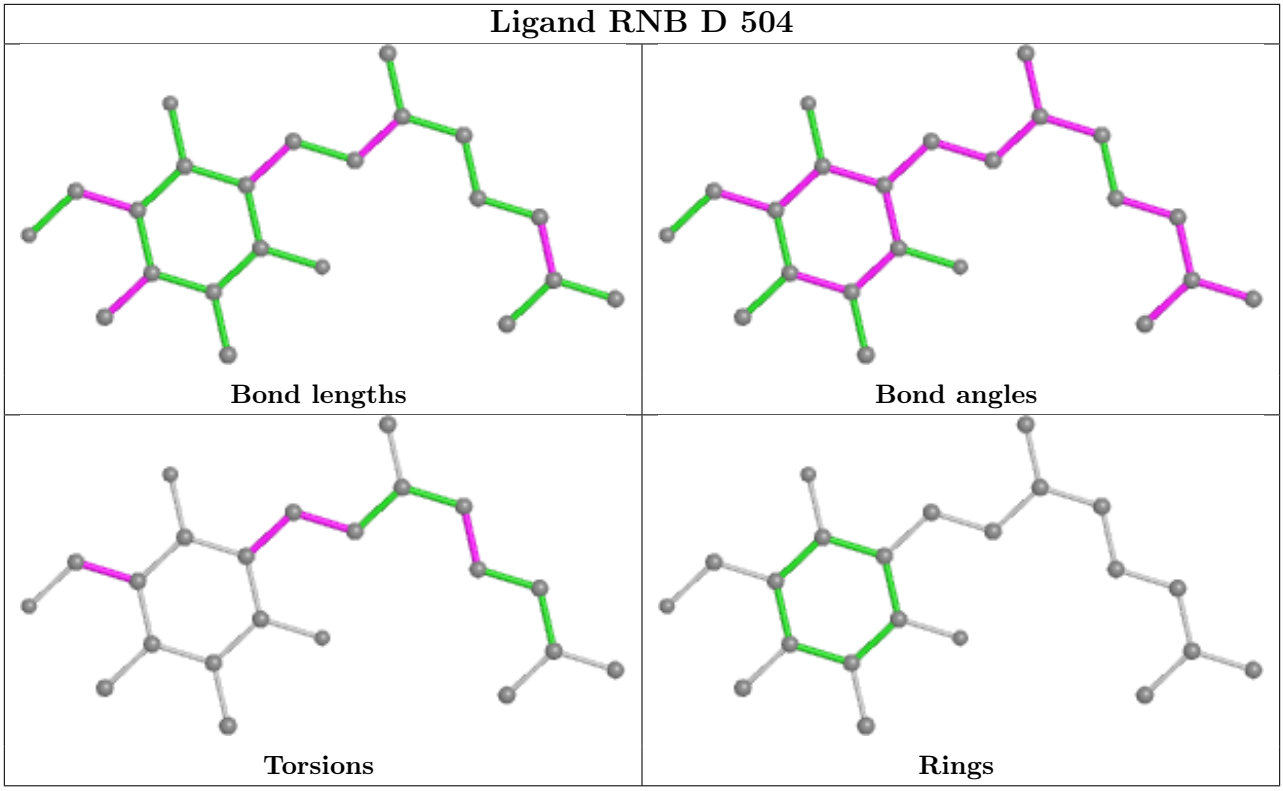
Bond angles



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	264/329 (80%)	0.03	8 (3%) 50 57	22, 33, 55, 83	0
1	B	266/329 (80%)	0.66	33 (12%) 4 5	30, 44, 82, 114	0
1	C	266/329 (80%)	0.66	34 (12%) 3 5	26, 45, 81, 116	0
1	D	263/329 (79%)	0.06	7 (2%) 54 62	24, 34, 52, 69	0
All	All	1059/1316 (80%)	0.35	82 (7%) 13 17	22, 39, 71, 116	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	TYR	8.9
1	C	235	THR	7.5
1	B	106	ARG	7.3
1	B	31	PRO	7.2
1	C	105	TYR	7.1
1	B	107	PHE	7.1
1	A	107	PHE	5.6
1	B	49	VAL	5.3
1	B	109	SER	5.3
1	C	104	LEU	5.0
1	B	235	THR	5.0
1	C	177	LEU	4.8
1	C	110	ILE	4.7
1	C	107	PHE	4.6
1	C	108	GLY	4.6
1	B	52	LEU	4.5
1	B	108	GLY	4.4
1	B	97	TRP	4.3
1	C	102	PHE	4.1
1	D	238	ASP	3.8
1	C	106	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	174	GLN	3.8
1	C	252	ASN	3.8
1	C	297	ASN	3.6
1	B	113	SER	3.5
1	B	252	ASN	3.5
1	A	49	VAL	3.5
1	C	293	VAL	3.5
1	A	32	VAL	3.4
1	A	251	LYS	3.4
1	A	238	ASP	3.4
1	C	172	LEU	3.4
1	D	252	ASN	3.4
1	C	178	PRO	3.3
1	D	32	VAL	3.3
1	B	104	LEU	3.2
1	C	109	SER	3.2
1	C	113	SER	3.1
1	C	48	PRO	3.1
1	C	174	GLN	3.1
1	C	179	LEU	3.1
1	C	99	PHE	3.1
1	B	102	PHE	3.0
1	C	32	VAL	3.0
1	B	177	LEU	3.0
1	B	110	ILE	2.9
1	C	173	ARG	2.8
1	D	47	VAL	2.7
1	B	251	LYS	2.6
1	D	251	LYS	2.6
1	B	253	ALA	2.6
1	C	111	THR	2.6
1	B	189	ILE	2.5
1	C	97	TRP	2.5
1	A	252	ASN	2.5
1	B	178	PRO	2.5
1	C	181	VAL	2.5
1	C	294	LEU	2.5
1	B	32	VAL	2.4
1	B	81	ASN	2.4
1	B	294	LEU	2.4
1	B	53	ARG	2.4
1	B	144	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	173	ARG	2.4
1	C	101	THR	2.3
1	B	84	VAL	2.3
1	D	283	ARG	2.3
1	B	111	THR	2.3
1	C	217	VAL	2.3
1	C	100	ASP	2.3
1	C	236	LYS	2.3
1	C	232	LEU	2.2
1	A	106	ARG	2.2
1	B	51	PRO	2.2
1	C	244	ARG	2.2
1	B	114	LYS	2.1
1	D	45[A]	GLU	2.1
1	B	267	ALA	2.1
1	B	238	ASP	2.0
1	C	103	SER	2.0
1	C	51	PRO	2.0
1	A	33	TRP	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
4	RNB	B	504	22/22	0.75	0.39	43,59,68,70	0
6	GOL	D	506	6/6	0.84	0.17	40,45,46,46	0
4	RNB	C	504	22/22	0.88	0.25	30,44,83,86	0
5	SO4	D	505	5/5	0.91	0.20	69,70,74,77	0

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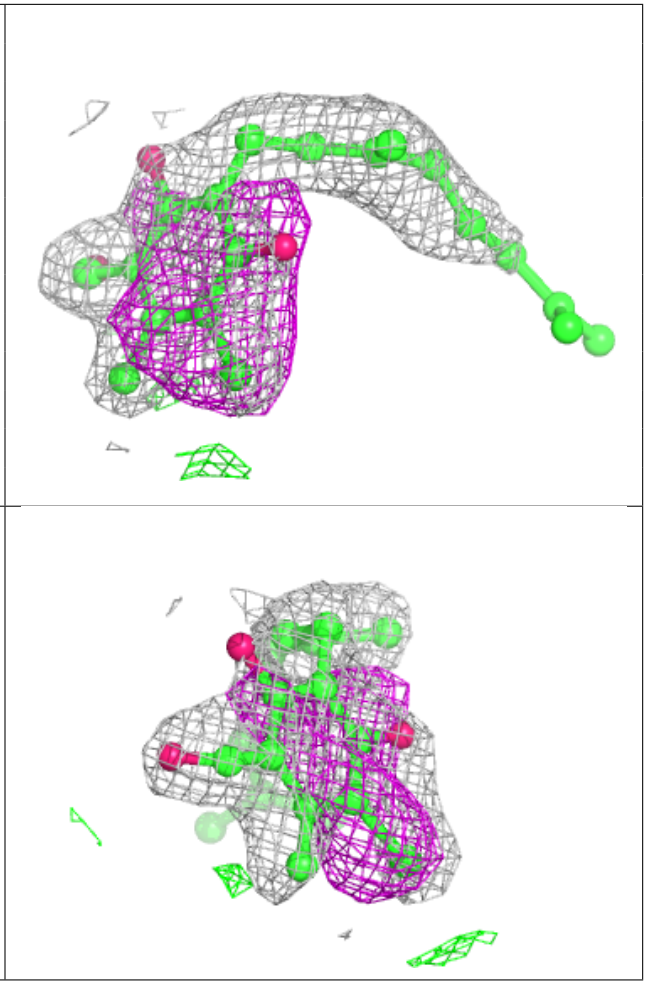
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	RNB	A	504	22/22	0.92	0.17	22,30,41,43	0
5	SO4	A	505	5/5	0.92	0.17	51,55,62,62	0
4	RNB	D	504	22/22	0.93	0.16	23,33,56,58	0
2	FE	C	502	1/1	0.97	0.19	34,34,34,34	0
2	FE	B	502	1/1	0.98	0.18	42,42,42,42	0
2	FE	C	501	1/1	0.99	0.14	44,44,44,44	0
2	FE	B	501	1/1	0.99	0.10	42,42,42,42	0
2	FE	D	502	1/1	0.99	0.14	27,27,27,27	0
3	OH	B	503	1/1	0.99	0.21	24,24,24,24	0
3	OH	C	503	1/1	0.99	0.23	19,19,19,19	0
2	FE	A	501	1/1	0.99	0.11	25,25,25,25	0
3	OH	D	503	1/1	1.00	0.20	14,14,14,14	0
3	OH	A	503	1/1	1.00	0.11	16,16,16,16	0
2	FE	D	501	1/1	1.00	0.13	31,31,31,31	0
2	FE	A	502	1/1	1.00	0.09	29,29,29,29	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.

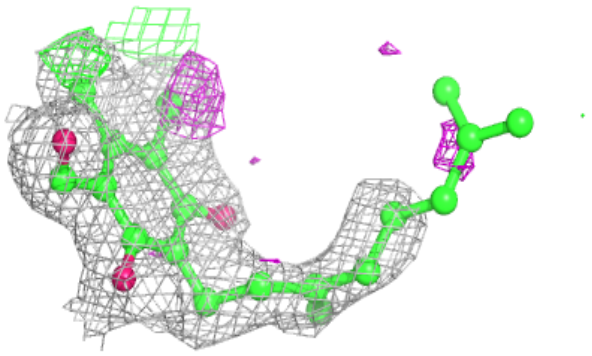
Electron density around RNB B 504:

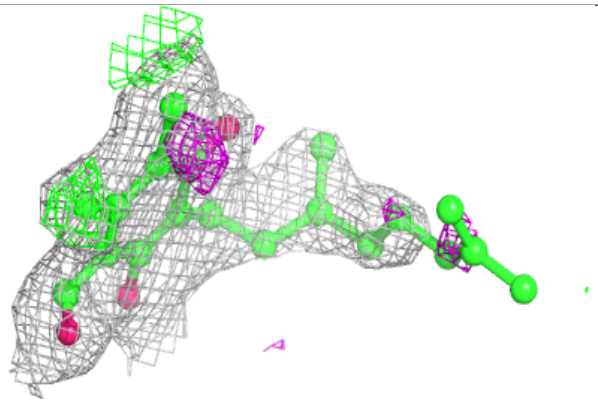
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

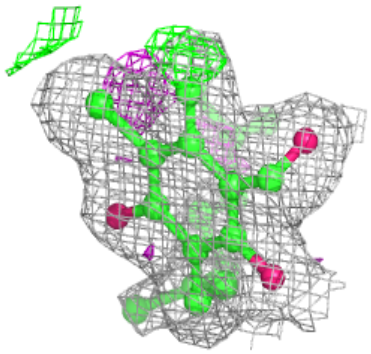


Electron density around RNB C 504:

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

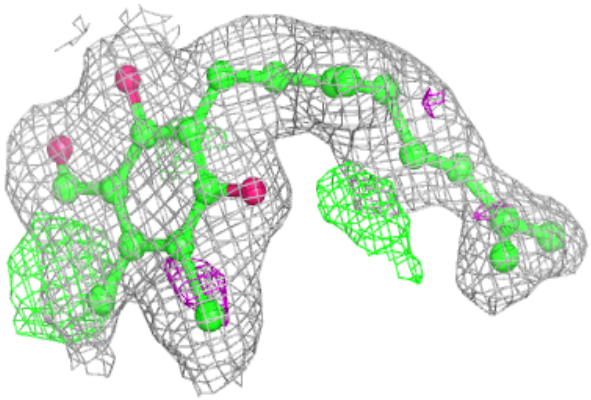


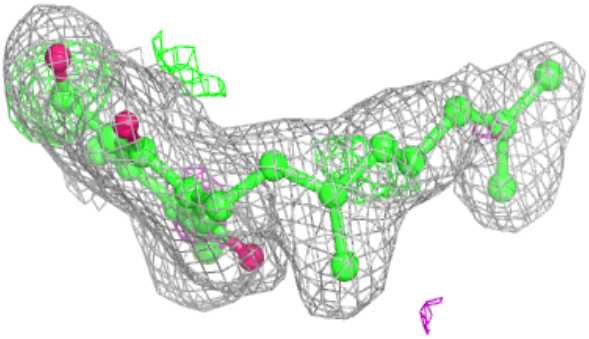


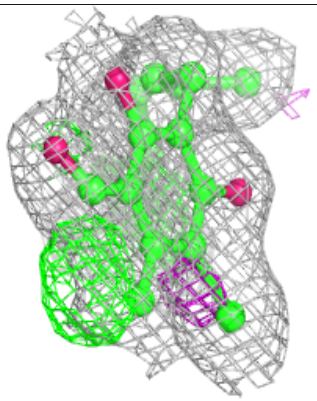


Electron density around RNB A 504:

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

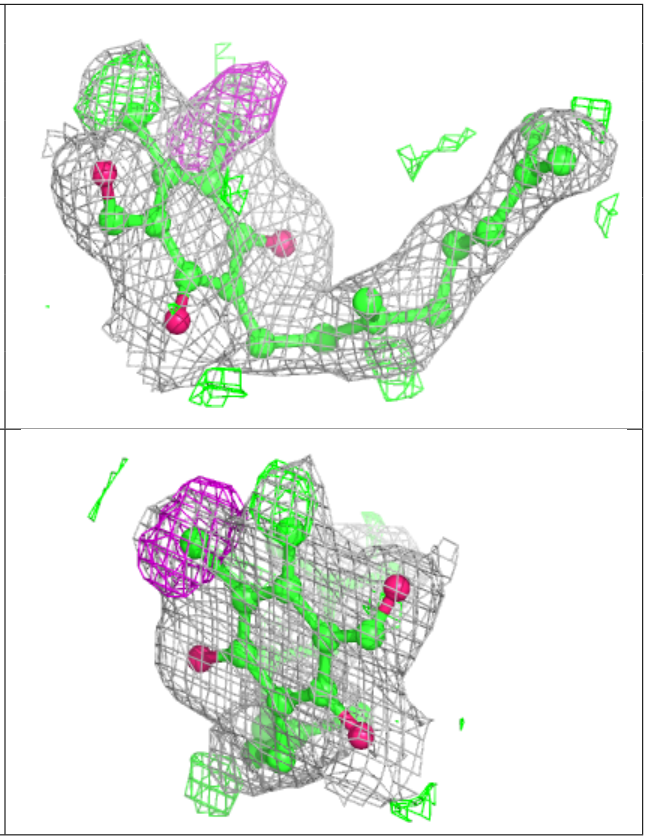






Electron density around RNB D 504:

$2mF_o$-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.