



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 5ZDQ / pdb_00005zdq
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

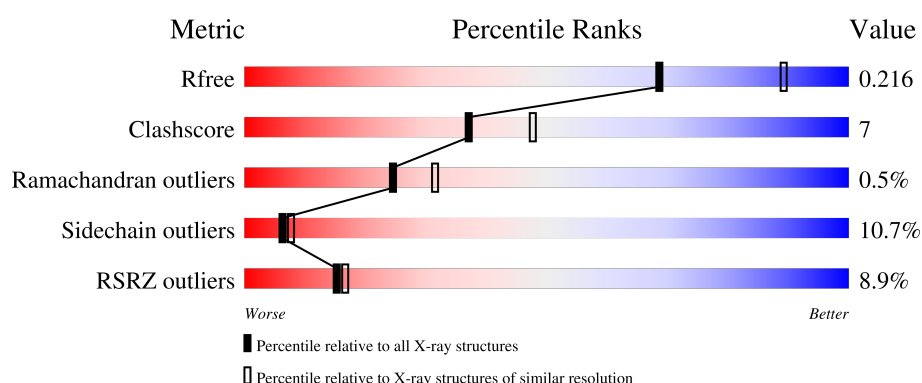
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	3% 62% 15% • 20%
1	B	329	11% 60% 19% •• 19%
1	C	329	11% 63% 16% • 19%
1	D	329	3% 63% 14% • 20%

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.

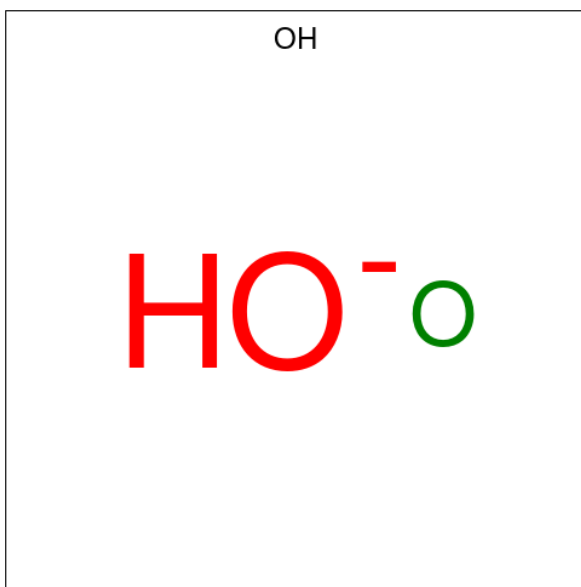
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

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 (CCD ID: FE) (formula: Fe).

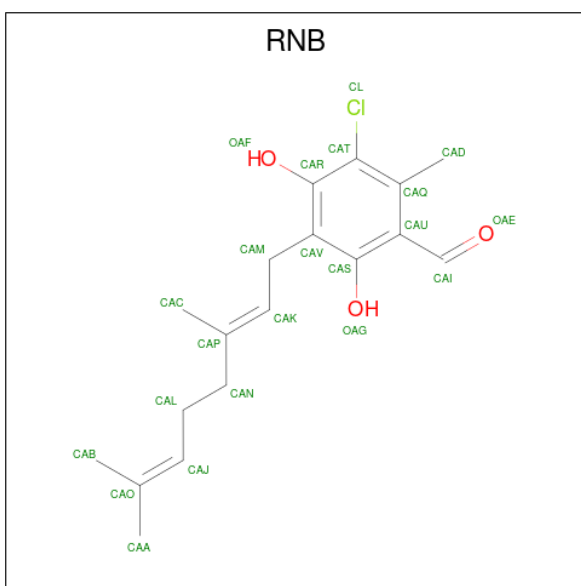
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



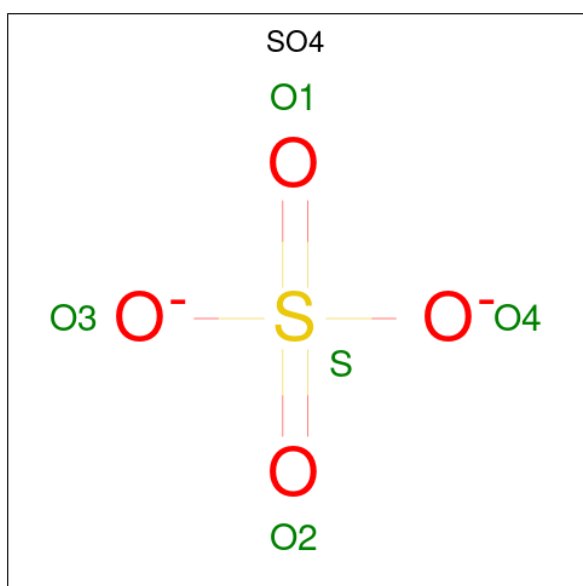
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

- Molecule 4 is 3-chloro-5-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-4,6-dihydroxy-2-methylbenzaldehyde (CCD ID: 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 (CCD ID: 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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

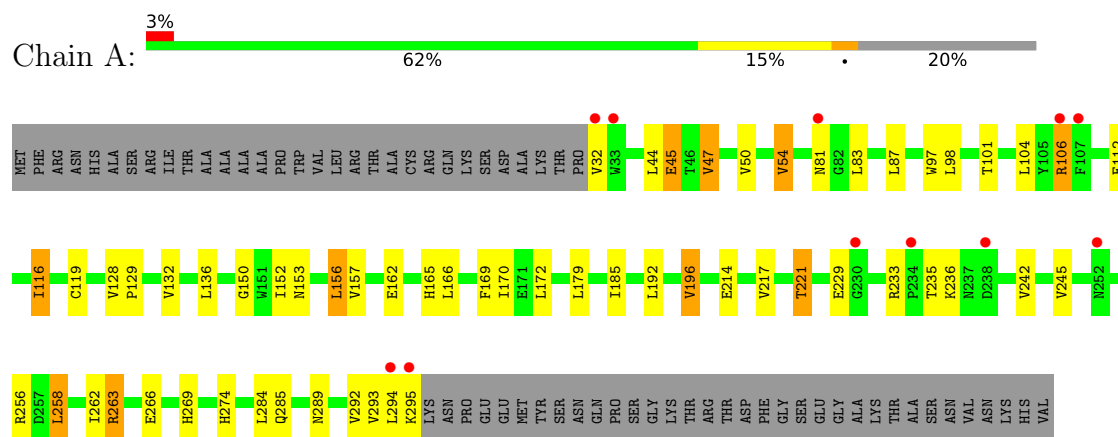
- Molecule 7 is water.

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		

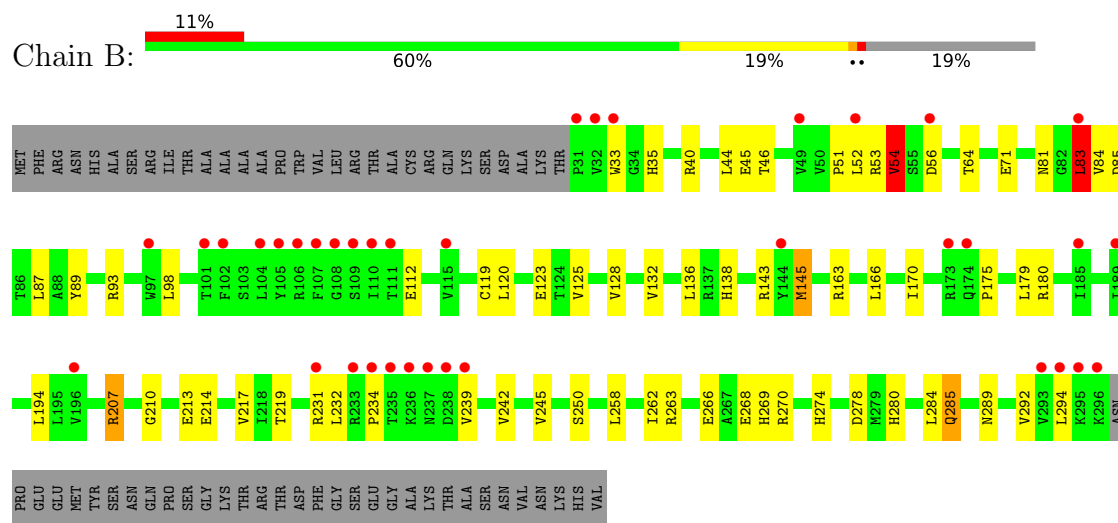
3 Residue-property plots

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.

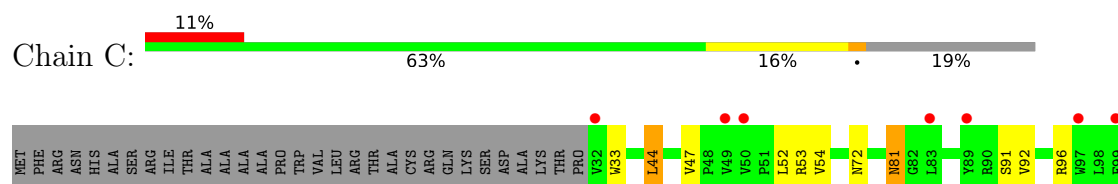
- Molecule 1: Alternative oxidase, mitochondrial

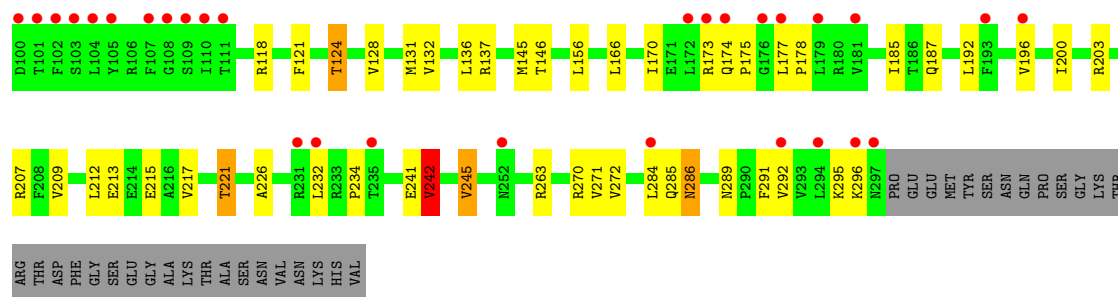


- Molecule 1: Alternative oxidase, mitochondrial

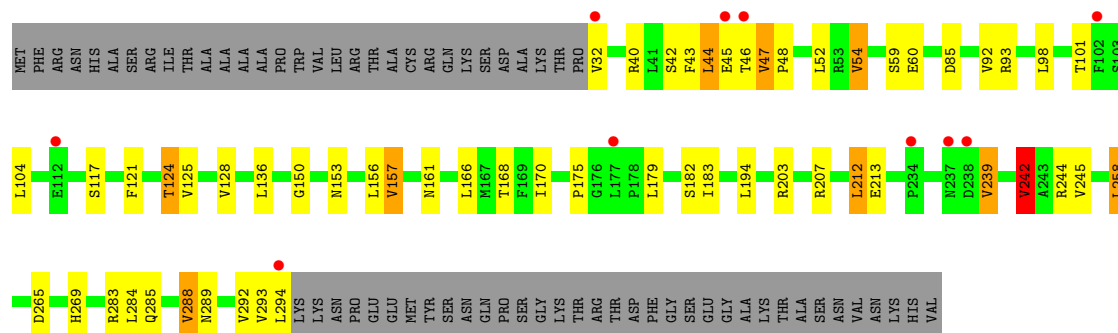


- Molecule 1: Alternative oxidase, mitochondrial





- 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 0.187 , 0.216	Depositor DCC
R_{free} test set	4089 reflections (4.92%)	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)	0.37 , 56.6	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*1,-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, RNB, FE, 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	0.63	1/2195 (0.0%)	0.91	2/2982 (0.1%)
1	B	0.55	1/2212 (0.0%)	0.84	0/3004
1	C	0.55	0/2212	0.86	1/3004 (0.0%)
1	D	0.60	0/2195	0.89	3/2983 (0.1%)
All	All	0.58	2/8814 (0.0%)	0.87	6/11973 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	HIS	C-O	-5.23	1.18	1.24
1	A	269	HIS	C-O	-5.17	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	VAL	N-CA-CB	7.37	115.14	110.50
1	A	47	VAL	N-CA-CB	7.10	114.97	110.50
1	D	242	VAL	CB-CA-C	-6.87	103.04	112.04
1	C	242	VAL	N-CA-CB	5.60	116.50	110.62
1	A	106	ARG	N-CA-C	5.46	117.23	111.28
1	D	242	VAL	N-CA-CB	5.07	116.81	110.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	30	0
1	B	2162	0	2196	35	0
1	C	2163	0	2194	35	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	125	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 (125) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:MET:HE3	1:C:170:ILE:HD13	1.75	0.68
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
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:A:258:LEU:C	1:A:258:LEU:HD23	2.25	0.61
1:C:81:ASN:CG	1:C:81:ASN:O	2.43	0.61
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: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:A:45:GLU:H	1:A:45:GLU:CD	2.15	0.55
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:B:138:HIS:CG	1:C:131:MET:HE3	2.42	0.54
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:NH1	1:B:56:ASP:OD2	2.43	0.52
1:B:81:ASN:HD22	1:B:81:ASN:C	2.18	0.51
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: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
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:89:TYR:O	1:B:93:ARG:HG2	2.12	0.48
1:B:262:ILE:O	1:B:266:GLU:HG2	2.14	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:B:145:MET:HE1	1:C:175:PRO:CG	2.44	0.47
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:32:VAL:O	1:A:32:VAL:HG13	2.13	0.47
1:A:229:GLU:OE2	1:B:89:TYR:OH	2.26	0.47
1:A:256:ARG:NE	7:A:604:HOH:O	2.47	0.47
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:HA	1:B:213:GLU:OE1	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:B:143:ARG:NH1	1:C:187:GLN:OE1	2.46	0.45
1:C:121:PHE:O	1:C:124:THR:HB	2.17	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:HA	1:D:213:GLU:OE1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:VAL:O	1:D:32:VAL:HG13	2.18	0.44
1:D:239:VAL:CG2	1:D:244:ARG:HG2	2.47	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
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:B:145:MET:HE1	1:C:175:PRO:HG3	2.01	0.42
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:A:258:LEU:C	1:A:258:LEU:CD2	2.93	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	30	38
1	B	264/329 (80%)	256 (97%)	5 (2%)	3 (1%)	11	13
1	C	264/329 (80%)	256 (97%)	8 (3%)	0	100	100
1	D	262/329 (80%)	255 (97%)	6 (2%)	1 (0%)	30	38
All	All	1052/1316 (80%)	1024 (97%)	23 (2%)	5 (0%)	24	31

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%)	211 (88%)	28 (12%)	5	6
1	B	241/292 (82%)	213 (88%)	28 (12%)	5	6
1	C	241/292 (82%)	219 (91%)	22 (9%)	9	11
1	D	239/292 (82%)	213 (89%)	26 (11%)	6	7
All	All	960/1168 (82%)	856 (89%)	104 (11%)	6	7

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	GLU
1	A	47	VAL
1	A	50	VAL
1	A	54	VAL
1	A	81	ASN
1	A	83	LEU
1	A	87	LEU
1	A	98	LEU
1	A	104	LEU
1	A	106	ARG
1	A	116	ILE
1	A	132	VAL
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	196	VAL
1	A	221	THR
1	A	233	ARG
1	A	235	THR
1	A	245	VAL
1	A	258	LEU
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	54	VAL
1	B	71	GLU
1	B	83	LEU
1	B	87	LEU
1	B	98	LEU
1	B	112	GLU
1	B	132	VAL
1	B	136	LEU
1	B	145	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	ARG
1	B	166	LEU
1	B	170	ILE
1	B	180	ARG
1	B	207	ARG
1	B	231	ARG
1	B	232	LEU
1	B	239	VAL
1	B	250	SER
1	B	258	LEU
1	B	263	ARG
1	B	284	LEU
1	B	285	GLN
1	B	294	LEU
1	C	44	LEU
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	136	LEU
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	245	VAL
1	C	284	LEU
1	C	286	ASN
1	D	44	LEU
1	D	45[A]	GLU
1	D	45[B]	GLU
1	D	52	LEU
1	D	54	VAL
1	D	60	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	157	VAL
1	D	166	LEU
1	D	170	ILE
1	D	182	SER
1	D	203	ARG
1	D	212	LEU
1	D	239	VAL
1	D	242	VAL
1	D	245	VAL
1	D	258	LEU
1	D	284	LEU
1	D	288	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	81	ASN
1	A	248	ASN
1	A	274	HIS
1	A	286	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	B	285	GLN
1	C	72	ASN
1	C	153	ASN
1	C	248	ASN
1	C	252	ASN
1	D	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	248	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
4	RNB	A	504	-	22,22,22	0.99	1 (4%)	30,30,30	1.82	7 (23%)
5	SO4	A	505	-	4,4,4	0.53	0	6,6,6	0.14	0
4	RNB	C	504	-	22,22,22	0.93	1 (4%)	30,30,30	1.37	3 (10%)
6	GOL	D	506	-	5,5,5	0.53	0	5,5,5	0.47	0
5	SO4	D	505	-	4,4,4	0.42	0	6,6,6	0.14	0
4	RNB	D	504	-	22,22,22	1.03	2 (9%)	30,30,30	1.30	4 (13%)
4	RNB	B	504	-	22,22,22	0.91	1 (4%)	30,30,30	1.48	3 (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
4	RNB	A	504	-	-	4/13/13/13	0/1/1/1
4	RNB	C	504	-	-	4/13/13/13	0/1/1/1
6	GOL	D	506	-	-	2/4/4/4	-
4	RNB	D	504	-	-	1/13/13/13	0/1/1/1
4	RNB	B	504	-	-	1/13/13/13	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	3.47	1.80	1.72
4	B	504	RNB	CAT-CL	3.34	1.79	1.72
4	C	504	RNB	CAT-CL	3.26	1.79	1.72
4	D	504	RNB	CAT-CL	2.38	1.77	1.72
4	D	504	RNB	CAR-CAV	-2.20	1.36	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	RNB	CAV-CAM-CAK	-5.44	102.77	112.06
4	A	504	RNB	CAV-CAM-CAK	4.77	120.21	112.06
4	D	504	RNB	CAV-CAM-CAK	-4.44	104.47	112.06
4	A	504	RNB	CAM-CAV-CAR	-3.85	114.76	120.85
4	A	504	RNB	CAM-CAV-CAS	3.75	126.77	120.85
4	C	504	RNB	CAC-CAP-CAN	3.26	120.89	115.23
4	A	504	RNB	CAC-CAP-CAK	-3.08	115.73	123.63
4	A	504	RNB	CAQ-CAT-CL	2.39	122.52	118.74
4	D	504	RNB	CAM-CAK-CAP	-2.31	124.11	127.42
4	B	504	RNB	CAM-CAK-CAP	-2.31	124.11	127.42
4	D	504	RNB	OAE-CAI-CAU	-2.30	119.34	124.80
4	C	504	RNB	CAC-CAP-CAK	-2.29	117.75	123.63
4	C	504	RNB	CAM-CAV-CAR	-2.29	117.24	120.85
4	A	504	RNB	CAN-CAP-CAK	2.15	126.00	121.17
4	D	504	RNB	CAD-CAQ-CAU	2.14	124.06	120.76
4	A	504	RNB	CAR-CAT-CAQ	-2.08	120.43	122.65
4	B	504	RNB	OAE-CAI-CAU	-2.07	119.90	124.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

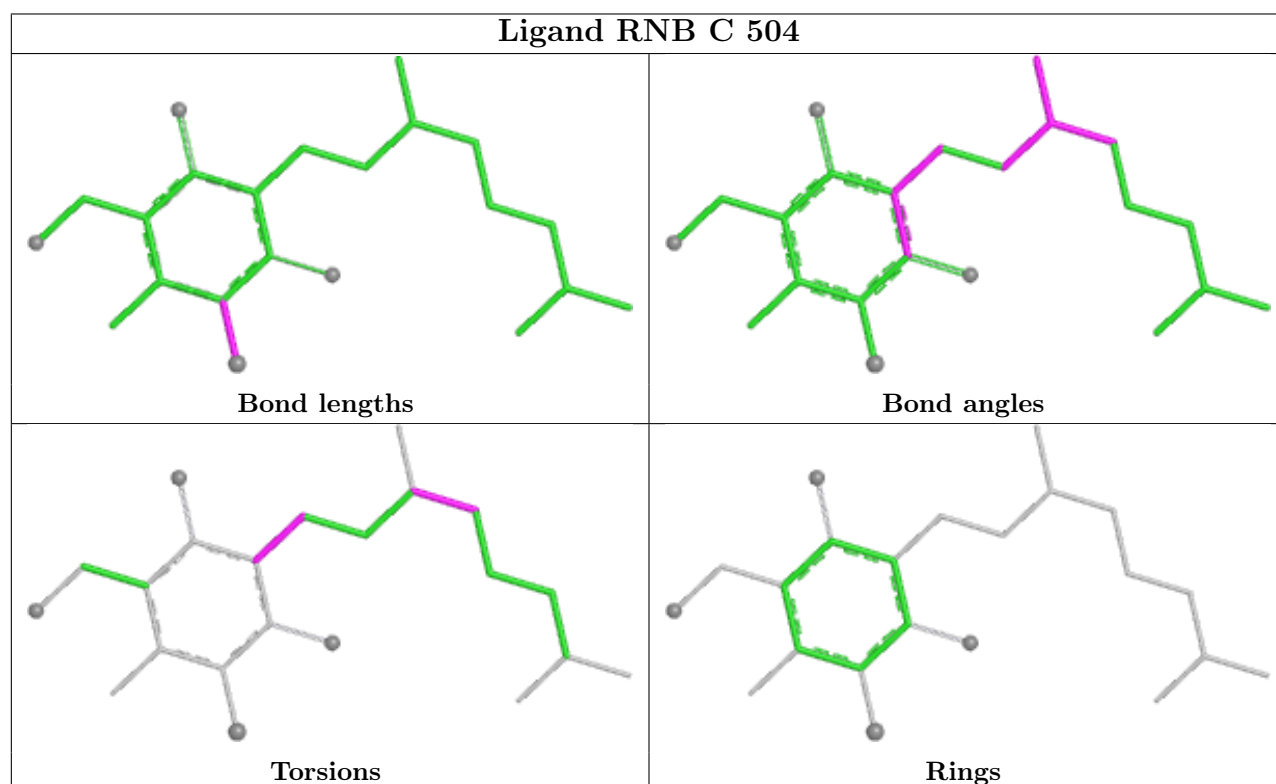
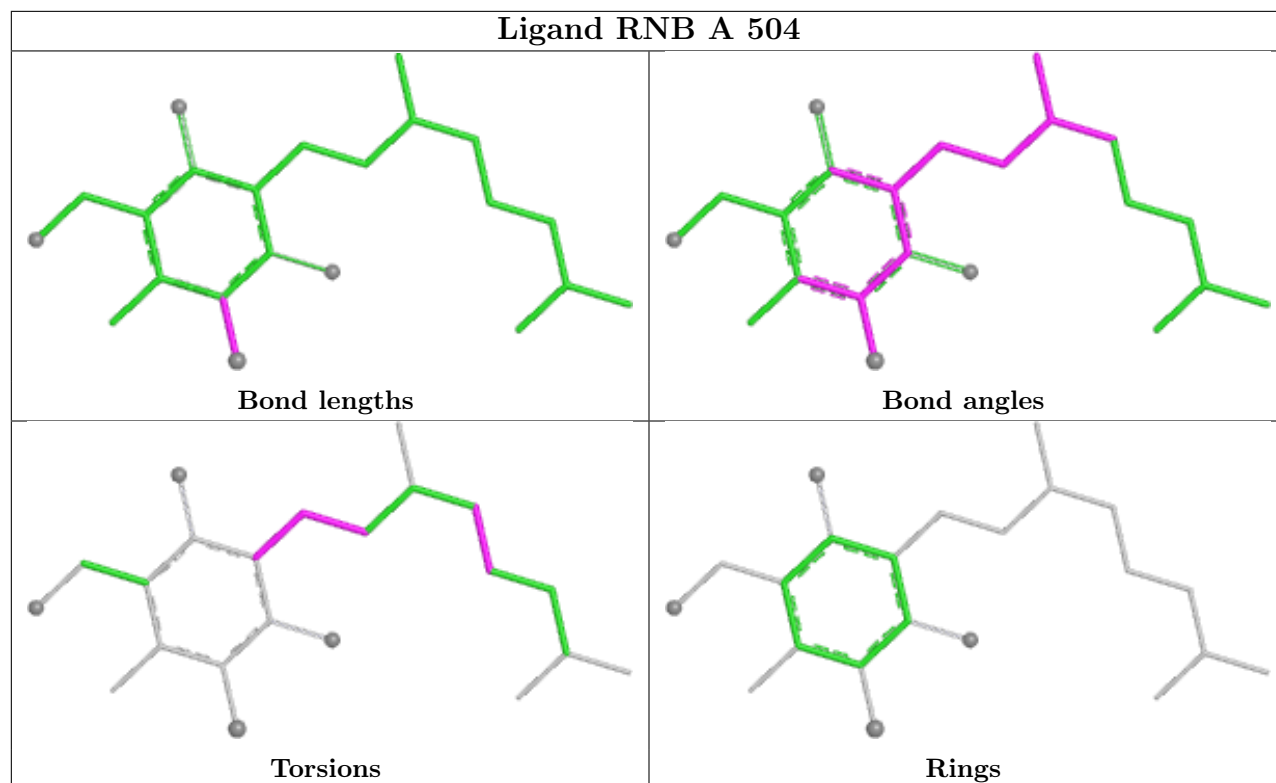
Mol	Chain	Res	Type	Atoms
4	A	504	RNB	CAK-CAM-CAV-CAS
4	A	504	RNB	CAK-CAM-CAV-CAR
4	C	504	RNB	CAK-CAM-CAV-CAS
6	D	506	GOL	C1-C2-C3-O3
4	C	504	RNB	CAL-CAN-CAP-CAC
4	C	504	RNB	CAL-CAN-CAP-CAK
4	B	504	RNB	CAJ-CAL-CAN-CAP
4	C	504	RNB	CAK-CAM-CAV-CAR
4	A	504	RNB	CAJ-CAL-CAN-CAP
4	D	504	RNB	CAJ-CAL-CAN-CAP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

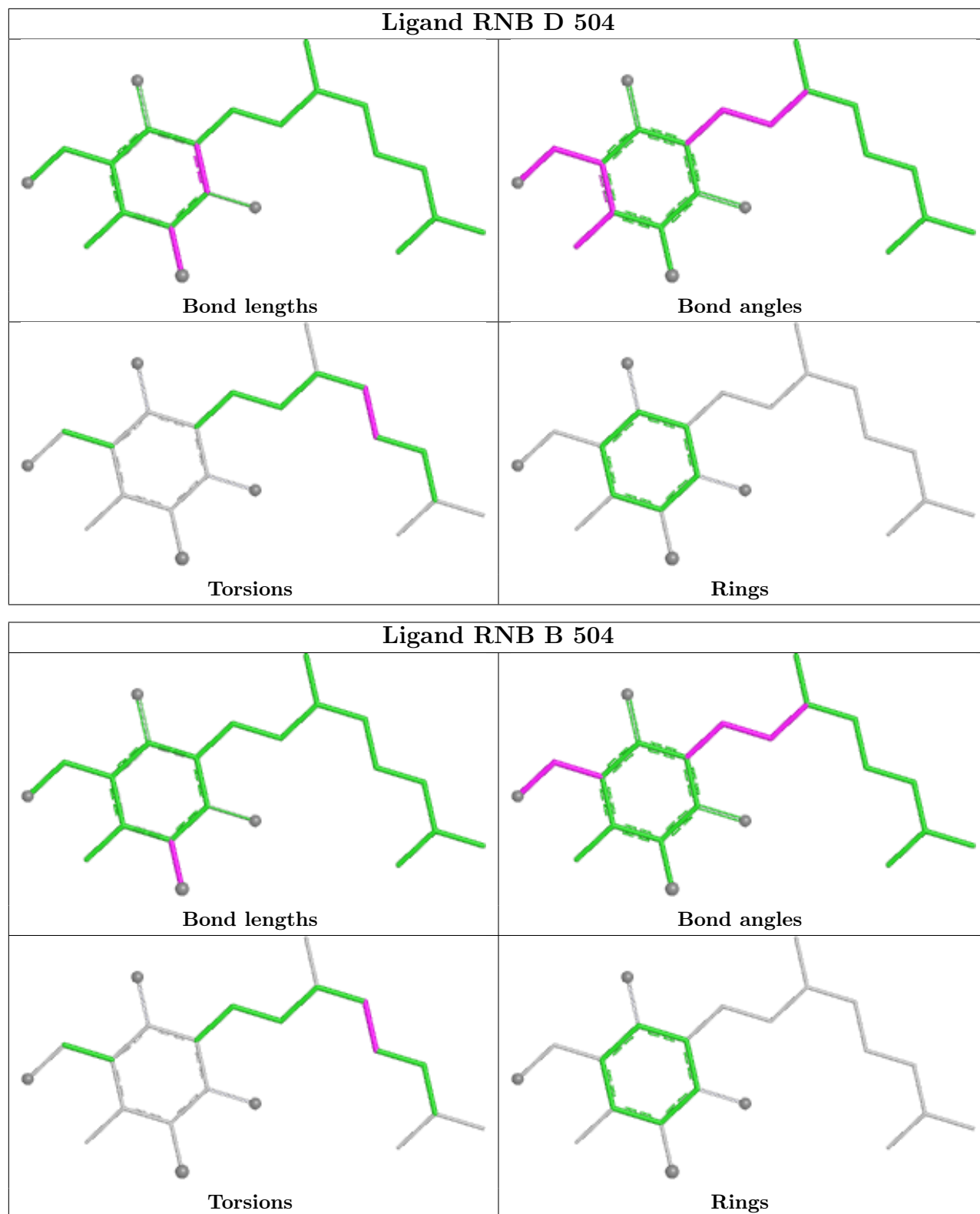
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	RNB	2	0
4	D	504	RNB	1	0
4	B	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%)	0.39	11 (4%) 40 42	22, 33, 53, 81	0
1	B	266/329 (80%)	0.92	37 (13%) 6 7	30, 44, 81, 113	0
1	C	266/329 (80%)	0.95	36 (13%) 7 8	27, 45, 80, 114	0
1	D	263/329 (79%)	0.39	10 (3%) 44 46	21, 33, 51, 67	1 (0%)
All	All	1059/1316 (80%)	0.66	94 (8%) 15 17	21, 39, 71, 114	1 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	107	PHE	6.9
1	C	104	LEU	6.7
1	D	238	ASP	6.3
1	B	104	LEU	5.5
1	D	294	LEU	5.4
1	C	110	ILE	5.4
1	B	110	ILE	5.2
1	B	107	PHE	5.0
1	A	32	VAL	5.0
1	B	105	TYR	4.7
1	A	238	ASP	4.4
1	A	294	LEU	4.4
1	C	235	THR	4.3
1	B	32	VAL	4.2
1	B	109	SER	4.1
1	B	236	LYS	3.9
1	C	105	TYR	3.9
1	B	174	GLN	3.8
1	C	101	THR	3.8
1	B	97	TRP	3.7
1	C	297	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	83	LEU	3.5
1	C	231	ARG	3.5
1	B	111	THR	3.4
1	B	235	THR	3.4
1	B	295	LYS	3.4
1	A	107	PHE	3.3
1	A	106	ARG	3.3
1	C	294	LEU	3.3
1	B	106	ARG	3.2
1	A	295	LYS	3.2
1	A	234	PRO	3.1
1	B	108	GLY	3.1
1	C	108	GLY	3.1
1	B	31	PRO	3.1
1	C	193	PHE	3.1
1	B	185	ILE	3.0
1	C	99	PHE	3.0
1	C	252	ASN	3.0
1	B	52	LEU	3.0
1	C	232	LEU	2.9
1	D	46	THR	2.9
1	C	32	VAL	2.9
1	D	45[A]	GLU	2.9
1	C	100	ASP	2.9
1	B	294	LEU	2.8
1	A	33	TRP	2.8
1	C	111	THR	2.7
1	B	56	ASP	2.7
1	A	230	GLY	2.7
1	B	233	ARG	2.7
1	C	97	TRP	2.7
1	D	237	ASN	2.7
1	C	179	LEU	2.7
1	B	238	ASP	2.6
1	C	109	SER	2.6
1	C	102	PHE	2.6
1	D	234	PRO	2.6
1	B	296	LYS	2.5
1	C	83	LEU	2.5
1	B	144	TYR	2.5
1	D	112	GLU	2.5
1	A	81	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	239	VAL	2.4
1	B	196	VAL	2.4
1	C	177	LEU	2.4
1	C	174	GLN	2.4
1	B	101	THR	2.3
1	C	89	TYR	2.3
1	C	176	GLY	2.3
1	C	49	VAL	2.3
1	D	177	LEU	2.3
1	B	237	ASN	2.3
1	B	173	ARG	2.3
1	C	181	VAL	2.3
1	C	284	LEU	2.2
1	A	252	ASN	2.2
1	C	172	LEU	2.2
1	C	196	VAL	2.2
1	B	33	TRP	2.2
1	B	189	ILE	2.2
1	B	231	ARG	2.2
1	B	49	VAL	2.2
1	B	115	VAL	2.2
1	D	32	VAL	2.2
1	B	234	PRO	2.2
1	C	296	LYS	2.2
1	C	103	SER	2.2
1	C	50	VAL	2.1
1	C	292	VAL	2.1
1	B	293	VAL	2.1
1	B	102	PHE	2.1
1	D	102	PHE	2.1
1	C	173	ARG	2.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

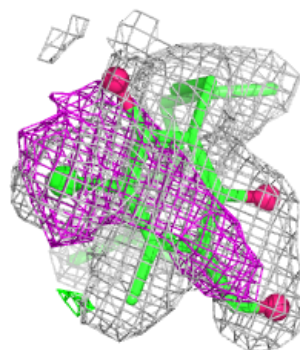
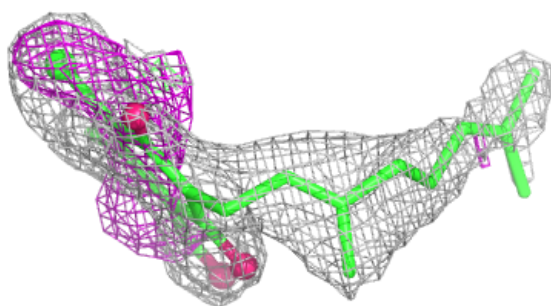
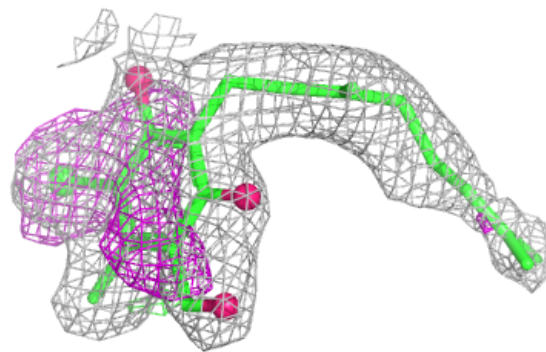
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	RNB	B	504	22/22	0.84	0.21	47,50,56,58	0
5	SO4	D	505	5/5	0.87	0.17	69,69,72,74	0
6	GOL	D	506	6/6	0.87	0.16	40,43,44,45	0
5	SO4	A	505	5/5	0.88	0.14	54,60,63,64	0
4	RNB	A	504	22/22	0.91	0.15	29,35,59,60	0
4	RNB	D	504	22/22	0.92	0.12	25,29,52,53	0
4	RNB	C	504	22/22	0.92	0.17	41,46,84,85	0
3	OH	C	503	1/1	0.98	0.06	17,17,17,17	0
3	OH	B	503	1/1	0.98	0.05	26,26,26,26	0
2	FE	B	501	1/1	0.99	0.03	45,45,45,45	0
2	FE	C	501	1/1	0.99	0.03	42,42,42,42	0
3	OH	A	503	1/1	0.99	0.03	16,16,16,16	0
2	FE	C	502	1/1	1.00	0.02	33,33,33,33	0
2	FE	D	501	1/1	1.00	0.01	28,28,28,28	0
2	FE	D	502	1/1	1.00	0.01	27,27,27,27	0
2	FE	A	501	1/1	1.00	0.02	27,27,27,27	0
2	FE	B	502	1/1	1.00	0.01	41,41,41,41	0
2	FE	A	502	1/1	1.00	0.02	28,28,28,28	0
3	OH	D	503	1/1	1.00	0.04	14,14,14,14	0

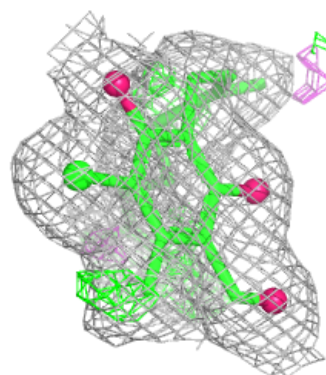
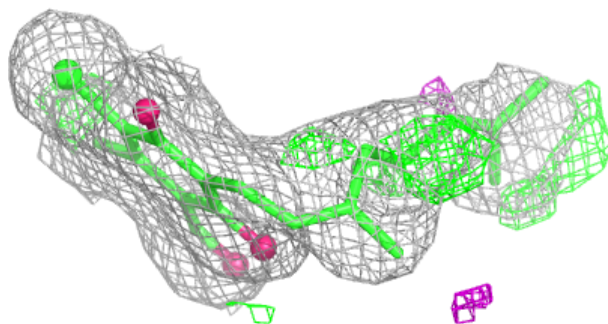
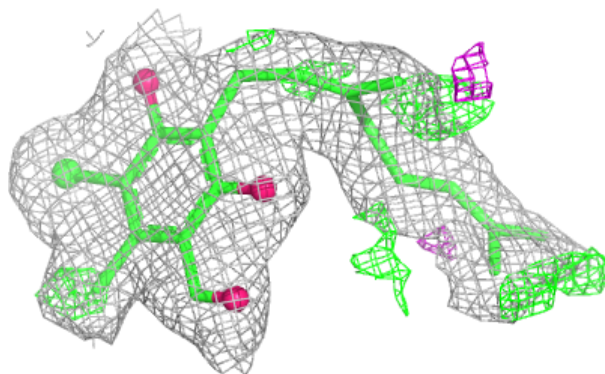
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

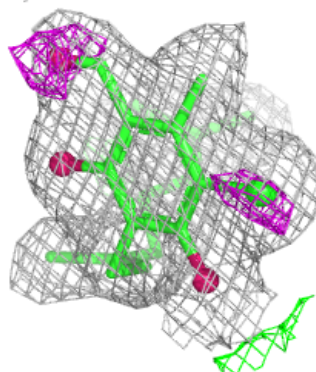
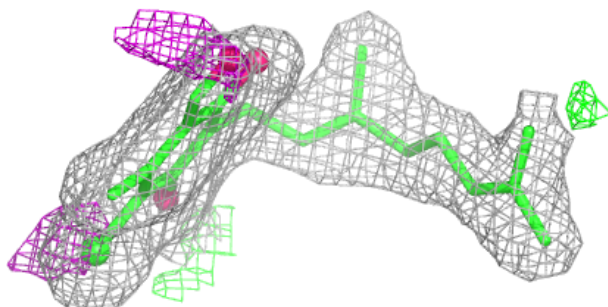
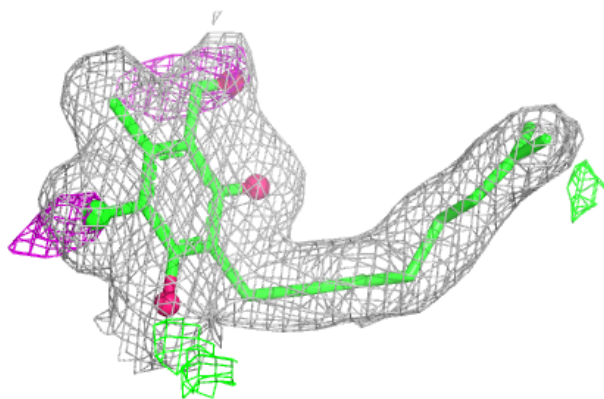
**Electron density around RNB A 504:**

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

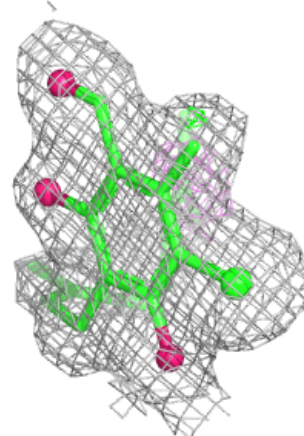
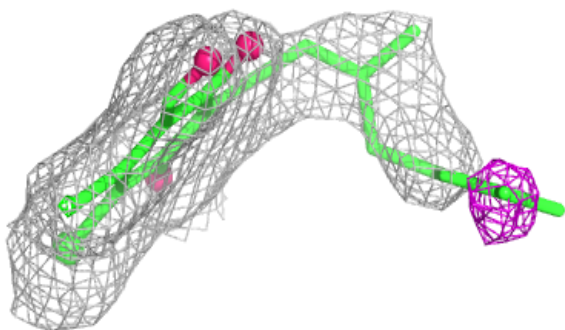
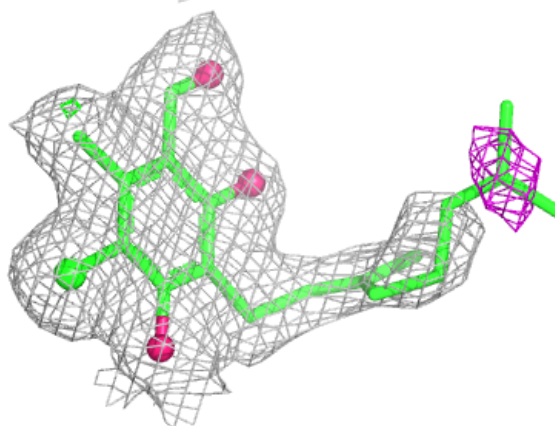


Electron density around RNB D 504:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.