



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 04:50 am BST

PDB ID : 5ZDQ
Title : Crystal structure of cyanide-insensitive alternative oxidase from *Trypanosoma brucei* with COLLETOCHLORIN B
Authors : Shiba, T.; Inaoka, D.K.; Takahashi, G.; Tsuge, C.; Kido, Y.; Young, L.; Ueda, S.; Balogun, E.O.; Nara, T.; Honma, T.; Tanaka, A.; Inoue, M.; Saimoto, H.; Harada, S.; Moore, A.L.; Kita, K.
Deposited on : 2018-02-23
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

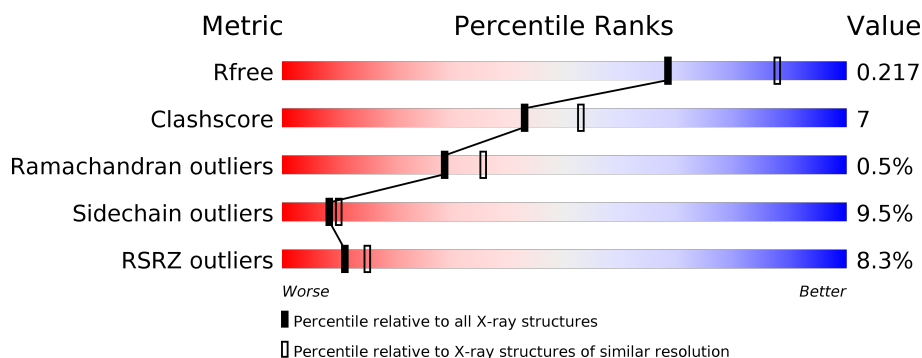
1 Overall quality at a glance ⓘ

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>15%</div> <div>•</div> <div>20%</div> </div> </div>
1	B	329	<div> <div>11%</div> <div> <div></div> <div>61%</div> <div>18%</div> <div>••</div> <div>19%</div> </div> </div>
1	C	329	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>16%</div> <div>•</div> <div>19%</div> </div> </div>
1	D	329	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>15%</div> <div>•</div> <div>20%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9026 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.

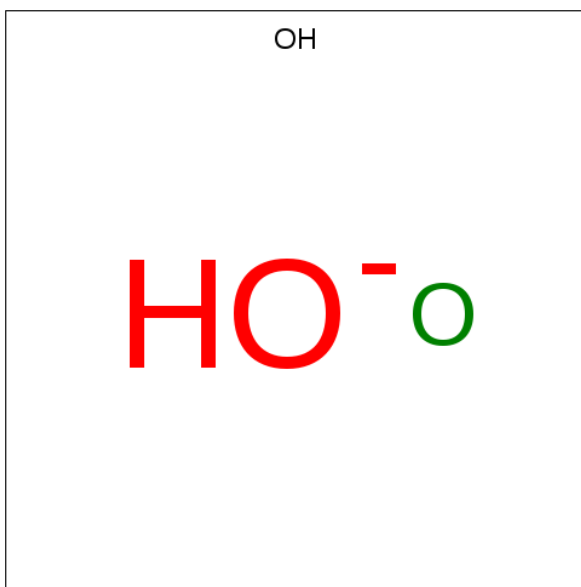
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

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

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

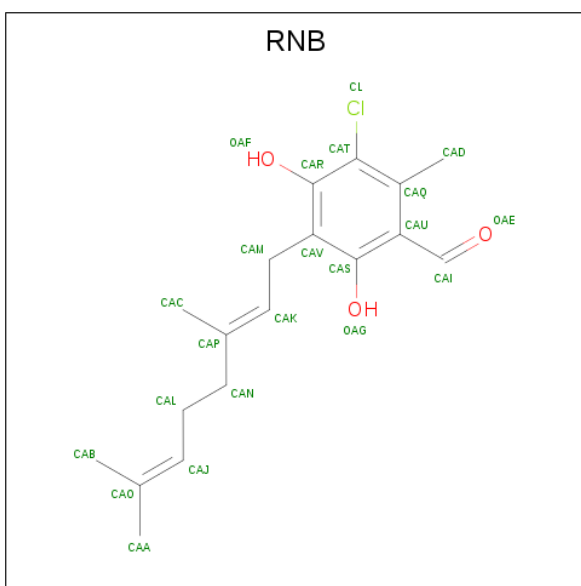
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		

- 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: C₁₈H₂₃ClO₃).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

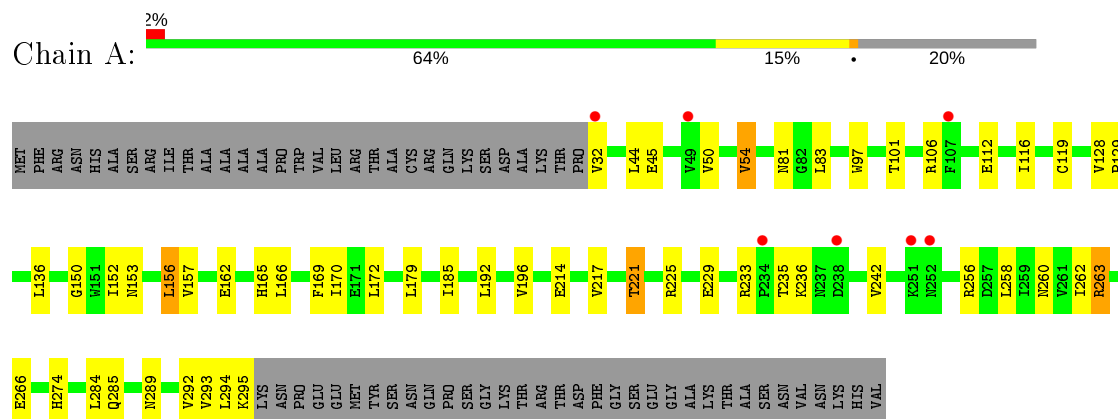
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	90	Total	O	0	0
			90	90		
7	B	65	Total	O	0	0
			65	65		
7	C	55	Total	O	0	0
			55	55		
7	D	83	Total	O	0	0
			83	83		

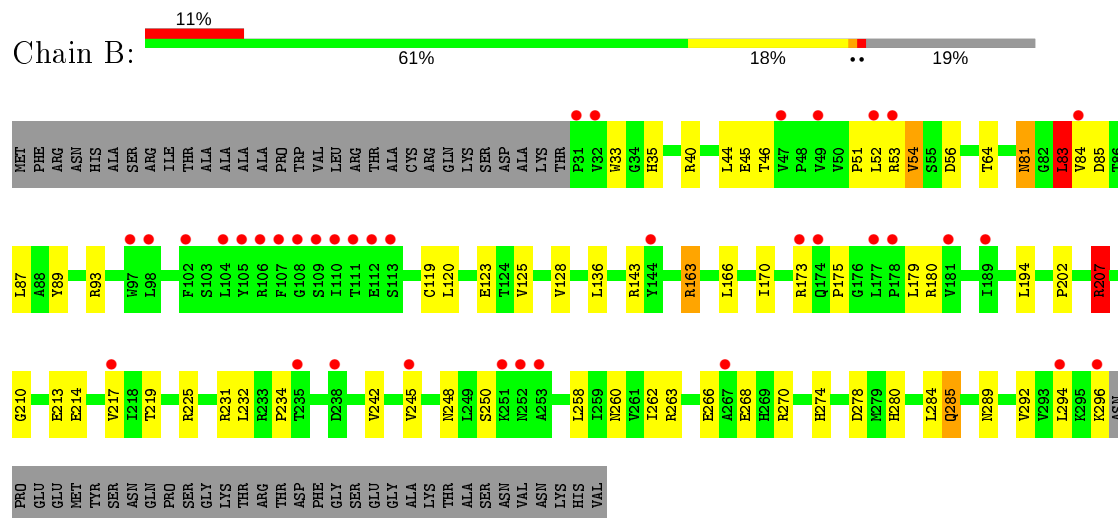
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

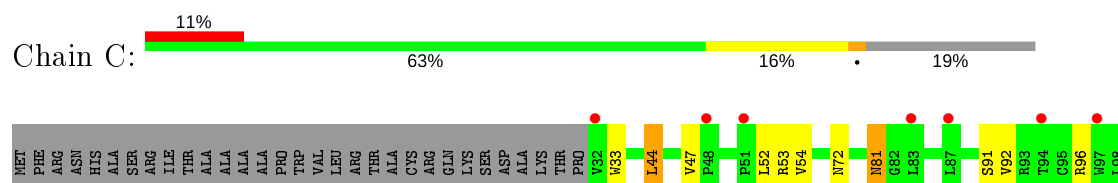
- Molecule 1: Alternative oxidase, mitochondrial

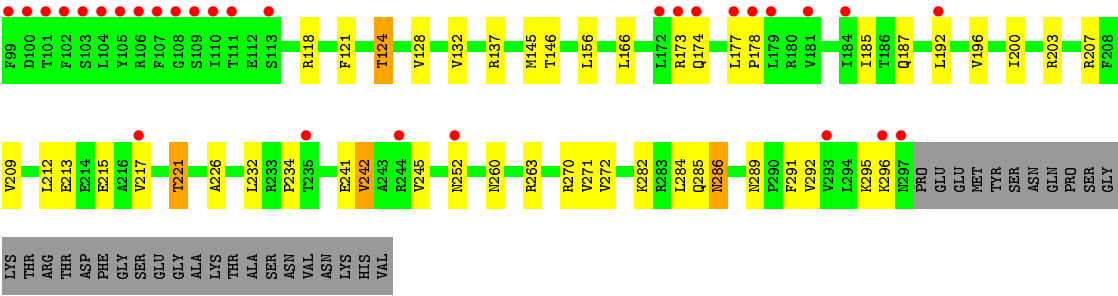


- Molecule 1: Alternative oxidase, mitochondrial

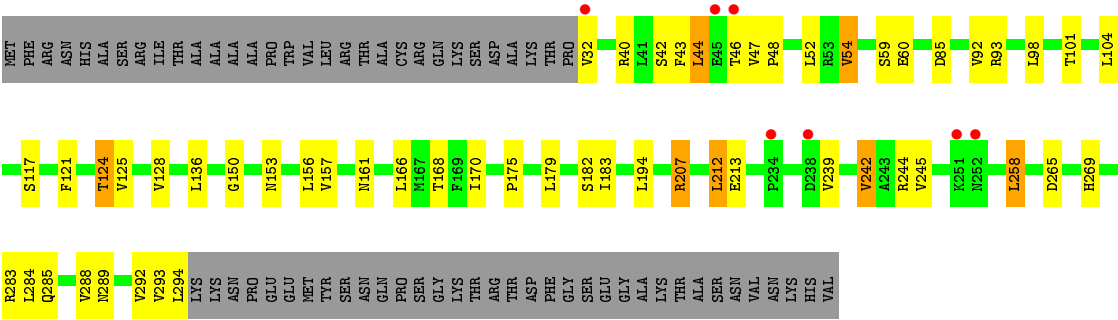


- Molecule 1: Alternative oxidase, mitochondrial





● Molecule 1: Alternative oxidase, mitochondrial



4 Data and refinement statistics

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) 99.7 (42.89-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.185 , 0.220 0.188 , 0.217	Depositor DCC
R_{free} test set	4089 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.247 for -h-2*k,l	Xtriage
Reported twinning fraction	0.477 for H, K, L 0.523 for H+4/2L, -K, -L	Depositor
Outliers	0 of 82820 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9026	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 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, RNB, FE, SO4, OH

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	0.45	0/2195	0.70	0/2982
1	B	0.38	0/2212	0.65	5/3004 (0.2%)
1	C	0.38	0/2212	0.62	0/3004
1	D	0.43	0/2195	0.71	0/2983
All	All	0.41	0/8814	0.67	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(°)	Ideal(°)
1	B	163	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	225	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	225	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	B	207	ARG	CG-CD-NE	5.02	122.35	111.80
1	B	207	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	29	0
1	B	2162	0	2196	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2163	0	2194	31	0
1	D	2146	0	2167	33	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	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	22	0	21	0	0
4	B	22	0	23	2	0
4	C	22	0	22	2	0
4	D	22	0	21	1	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
6	D	6	0	8	0	0
7	A	90	0	0	3	0
7	B	65	0	0	0	0
7	C	55	0	0	3	0
7	D	83	0	0	2	0
All	All	9026	0	8827	120	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 7.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:O	1:A:221:THR:CG2	2.36	0.74
1:A:217:VAL:O	1:A:221:THR:HG22	1.88	0.74
1:D:124:THR:HG21	1:D:183:ILE:HG23	1.69	0.74
1:D:54:VAL:HG22	1:D:242:VAL:HG13	1.70	0.73
1:A:293:VAL:O	1:A:295:LYS:N	2.22	0.73
1:C:207:ARG:CZ	7:C:604:HOH:O	2.37	0.72
1:D:125:VAL:O	1:D:128:VAL:HG22	1.92	0.70
1:C:217:VAL:O	1:C:221:THR:HG23	1.92	0.69
1:D:153:ASN:O	1:D:157:VAL:HG13	1.96	0.65
1:C:221:THR:HG22	1:C:263:ARG:HD2	1.79	0.64
1:B:268:GLU:OE2	1:C:33:TRP:NE1	2.25	0.64
1:D:239:VAL:HA	7:D:621:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:VAL:O	1:B:128:VAL:HG12	2.00	0.62
1:A:54:VAL:CG2	1:A:242:VAL:HG12	2.29	0.62
1:D:161:ASN:HD22	1:D:269:HIS:CE1	2.18	0.61
1:D:44:LEU:O	1:D:47:VAL:HG12	2.02	0.60
1:D:85:ASP:OD1	1:D:207:ARG:HD2	2.01	0.60
1:D:289:ASN:O	1:D:292:VAL:HG22	2.01	0.60
1:B:128:VAL:HG13	1:B:194:LEU:CD1	2.32	0.59
1:D:128:VAL:HG23	1:D:194:LEU:CD1	2.33	0.59
1:B:40:ARG:O	1:C:271:VAL:HG12	2.02	0.59
1:C:92:VAL:HG22	1:C:212:LEU:CD2	2.31	0.58
1:D:92:VAL:HG22	1:D:212:LEU:HD23	1.85	0.58
1:A:214:GLU:OE1	1:A:274:HIS:HE1	1.87	0.57
1:B:85:ASP:OD1	1:B:207:ARG:NH1	2.38	0.57
1:A:192:LEU:O	1:A:196:VAL:HG13	2.05	0.57
1:C:81:ASN:CG	1:C:81:ASN:O	2.43	0.56
1:A:258:LEU:HD23	1:A:258:LEU:C	2.25	0.56
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.71	0.56
1:D:175:PRO:HB3	1:D:179:LEU:HD23	1.88	0.56
1:B:120:LEU:HD11	1:C:145:MET:SD	2.46	0.55
1:C:137:ARG:NH2	1:C:285:GLN:O	2.33	0.55
1:B:219:THR:HG21	4:B:504:RNB:CL	2.43	0.55
1:D:43:PHE:O	1:D:46:THR:HG22	2.07	0.55
1:A:217:VAL:O	1:A:221:THR:HG23	2.07	0.54
1:C:54:VAL:CG2	1:C:242:VAL:HG13	2.37	0.54
1:C:118:ARG:NH2	4:C:504:RNB:OAF	2.40	0.54
1:B:64:THR:HG22	1:B:64:THR:O	2.06	0.54
1:C:286:ASN:HB2	7:C:610:HOH:O	2.07	0.54
1:B:54:VAL:HG12	1:B:245:VAL:HG11	1.90	0.54
1:A:221:THR:HB	1:A:263:ARG:HH21	1.73	0.53
1:B:54:VAL:HG22	1:B:242:VAL:HG12	1.91	0.53
1:D:161:ASN:HD22	1:D:269:HIS:HE1	1.56	0.53
1:A:152:ILE:HG22	1:A:156:LEU:HD22	1.91	0.53
1:D:161:ASN:HD21	1:D:265:ASP:HB3	1.73	0.53
1:C:291:PHE:O	1:C:295:LYS:HB2	2.09	0.52
1:B:53:ARG:NH1	1:B:56:ASP:OD2	2.43	0.52
1:C:289:ASN:O	1:C:292:VAL:HG22	2.11	0.51
1:D:128:VAL:HG23	1:D:194:LEU:HD13	1.93	0.51
1:A:45:GLU:CD	1:A:45:GLU:H	2.15	0.50
1:A:289:ASN:O	1:A:292:VAL:HG22	2.12	0.50
1:D:40:ARG:NH2	1:D:42:SER:O	2.44	0.50
1:A:54:VAL:HG22	1:A:242:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ARG:HA	1:D:285:GLN:NE2	2.27	0.49
1:D:293:VAL:O	1:D:294:LEU:HG	2.11	0.49
4:C:504:RNB:CAK	4:C:504:RNB:OAG	2.60	0.49
1:D:150:GLY:HA3	1:D:292:VAL:HG11	1.95	0.48
1:B:262:ILE:O	1:B:266:GLU:HG2	2.14	0.48
1:B:89:TYR:O	1:B:93:ARG:HG2	2.12	0.48
1:B:278:ASP:HB3	1:C:44:LEU:HG	1.96	0.48
1:B:217:VAL:HG11	1:B:270:ARG:NH2	2.29	0.48
1:A:162:GLU:O	1:A:165:HIS:HB2	2.14	0.47
1:B:35:HIS:CG	1:C:72:ASN:HB3	2.50	0.47
1:A:153:ASN:O	1:A:157:VAL:HG22	2.14	0.47
1:D:47:VAL:HG13	1:D:48:PRO:HD3	1.96	0.47
1:C:292:VAL:O	1:C:296:LYS:HG2	2.14	0.47
1:A:229:GLU:OE2	1:B:89:TYR:OH	2.26	0.47
1:A:32:VAL:O	1:A:32:VAL:HG13	2.13	0.47
1:A:256:ARG:NE	7:A:604:HOH:O	2.47	0.47
1:B:81:ASN:HD22	1:B:81:ASN:C	2.18	0.46
1:B:207:ARG:HH11	1:B:207:ARG:CG	2.28	0.46
1:C:221:THR:HG22	1:C:263:ARG:CD	2.44	0.46
1:A:172:LEU:O	1:A:236:LYS:NZ	2.48	0.46
1:B:213:GLU:OE1	1:B:213:GLU:HA	2.16	0.46
1:C:96:ARG:NE	1:C:215:GLU:OE1	2.40	0.46
1:B:54:VAL:HG13	1:B:242:VAL:HA	1.97	0.45
1:C:54:VAL:HG22	1:C:242:VAL:HG13	1.97	0.45
1:D:175:PRO:CB	1:D:179:LEU:HD23	2.46	0.45
1:D:121:PHE:O	1:D:124:THR:HB	2.16	0.45
1:A:97:TRP:O	1:A:101:THR:HG23	2.16	0.45
1:C:121:PHE:O	1:C:124:THR:HB	2.17	0.45
1:B:143:ARG:NH1	1:C:187:GLN:OE1	2.46	0.45
1:B:83:LEU:HD12	1:B:84:VAL:H	1.82	0.45
1:C:209:VAL:O	1:C:213:GLU:HG2	2.17	0.45
1:D:213:GLU:OE1	1:D:213:GLU:HA	2.17	0.44
1:A:150:GLY:HA3	1:A:292:VAL:HG11	2.00	0.44
1:C:226:ALA:HB3	1:C:232:LEU:HD23	1.99	0.44
1:D:239:VAL:CG2	1:D:244:ARG:HG2	2.47	0.44
1:D:32:VAL:O	1:D:32:VAL:HG13	2.18	0.44
1:B:175:PRO:HB3	1:B:179:LEU:HD23	2.00	0.44
1:D:168:THR:HG21	1:D:258:LEU:HD11	1.99	0.44
1:D:288:VAL:HG13	7:D:633:HOH:O	2.16	0.43
1:C:177:LEU:N	1:C:178:PRO:HD2	2.33	0.43
4:D:504:RNB:H17	4:D:504:RNB:H12	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:VAL:O	1:D:294:LEU:CG	2.66	0.43
1:A:242:VAL:HG13	7:A:621:HOH:O	2.18	0.43
1:B:119:CYS:O	1:B:123:GLU:HG2	2.18	0.43
4:B:504:RNB:H12	4:B:504:RNB:H17	1.86	0.43
1:A:292:VAL:HG23	1:A:293:VAL:HG23	2.01	0.43
1:C:232:LEU:HD12	1:C:234:PRO:HD3	1.99	0.43
1:A:119:CYS:HB3	1:A:169:PHE:CE2	2.54	0.42
1:D:124:THR:CG2	1:D:183:ILE:HG23	2.45	0.42
1:B:207:ARG:HD3	1:B:274:HIS:CD2	2.54	0.42
1:C:241:GLU:O	1:C:245:VAL:HG13	2.19	0.42
1:C:270:ARG:NE	7:C:606:HOH:O	2.52	0.42
1:A:128:VAL:HB	1:A:129:PRO:HD3	2.01	0.42
1:A:262:ILE:O	1:A:266:GLU:HG2	2.19	0.42
1:B:280:HIS:HA	1:B:285:GLN:HG3	2.00	0.42
1:C:272:VAL:HA	1:C:291:PHE:CE2	2.55	0.42
1:D:283:ARG:HA	1:D:285:GLN:HE22	1.84	0.42
1:C:196:VAL:O	1:C:200:ILE:HG12	2.20	0.41
1:C:192:LEU:O	1:C:196:VAL:HG12	2.19	0.41
1:D:244:ARG:HB3	1:D:244:ARG:NH1	2.35	0.41
1:D:293:VAL:O	1:D:294:LEU:CB	2.69	0.41
1:A:112:GLU:O	1:A:116:ILE:HD13	2.21	0.41
1:B:210:GLY:O	1:B:214:GLU:HG3	2.20	0.41
1:A:54:VAL:HG22	1:A:242:VAL:HA	2.03	0.41
1:B:51:PRO:HG2	1:B:53:ARG:HD3	2.03	0.40
1:B:289:ASN:O	1:B:292:VAL:HG22	2.21	0.40
1:A:263:ARG:NH2	7:A:601:HOH:O	2.40	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%)	257 (98%)	4 (2%)	1 (0%)	34	42
1	B	264/329 (80%)	256 (97%)	5 (2%)	3 (1%)	14	15
1	C	264/329 (80%)	256 (97%)	8 (3%)	0	100	100
1	D	262/329 (80%)	255 (97%)	6 (2%)	1 (0%)	34	42
All	All	1052/1316 (80%)	1024 (97%)	23 (2%)	5 (0%)	29	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	LEU
1	B	54	VAL
1	B	83	LEU
1	D	59	SER
1	B	234	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/292 (82%)	219 (92%)	20 (8%)	11	13
1	B	241/292 (82%)	214 (89%)	27 (11%)	6	6
1	C	241/292 (82%)	218 (90%)	23 (10%)	8	10
1	D	239/292 (82%)	218 (91%)	21 (9%)	10	12
All	All	960/1168 (82%)	869 (90%)	91 (10%)	8	10

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	50	VAL
1	A	54	VAL
1	A	81	ASN
1	A	83	LEU
1	A	106	ARG

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Mol	Chain	Res	Type
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	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
1	B	44	LEU
1	B	45	GLU
1	B	46	THR
1	B	52	LEU
1	B	81	ASN
1	B	83	LEU
1	B	87	LEU
1	B	136	LEU
1	B	163	ARG
1	B	166	LEU
1	B	170	ILE
1	B	173	ARG
1	B	180	ARG
1	B	202	PRO
1	B	207	ARG
1	B	231	ARG
1	B	232	LEU
1	B	248	ASN
1	B	250	SER
1	B	258	LEU
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

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Mol	Chain	Res	Type
1	C	47	VAL
1	C	52	LEU
1	C	53	ARG
1	C	81	ASN
1	C	91	SER
1	C	124	THR
1	C	128	VAL
1	C	132	VAL
1	C	146	THR
1	C	156	LEU
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	242	VAL
1	C	252	ASN
1	C	260	ASN
1	C	282	LYS
1	C	284	LEU
1	C	286	ASN
1	D	44	LEU
1	D	52	LEU
1	D	54	VAL
1	D	60	GLU
1	D	93	ARG
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	207	ARG
1	D	212	LEU
1	D	242	VAL
1	D	245	VAL
1	D	258	LEU

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Mol	Chain	Res	Type
1	D	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	248	ASN
1	A	260	ASN
1	A	274	HIS
1	A	280	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	273	ASN
1	B	274	HIS
1	C	37	GLN
1	C	72	ASN
1	C	252	ASN
1	C	260	ASN
1	D	72	ASN
1	D	161	ASN
1	D	248	ASN
1	D	260	ASN
1	D	269	HIS
1	D	273	ASN
1	D	274	HIS
1	D	280	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are modelled with single atom and 8 are monoatomic - 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
4	RNB	D	504	-	22,22,22	1.03	2 (9%)	29,30,30	1.36	4 (13%)
5	SO4	A	505	-	4,4,4	0.44	0	6,6,6	0.12	0
4	RNB	B	504	-	22,22,22	0.90	1 (4%)	29,30,30	1.59	4 (13%)
4	RNB	C	504	-	22,22,22	0.93	1 (4%)	29,30,30	1.49	7 (24%)
6	GOL	D	506	-	5,5,5	0.52	0	5,5,5	0.46	0
4	RNB	A	504	-	22,22,22	0.99	1 (4%)	29,30,30	2.07	7 (24%)
5	SO4	D	505	-	4,4,4	0.32	0	6,6,6	0.16	0

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	RNB	CAT-CL	3.40	1.80	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	RNB	CAT-CL	3.27	1.79	1.72
4	C	504	RNB	CAT-CL	3.20	1.79	1.72
4	D	504	RNB	CAT-CL	2.34	1.77	1.72
4	D	504	RNB	CAR-CAV	-2.11	1.36	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	RNB	CAV-CAM-CAK	-5.93	102.77	112.17
4	A	504	RNB	CAV-CAM-CAK	5.08	120.21	112.17
4	D	504	RNB	CAV-CAM-CAK	-4.86	104.47	112.17
4	A	504	RNB	CAM-CAV-CAR	-4.60	114.76	120.82
4	A	504	RNB	CAM-CAV-CAS	4.52	126.77	120.82
4	A	504	RNB	CAR-CAT-CAQ	-3.72	120.43	122.79
4	C	504	RNB	CAC-CAP-CAN	3.34	120.89	115.27
4	A	504	RNB	CAC-CAP-CAK	-3.10	115.73	123.68
4	C	504	RNB	CAR-CAT-CAQ	-2.82	121.00	122.79
4	B	504	RNB	CAR-CAT-CAQ	-2.74	121.05	122.79
4	C	504	RNB	CAM-CAV-CAR	-2.72	117.24	120.82
4	A	504	RNB	CAQ-CAT-CL	2.60	122.52	118.58
4	D	504	RNB	OAE-CAI-CAU	-2.56	119.34	124.91
4	A	504	RNB	CAN-CAP-CAK	2.41	126.00	121.12
4	D	504	RNB	CAD-CAQ-CAU	2.31	124.06	120.62
4	C	504	RNB	CAC-CAP-CAK	-2.31	117.75	123.68
4	B	504	RNB	OAE-CAI-CAU	-2.30	119.90	124.91
4	C	504	RNB	CAM-CAV-CAS	2.23	123.75	120.82
4	C	504	RNB	OAE-CAI-CAU	-2.11	120.32	124.91
4	C	504	RNB	CAQ-CAT-CL	2.05	121.69	118.58
4	D	504	RNB	CAM-CAK-CAP	-2.02	124.11	127.24
4	B	504	RNB	CAM-CAK-CAP	-2.02	124.11	127.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

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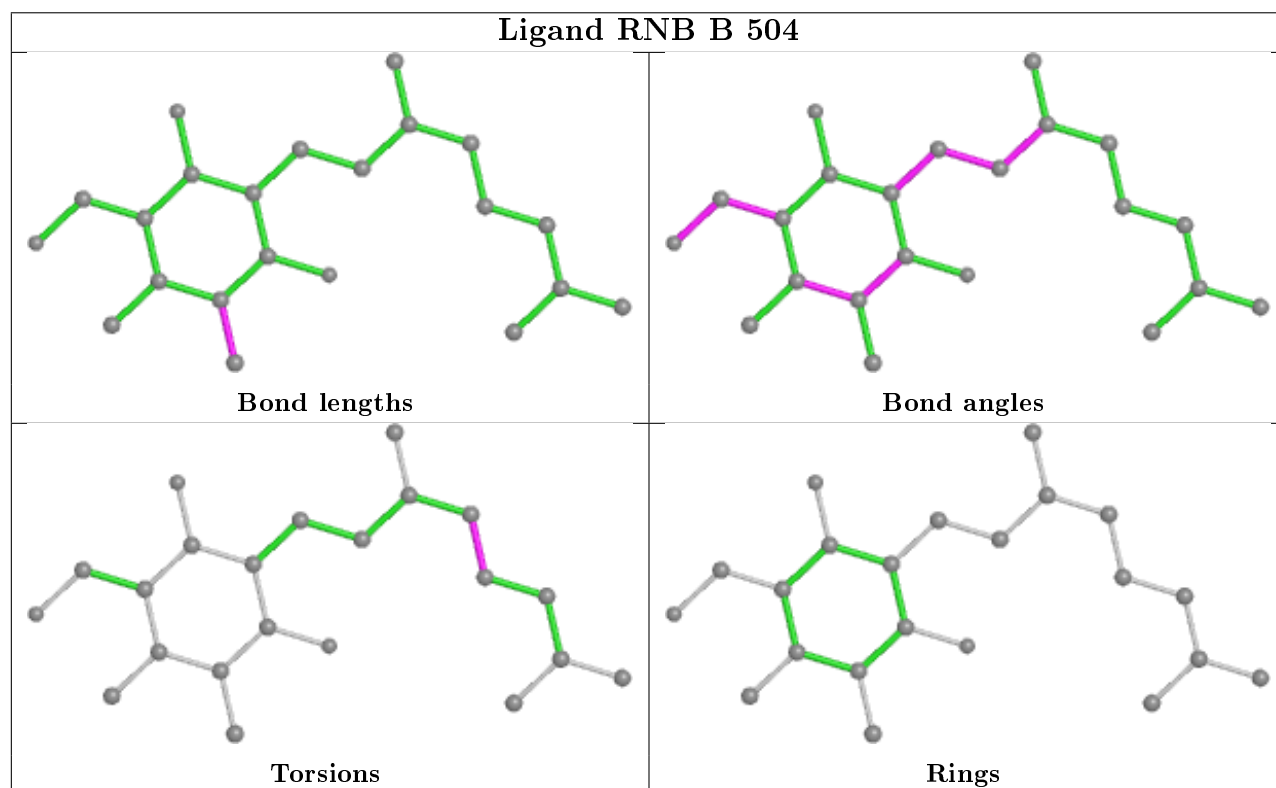
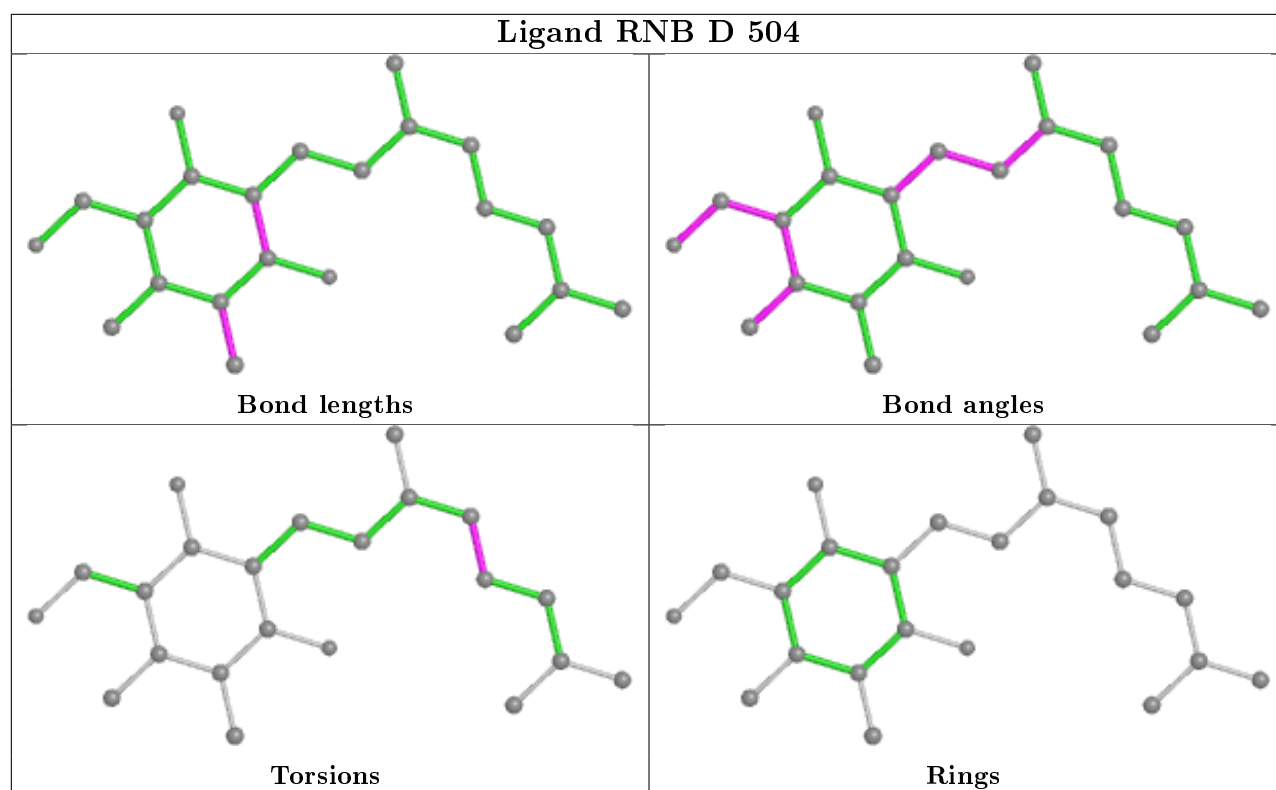
Mol	Chain	Res	Type	Atoms
4	C	504	RNB	CAK-CAM-CAV-CAR
4	D	504	RNB	CAJ-CAL-CAN-CAP
4	A	504	RNB	CAJ-CAL-CAN-CAP
4	A	504	RNB	CAP-CAK-CAM-CAV
6	D	506	GOL	O2-C2-C3-O3
4	C	504	RNB	CAP-CAK-CAM-CAV

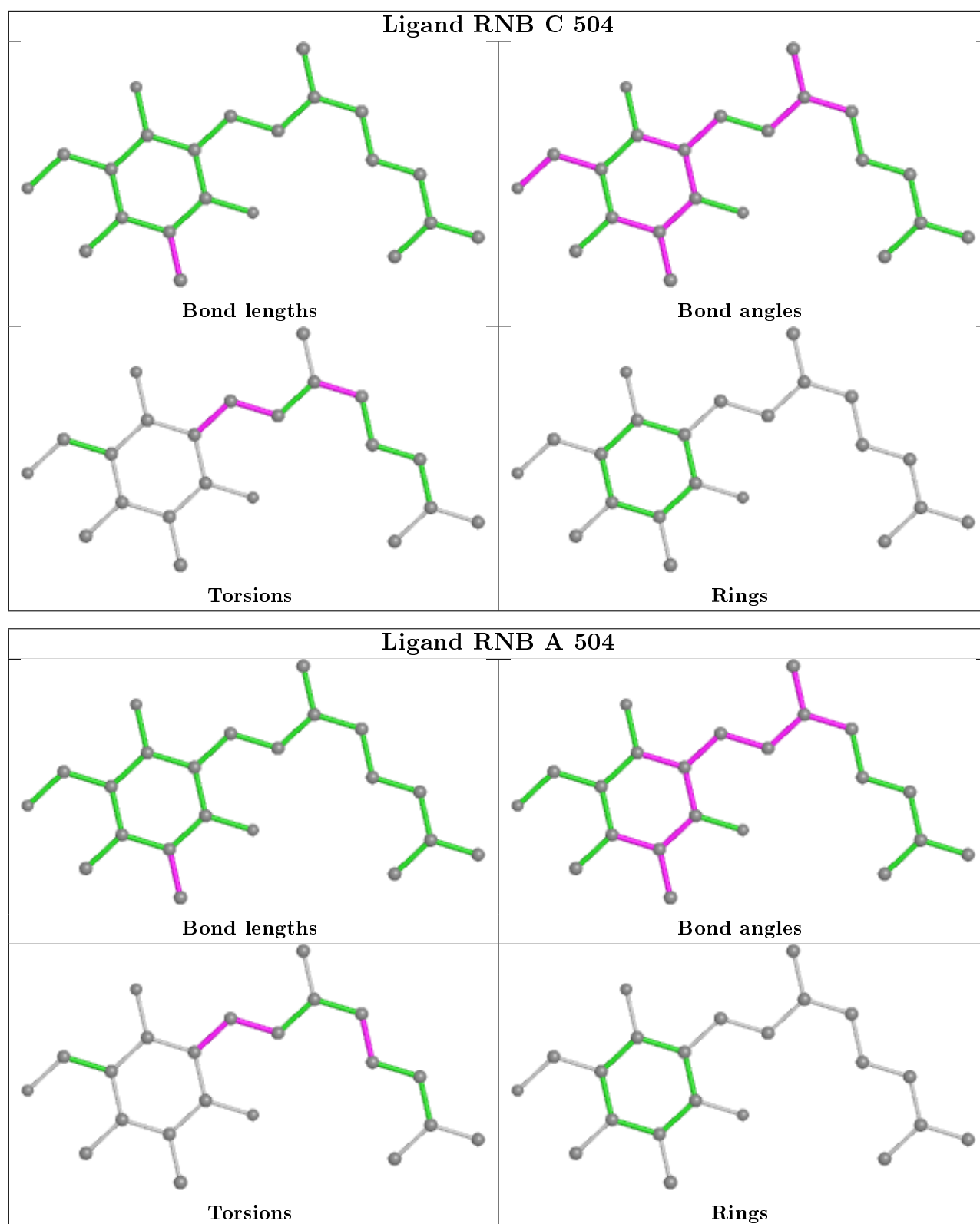
There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/329 (80%)	0.00	7 (2%) 54 62	22, 33, 53, 81	0
1	B	266/329 (80%)	0.65	37 (13%) 2 4	30, 44, 81, 113	0
1	C	266/329 (80%)	0.68	37 (13%) 2 4	27, 45, 80, 114	0
1	D	263/329 (79%)	0.02	7 (2%) 54 62	24, 33, 51, 67	0
All	All	1059/1316 (80%)	0.34	88 (8%) 11 15	22, 39, 71, 114	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	TYR	9.2
1	B	106	ARG	7.3
1	C	105	TYR	6.9
1	B	107	PHE	6.2
1	B	31	PRO	6.2
1	C	235	THR	5.7
1	A	107	PHE	5.7
1	B	109	SER	5.3
1	C	177	LEU	5.2
1	C	107	PHE	5.1
1	C	104	LEU	5.0
1	B	52	LEU	4.9
1	C	108	GLY	4.9
1	B	235	THR	4.4
1	A	32	VAL	4.4
1	B	174	GLN	4.3
1	D	238	ASP	4.2
1	B	49	VAL	4.2
1	C	102	PHE	4.2
1	C	106	ARG	4.1
1	C	252	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	178	PRO	3.9
1	B	97	TRP	3.9
1	B	113	SER	3.8
1	B	177	LEU	3.8
1	B	108	GLY	3.6
1	C	110	ILE	3.6
1	A	251	LYS	3.6
1	C	109	SER	3.5
1	C	99	PHE	3.5
1	C	48	PRO	3.5
1	C	179	LEU	3.4
1	D	32	VAL	3.4
1	D	252	ASN	3.3
1	B	252	ASN	3.3
1	B	110	ILE	3.3
1	B	102	PHE	3.3
1	A	238	ASP	3.3
1	C	173	ARG	3.2
1	C	293	VAL	3.0
1	C	297	ASN	2.9
1	C	101	THR	2.9
1	B	251	LYS	2.9
1	C	111	THR	2.8
1	C	97	TRP	2.8
1	A	234	PRO	2.8
1	B	32	VAL	2.8
1	B	104	LEU	2.8
1	C	113	SER	2.7
1	B	253	ALA	2.7
1	C	174	GLN	2.7
1	C	32	VAL	2.6
1	B	238	ASP	2.6
1	B	47	VAL	2.6
1	C	192	LEU	2.6
1	C	103	SER	2.6
1	A	252	ASN	2.6
1	B	84	VAL	2.5
1	C	181	VAL	2.5
1	C	100	ASP	2.4
1	B	189	ILE	2.4
1	B	181	VAL	2.4
1	B	112	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	251	LYS	2.3
1	B	294	LEU	2.3
1	D	46	THR	2.3
1	D	45[A]	GLU	2.3
1	C	172	LEU	2.3
1	B	111	THR	2.3
1	C	217	VAL	2.3
1	B	178	PRO	2.3
1	A	49	VAL	2.2
1	B	53	ARG	2.2
1	B	173	ARG	2.2
1	C	94	THR	2.2
1	C	244	ARG	2.2
1	C	83	LEU	2.2
1	B	245	VAL	2.1
1	B	144	TYR	2.1
1	B	296	LYS	2.1
1	C	51	PRO	2.1
1	C	184	ILE	2.1
1	B	267	ALA	2.1
1	C	296	LYS	2.1
1	C	87	LEU	2.1
1	B	217	VAL	2.1
1	D	234	PRO	2.0
1	B	98	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

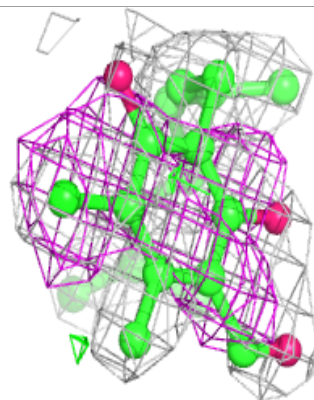
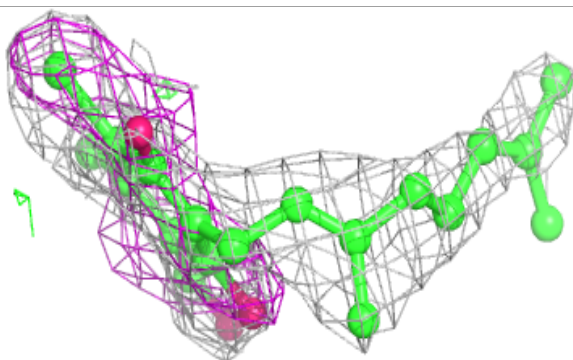
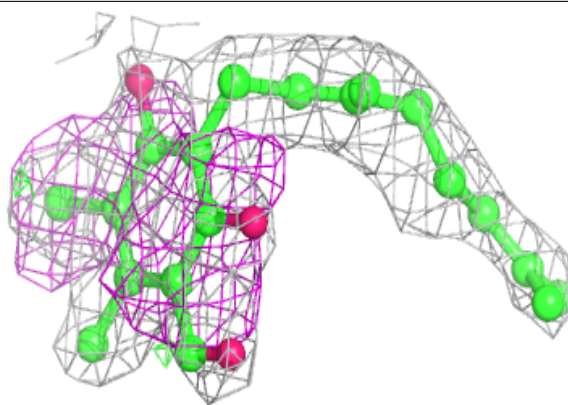
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	RNB	B	504	22/22	0.82	0.32	47,50,56,58	0
6	GOL	D	506	6/6	0.86	0.14	40,43,44,45	0
5	SO4	D	505	5/5	0.87	0.23	69,69,72,74	0
4	RNB	C	504	22/22	0.88	0.24	41,46,84,85	0
4	RNB	A	504	22/22	0.91	0.18	29,35,59,60	0
5	SO4	A	505	5/5	0.92	0.17	54,60,63,64	0
4	RNB	D	504	22/22	0.94	0.14	25,29,52,53	0
3	OH	C	503	1/1	0.99	0.15	17,17,17,17	0
2	FE	B	501	1/1	0.99	0.08	45,45,45,45	0
2	FE	D	502	1/1	0.99	0.13	27,27,27,27	0
2	FE	C	501	1/1	0.99	0.13	42,42,42,42	0
3	OH	B	503	1/1	0.99	0.19	26,26,26,26	0
3	OH	A	503	1/1	1.00	0.12	16,16,16,16	0
2	FE	A	501	1/1	1.00	0.10	27,27,27,27	0
2	FE	C	502	1/1	1.00	0.14	33,33,33,33	0
3	OH	D	503	1/1	1.00	0.16	14,14,14,14	0
2	FE	D	501	1/1	1.00	0.13	28,28,28,28	0
2	FE	A	502	1/1	1.00	0.09	28,28,28,28	0
2	FE	B	502	1/1	1.00	0.13	41,41,41,41	0

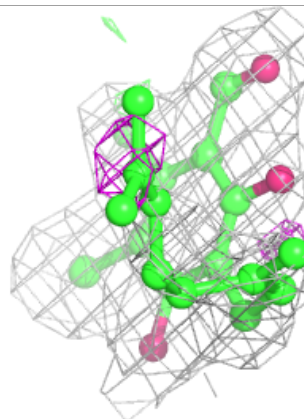
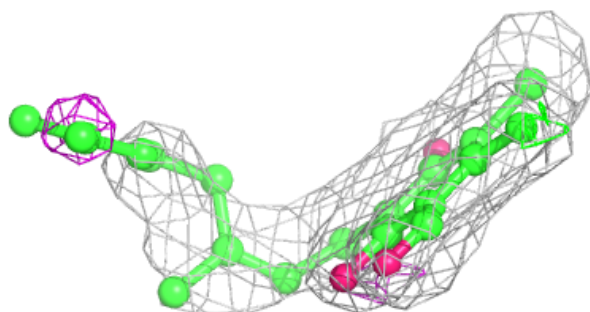
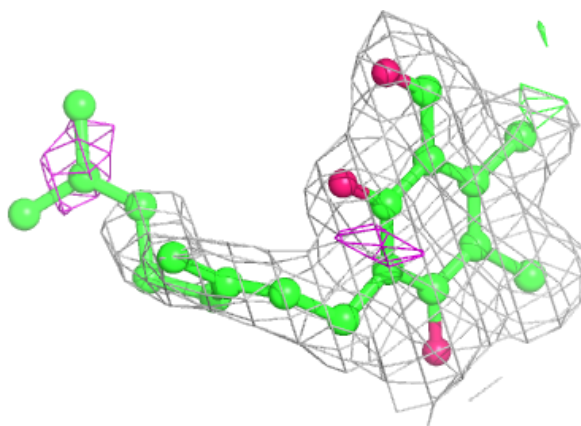
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

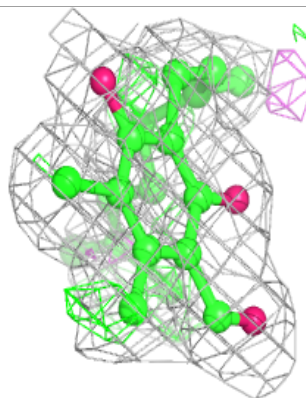
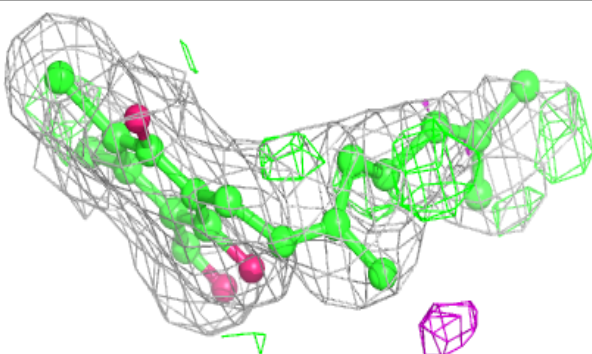
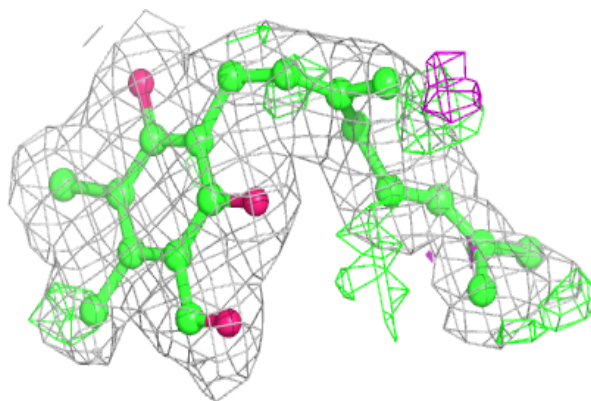
**Electron density around RNB C 504:**

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

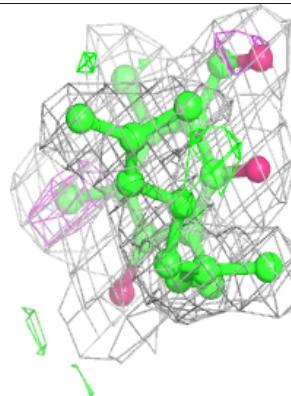
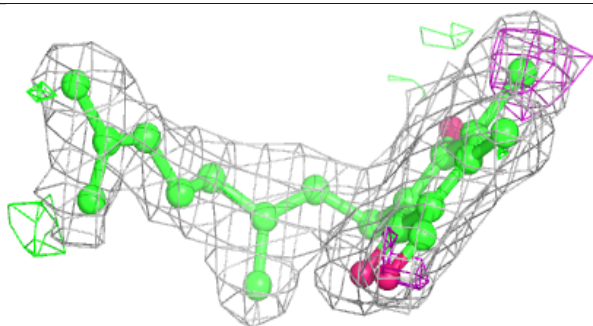
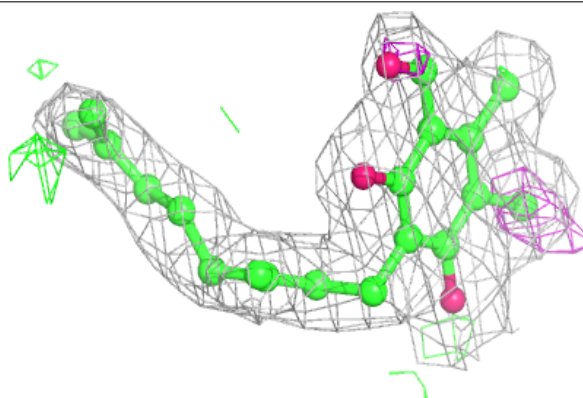


Electron density around RNB A 504:

$2mF_o-DF_c$ (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

There are no such residues in this entry.