



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2025 – 06:18 PM JST

PDB ID : 5ZDR
Title : Crystal structure of cyanide-insensitive alternative oxidase from *Trypanosoma brucei* with ascofuranone derivative
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 : 2.59 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

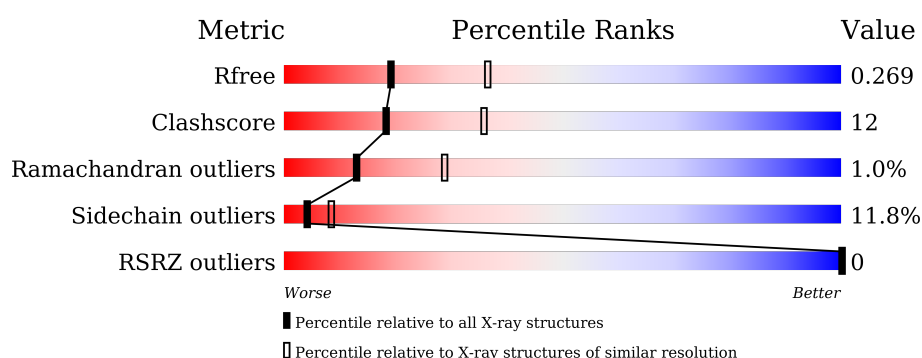
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	<div> <div>52%</div> <div>24%</div> <div>5%</div> <div>19%</div> </div>
1	B	329	<div> <div>58%</div> <div>19%</div> <div>.</div> <div>19%</div> </div>
1	C	329	<div> <div>56%</div> <div>20%</div> <div>5%</div> <div>19%</div> </div>
1	D	329	<div> <div>53%</div> <div>23%</div> <div>5%</div> <div>19%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8878 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.

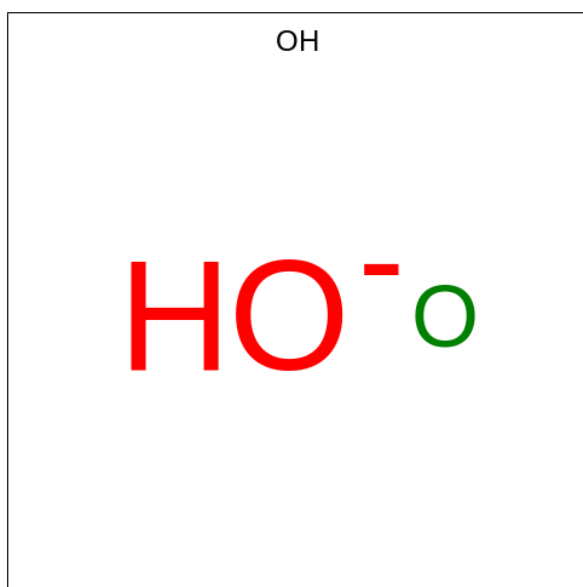
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2160	1384	383	383	10			
1	B	265	Total	C	N	O	S	0	0	0
			2155	1381	383	381	10			
1	C	266	Total	C	N	O	S	0	0	0
			2162	1386	384	382	10			
1	D	266	Total	C	N	O	S	0	0	0
			2160	1384	383	383	10			

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

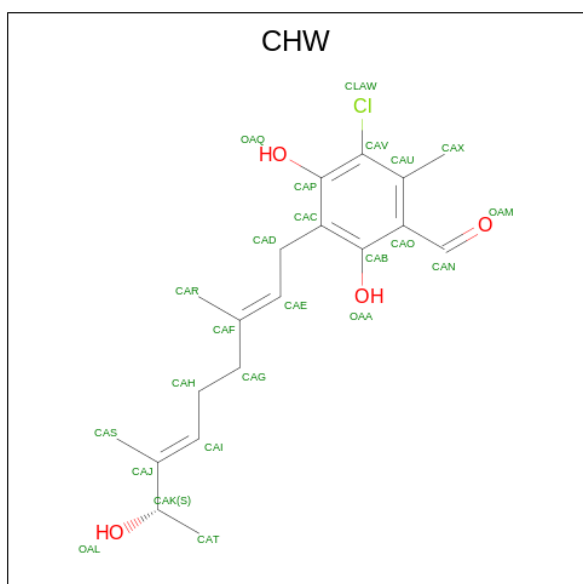
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (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-4,6-dihydroxy-5-[(2E,6E,8S)-8-hydroxy-3,7-dimethylnona-2,6-dien-1-yl]-2-methylbenzaldehyde (three-letter code: CHW) (formula: C₁₉H₂₅ClO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			24	19	1	4		
4	B	1	Total	C	Cl	O	0	0
			24	19	1	4		
4	C	1	Total	C	Cl	O	0	0
			24	19	1	4		
4	D	1	Total	C	Cl	O	0	0
			24	19	1	4		

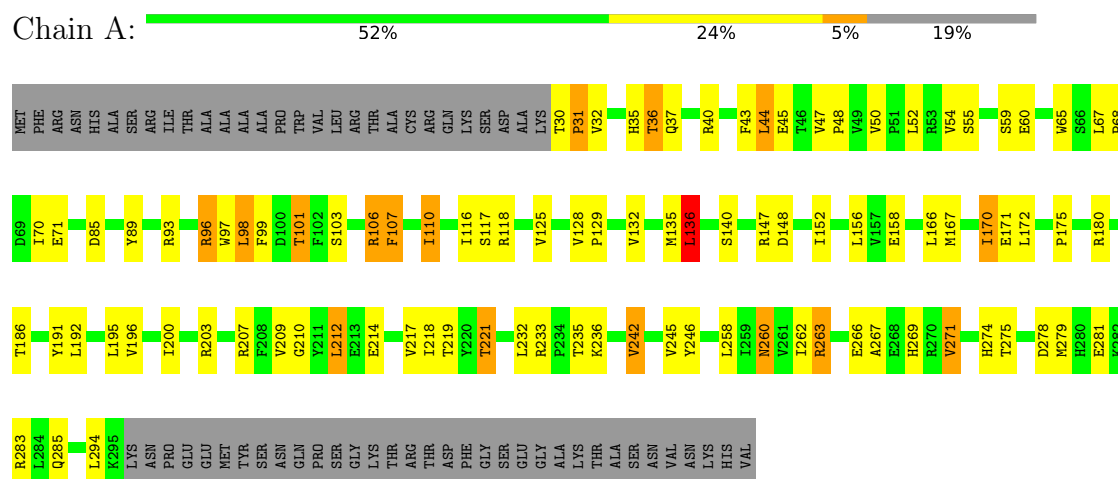
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	38	Total	O	0	0
			38	38		
5	C	22	Total	O	0	0
			22	22		
5	D	36	Total	O	0	0
			36	36		

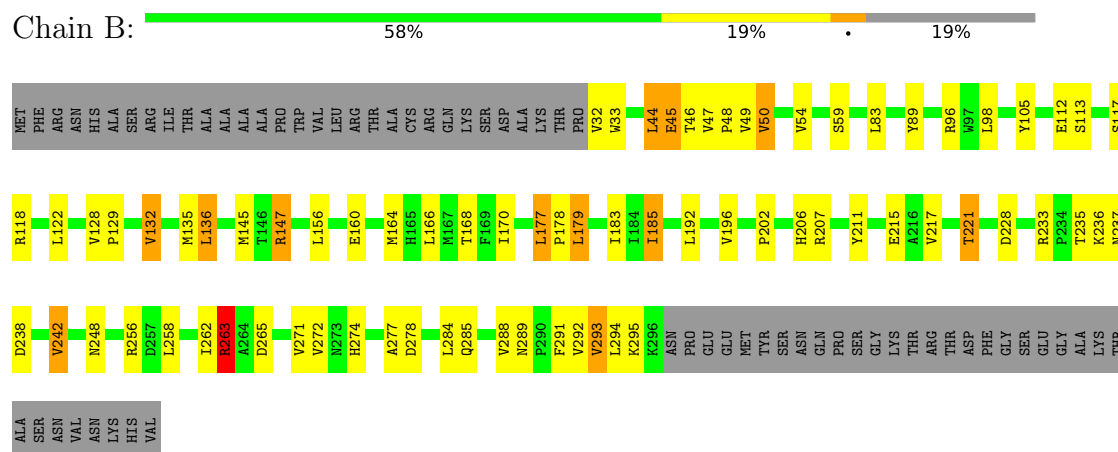
3 Residue-property plots

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.

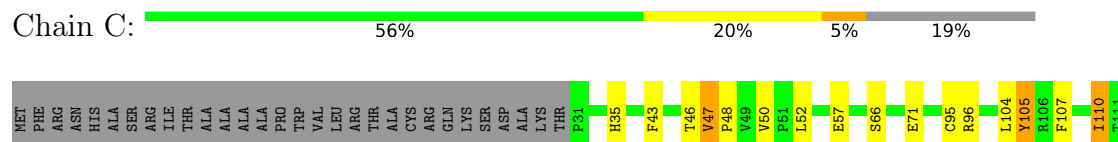
- Molecule 1: Alternative oxidase, mitochondrial



- Molecule 1: Alternative oxidase, mitochondrial



- Molecule 1: Alternative oxidase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.31Å 219.68Å 63.48Å 90.00° 114.89° 90.00°	Depositor
Resolution (Å)	39.81 – 2.59 39.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	92.2 (39.81-2.59) 97.2 (39.81-2.59)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.206 , 0.257 0.217 , 0.269	Depositor DCC
R_{free} test set	2887 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.138 for -h-2*1,-k,l	Xtriage
Reported twinning fraction	0.443 for H, K, L 0.557 for H+4/2L, -K, -L	Depositor
Outliers	0 of 56974 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8878	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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: CHW, OH, FE

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	0.70	0/2210	0.86	2/3004 (0.1%)
1	B	0.62	0/2204	0.82	2/2993 (0.1%)
1	C	0.57	0/2212	0.77	0/3004
1	D	0.57	0/2210	0.77	0/3004
All	All	0.62	0/8836	0.81	4/12005 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	147	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	136	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	147	ARG	NE-CZ-NH1	-5.25	117.67	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	ASN	Peptide
1	D	237	ASN	Peptide
1	D	238	ASP	Peptide

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	2160	0	2189	66	0
1	B	2155	0	2188	55	0
1	C	2162	0	2196	55	0
1	D	2160	0	2189	54	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	1	0
4	A	24	0	23	1	0
4	B	24	0	25	2	0
4	C	24	0	24	5	0
4	D	24	0	23	1	0
5	A	37	0	0	1	0
5	B	38	0	0	1	0
5	C	22	0	0	1	0
5	D	36	0	0	2	0
All	All	8878	0	8857	210	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 12.

All (210) 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:217:VAL:O	1:B:221:THR:HG23	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:HD12	1:B:185:ILE:C	2.07	0.75
1:C:192:LEU:O	1:C:196:VAL:HG12	1.89	0.72
1:C:221:THR:HG22	1:C:263:ARG:NE	2.03	0.72
1:A:110:ILE:HG12	1:A:232:LEU:HD22	1.76	0.68
1:D:233:ARG:O	1:D:234:PRO:C	2.30	0.68
1:C:46:THR:O	1:C:50:VAL:HG12	1.94	0.66
1:B:202:PRO:HD2	5:B:621:HOH:O	1.94	0.65
1:D:75:ILE:HD11	1:D:221:THR:HG21	1.80	0.64
1:A:135:MET:SD	1:A:135:MET:C	2.77	0.64
1:B:228:ASP:CG	1:B:256:ARG:HH11	2.02	0.62
1:D:200:ILE:N	1:D:200:ILE:HD13	2.15	0.62
1:A:135:MET:HG3	1:B:135:MET:HE3	1.81	0.62
1:D:252:ASN:OD1	1:D:252:ASN:N	2.33	0.61
1:A:40:ARG:HD3	1:A:43:PHE:CZ	2.35	0.61
1:C:219:THR:O	1:C:223:VAL:HG23	2.01	0.61
1:B:45:GLU:CD	1:B:45:GLU:H	2.04	0.61
1:C:215:GLU:HB3	4:C:504:CHW:HAD	1.82	0.61
1:D:269:HIS:O	1:D:273:ASN:HB2	2.00	0.61
1:A:135:MET:HG3	1:B:135:MET:CE	2.32	0.59
1:C:177:LEU:O	1:C:181:VAL:HG23	2.01	0.59
1:A:44:LEU:HG	1:B:278:ASP:HB3	1.84	0.59
1:A:54:VAL:HG21	1:A:242:VAL:HA	1.84	0.59
1:D:54:VAL:CG2	1:D:242:VAL:HG13	2.33	0.59
1:D:262:ILE:O	1:D:266:GLU:HG2	2.03	0.59
1:B:236:LYS:C	1:B:238:ASP:H	2.05	0.59
1:B:46:THR:O	1:B:50:VAL:HG12	2.03	0.59
1:C:236:LYS:C	1:C:238:ASP:H	2.05	0.59
1:A:40:ARG:O	1:B:271:VAL:HG12	2.03	0.58
1:D:217:VAL:O	1:D:221:THR:HG22	2.03	0.58
1:C:235:THR:C	1:C:237:ASN:H	2.07	0.58
1:A:294:LEU:HD22	1:B:33:TRP:CZ3	2.38	0.58
1:B:122:LEU:HD11	4:B:504:CHW:HARB	1.86	0.57
1:D:96:ARG:NH1	1:D:215:GLU:OE1	2.36	0.57
1:C:221:THR:HG22	1:C:263:ARG:CZ	2.34	0.57
1:D:162:GLU:OE1	3:D:503:OH:O	2.22	0.57
1:B:293:VAL:C	1:B:295:LYS:H	2.07	0.56
1:D:85:ASP:CG	1:D:207:ARG:HE	2.08	0.56
1:A:214:GLU:O	1:A:218:ILE:HG13	2.05	0.56
1:B:293:VAL:O	1:B:295:LYS:N	2.34	0.56
1:B:128:VAL:HB	1:B:129:PRO:HD3	1.88	0.56
1:A:175:PRO:HG2	1:A:180:ARG:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:O	1:A:221:THR:HG23	2.05	0.55
1:C:217:VAL:O	1:C:221:THR:HG23	2.07	0.55
1:C:271:VAL:HG23	1:C:272:VAL:N	2.23	0.54
1:B:179:LEU:HD13	1:B:183:ILE:HD12	1.89	0.54
1:B:217:VAL:O	1:B:221:THR:CG2	2.46	0.54
1:C:50:VAL:HG23	1:D:293:VAL:HG21	1.90	0.54
1:D:288:VAL:HG23	5:D:611:HOH:O	2.06	0.54
1:B:32:VAL:O	1:B:32:VAL:HG13	2.07	0.54
1:D:289:ASN:O	1:D:292:VAL:HG22	2.08	0.54
1:A:191:TYR:CE1	1:A:195:LEU:HD22	2.43	0.54
1:A:135:MET:CE	1:A:136:LEU:HD13	2.37	0.54
4:A:504:CHW:OAM	4:A:504:CHW:OAA	2.21	0.54
1:C:241:GLU:HA	1:C:244:ARG:HB2	1.89	0.54
1:A:200:ILE:N	1:A:200:ILE:HD13	2.24	0.53
1:C:172:LEU:O	1:C:173:ARG:HB2	2.08	0.53
1:C:271:VAL:HG12	1:D:40:ARG:O	2.06	0.53
1:D:233:ARG:HD3	1:D:234:PRO:HD2	1.90	0.53
1:C:219:THR:HG21	4:C:504:CHW:CLAW	2.45	0.53
1:A:45:GLU:N	1:A:45:GLU:OE1	2.42	0.53
1:A:262:ILE:O	1:A:266:GLU:HG2	2.08	0.53
1:A:283:ARG:HA	1:A:285:GLN:NE2	2.23	0.53
1:C:71:GLU:OE1	1:C:260:ASN:OD1	2.27	0.53
1:C:221:THR:HG22	1:C:263:ARG:HE	1.73	0.52
1:B:272:VAL:HA	1:B:291:PHE:CZ	2.45	0.52
1:C:280:HIS:CE1	1:C:285:GLN:HB3	2.44	0.52
1:D:136:LEU:O	1:D:140:SER:OG	2.26	0.52
1:A:96:ARG:NH2	1:A:219:THR:OG1	2.42	0.52
1:D:292:VAL:HG23	1:D:293:VAL:HG23	1.92	0.52
1:C:236:LYS:O	1:C:238:ASP:N	2.36	0.52
1:A:171:GLU:OE1	1:A:171:GLU:HA	2.10	0.51
1:B:59:SER:N	1:B:160:GLU:OE2	2.35	0.51
1:C:151:TRP:CD1	1:C:289:ASN:HB2	2.45	0.51
1:D:73:VAL:HG11	1:D:263:ARG:HD3	1.93	0.51
1:A:97:TRP:O	1:A:101:THR:OG1	2.29	0.51
1:A:106:ARG:HD3	1:A:107:PHE:H	1.76	0.51
1:B:235:THR:O	1:B:235:THR:HG22	2.10	0.51
1:C:138:HIS:CE1	1:D:159:ALA:HB1	2.46	0.51
1:A:209:VAL:HA	1:A:212:LEU:HB2	1.93	0.51
1:B:132:VAL:HG23	1:B:136:LEU:HD23	1.93	0.50
1:C:50:VAL:HG13	1:D:288:VAL:HG11	1.93	0.50
1:A:54:VAL:HG13	1:A:245:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:THR:HG21	1:B:258:LEU:HD21	1.92	0.50
1:C:149:LYS:HB2	1:C:288:VAL:HA	1.93	0.50
1:A:221:THR:HG22	1:A:263:ARG:HE	1.77	0.50
1:D:133:GLY:O	1:D:134:GLY:C	2.49	0.50
1:D:144:TYR:O	1:D:146:THR:HG23	2.12	0.50
1:B:236:LYS:C	1:B:238:ASP:N	2.65	0.49
1:C:50:VAL:HG13	1:D:288:VAL:CG1	2.42	0.49
1:C:112:GLU:HA	1:C:232:LEU:HD11	1.93	0.49
1:A:207:ARG:HH11	1:A:274:HIS:HD2	1.60	0.49
1:B:289:ASN:O	1:B:292:VAL:HG22	2.13	0.49
1:A:171:GLU:OE2	1:B:147:ARG:NH2	2.45	0.49
1:D:110:ILE:HA	1:D:114:LYS:HD3	1.94	0.49
1:D:219:THR:HG21	4:D:504:CHW:CLAW	2.49	0.49
1:B:228:ASP:OD2	1:B:256:ARG:NH1	2.37	0.49
1:A:85:ASP:HA	1:A:207:ARG:HG2	1.94	0.49
1:A:135:MET:HE1	1:A:136:LEU:HD13	1.94	0.49
1:A:170:ILE:HD12	1:B:145:MET:HB3	1.96	0.48
1:A:172:LEU:HD22	1:A:236:LYS:HD2	1.95	0.48
1:C:35:HIS:ND1	1:D:69:ASP:OD1	2.42	0.48
1:A:50:VAL:HG13	1:B:288:VAL:HG22	1.94	0.48
1:A:148:ASP:OD1	1:A:152:ILE:HG13	2.14	0.48
1:A:209:VAL:O	1:A:210:GLY:C	2.49	0.48
1:A:36:THR:HG22	1:A:37:GLN:NE2	2.29	0.48
1:A:99:PHE:O	1:A:103:SER:OG	2.30	0.48
1:A:275:THR:O	1:A:279:MET:HG3	2.13	0.48
1:C:278:ASP:OD2	1:D:42:SER:OG	2.23	0.48
1:D:129:PRO:O	1:D:132:VAL:HG22	2.13	0.48
1:B:262:ILE:O	1:B:265:ASP:HB2	2.14	0.47
1:A:128:VAL:N	1:A:129:PRO:HD2	2.30	0.47
1:D:138:HIS:O	1:D:142:LEU:HG	2.14	0.47
1:D:268:GLU:O	1:D:272:VAL:HG23	2.14	0.47
1:D:71:GLU:OE2	1:D:256:ARG:NH2	2.44	0.47
1:A:116:ILE:N	1:A:116:ILE:HD12	2.30	0.47
1:A:32:VAL:HG22	1:A:32:VAL:O	2.15	0.47
1:B:207:ARG:HH11	1:B:274:HIS:HD2	1.63	0.46
1:C:112:GLU:OE1	1:C:232:LEU:HG	2.15	0.46
1:A:267:ALA:O	1:A:271:VAL:HG23	2.15	0.46
1:C:47:VAL:N	1:C:48:PRO:HD2	2.30	0.46
1:D:44:LEU:HD23	1:D:45:GLU:N	2.30	0.46
1:A:135:MET:SD	1:A:135:MET:O	2.74	0.46
1:A:170:ILE:HG12	1:A:170:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLU:HA	5:D:615:HOH:O	2.16	0.46
1:B:54:VAL:HG22	1:B:242:VAL:CG1	2.46	0.46
1:C:280:HIS:CD2	1:C:285:GLN:HG2	2.51	0.46
1:B:185:ILE:HD12	1:B:185:ILE:O	2.14	0.46
1:A:67:LEU:HB2	1:A:68:PRO:HD3	1.97	0.46
1:A:260:ASN:C	1:A:260:ASN:HD22	2.19	0.46
1:C:266:GLU:OE2	1:C:266:GLU:HA	2.16	0.46
1:D:206:HIS:HB2	1:D:277:ALA:HB2	1.97	0.45
1:D:79:LYS:HG3	1:D:79:LYS:O	2.17	0.45
1:D:226:ALA:CB	1:D:232:LEU:HD22	2.46	0.45
1:A:60:GLU:OE1	1:A:60:GLU:N	2.50	0.45
1:B:96:ARG:HH11	1:B:215:GLU:HB3	1.82	0.45
1:C:57:GLU:O	1:C:163:ARG:NH1	2.49	0.45
1:B:113:SER:O	1:B:117:SER:HB2	2.17	0.44
1:B:177:LEU:O	1:B:178:PRO:C	2.55	0.44
1:C:206:HIS:O	1:C:209:VAL:N	2.50	0.44
1:A:30:THR:N	1:A:31:PRO:HD2	2.32	0.44
1:D:291:PHE:O	1:D:295:LYS:HB2	2.18	0.44
1:A:172:LEU:O	1:A:236:LYS:NZ	2.33	0.44
1:B:112:GLU:OE2	1:B:236:LYS:HG2	2.17	0.44
1:C:140:SER:OG	1:C:143:ARG:NH2	2.50	0.44
1:D:44:LEU:O	1:D:45:GLU:C	2.56	0.44
1:B:160:GLU:O	1:B:164:MET:HG2	2.18	0.44
1:C:158:GLU:OE2	1:C:273:ASN:OD1	2.35	0.44
1:A:50:VAL:HG13	1:B:288:VAL:CG2	2.48	0.43
1:C:105:TYR:CE1	1:C:118:ARG:HD2	2.54	0.43
1:C:143:ARG:HH11	1:D:187:GLN:NE2	2.16	0.43
1:D:44:LEU:O	1:D:47:VAL:HG12	2.18	0.43
1:A:203:ARG:NH1	1:A:281:GLU:OE2	2.50	0.43
1:C:43:PHE:HE2	1:D:271:VAL:HG11	1.84	0.43
1:D:85:ASP:O	1:D:88:ALA:HB3	2.17	0.43
1:D:289:ASN:C	1:D:289:ASN:OD1	2.57	0.43
1:D:162:GLU:O	1:D:165:HIS:HB2	2.18	0.43
1:C:147:ARG:HA	1:D:167:MET:HE2	2.01	0.43
1:B:206:HIS:CB	1:B:277:ALA:HB2	2.49	0.42
1:D:165:HIS:O	1:D:168:THR:HB	2.18	0.42
1:B:235:THR:O	1:B:235:THR:CG2	2.66	0.42
1:C:122:LEU:HD11	4:C:504:CHW:HARB	2.01	0.42
1:D:54:VAL:HG13	1:D:245:VAL:HG21	2.01	0.42
1:B:236:LYS:O	1:B:238:ASP:N	2.52	0.42
1:C:280:HIS:CD2	1:C:285:GLN:CG	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TYR:OH	1:C:225:ARG:HG2	2.19	0.42
1:A:158:GLU:HG3	1:A:269:HIS:CD2	2.54	0.42
1:B:122:LEU:HD13	4:B:504:CHW:CAP	2.50	0.42
1:D:123:GLU:OE2	1:D:123:GLU:HA	2.19	0.42
1:C:235:THR:C	1:C:237:ASN:N	2.71	0.42
1:C:139:LEU:O	1:C:142:LEU:HB2	2.20	0.42
1:B:89:TYR:HB2	1:B:211:TYR:CE2	2.55	0.42
1:B:221:THR:HB	1:B:263:ARG:HH21	1.84	0.42
1:C:262:ILE:O	1:C:266:GLU:HG2	2.19	0.42
1:A:278:ASP:HB3	1:B:44:LEU:HG	2.02	0.42
1:A:35:HIS:CD2	1:A:35:HIS:C	2.94	0.41
1:A:110:ILE:CG1	1:A:232:LEU:HD22	2.48	0.41
1:A:128:VAL:N	1:A:129:PRO:CD	2.82	0.41
1:C:221:THR:HG22	1:C:263:ARG:NH2	2.35	0.41
1:A:129:PRO:O	1:A:132:VAL:HG22	2.19	0.41
1:D:117:SER:HB2	1:D:173:ARG:CZ	2.50	0.41
1:D:200:ILE:N	1:D:200:ILE:CD1	2.83	0.41
1:A:167:MET:HE2	1:B:147:ARG:HH11	1.85	0.41
1:A:196:VAL:O	1:A:200:ILE:HG12	2.19	0.41
1:C:118:ARG:NH2	4:C:504:CHW:OAQ	2.51	0.41
1:D:134:GLY:HA3	1:D:156:LEU:CD1	2.50	0.41
1:A:245:VAL:HG23	1:A:246:TYR:N	2.35	0.41
1:D:206:HIS:CB	1:D:277:ALA:HB2	2.51	0.41
1:A:192:LEU:HD22	5:A:625:HOH:O	2.20	0.41
1:B:179:LEU:HD13	1:B:183:ILE:CD1	2.51	0.41
1:B:271:VAL:HG23	1:B:272:VAL:N	2.36	0.41
1:C:167:MET:HA	1:C:167:MET:CE	2.50	0.41
1:D:116:ILE:HG21	1:D:173:ARG:HB2	2.02	0.41
1:A:89:TYR:O	1:A:93:ARG:HG2	2.21	0.41
1:B:47:VAL:HB	1:B:48:PRO:HD3	2.03	0.41
1:B:105:TYR:CE1	1:B:118:ARG:HD2	2.56	0.41
1:D:186:THR:O	1:D:187:GLN:C	2.59	0.41
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.91	0.41
1:B:132:VAL:HG23	1:B:136:LEU:CD2	2.50	0.41
1:C:110:ILE:HA	1:C:114:LYS:HE3	2.03	0.41
1:C:258:LEU:HA	1:C:261:VAL:HG22	2.03	0.41
1:A:47:VAL:HB	1:A:48:PRO:HD3	2.03	0.41
1:A:96:ARG:HH21	1:A:118:ARG:NH2	2.19	0.41
1:B:185:ILE:C	1:B:185:ILE:CD1	2.78	0.40
1:A:65:TRP:HB3	1:A:70:ILE:HD13	2.03	0.40
1:C:179:LEU:HD23	5:C:616:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:GLY:O	1:C:233:ARG:NH2	2.53	0.40
4:C:504:CHW:HATB	4:C:504:CHW:HAS	1.83	0.40
1:C:247:TRP:CD1	1:C:261:VAL:HB	2.57	0.40
1:A:125:VAL:HG21	1:A:186:THR:HG21	2.04	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	264/329 (80%)	235 (89%)	26 (10%)	3 (1%)	12	26
1	B	263/329 (80%)	238 (90%)	23 (9%)	2 (1%)	16	34
1	C	264/329 (80%)	238 (90%)	23 (9%)	3 (1%)	12	26
1	D	264/329 (80%)	240 (91%)	21 (8%)	3 (1%)	12	26
All	All	1055/1316 (80%)	951 (90%)	93 (9%)	11 (1%)	13	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	LEU
1	C	236	LYS
1	C	237	ASN
1	A	31	PRO
1	A	59	SER
1	A	71	GLU
1	B	263	ARG
1	C	147	ARG
1	D	44	LEU
1	D	175	PRO
1	D	134	GLY

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	241/292 (82%)	216 (90%)	25 (10%)	5	11
1	B	240/292 (82%)	216 (90%)	24 (10%)	6	13
1	C	241/292 (82%)	208 (86%)	33 (14%)	3	5
1	D	241/292 (82%)	209 (87%)	32 (13%)	3	6
All	All	963/1168 (82%)	849 (88%)	114 (12%)	4	8

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	44	LEU
1	A	52	LEU
1	A	55	SER
1	A	96	ARG
1	A	98	LEU
1	A	101	THR
1	A	106	ARG
1	A	107	PHE
1	A	110	ILE
1	A	117	SER
1	A	136	LEU
1	A	140	SER
1	A	156	LEU
1	A	166	LEU
1	A	170	ILE
1	A	212	LEU
1	A	221	THR
1	A	233	ARG
1	A	235	THR
1	A	242	VAL
1	A	258	LEU
1	A	260	ASN
1	A	263	ARG

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Mol	Chain	Res	Type
1	A	271	VAL
1	B	44	LEU
1	B	45	GLU
1	B	49	VAL
1	B	50	VAL
1	B	83	LEU
1	B	98	LEU
1	B	132	VAL
1	B	136	LEU
1	B	156	LEU
1	B	166	LEU
1	B	170	ILE
1	B	177	LEU
1	B	179	LEU
1	B	185	ILE
1	B	192	LEU
1	B	196	VAL
1	B	221	THR
1	B	233	ARG
1	B	242	VAL
1	B	248	ASN
1	B	263	ARG
1	B	284	LEU
1	B	285	GLN
1	B	293	VAL
1	C	47	VAL
1	C	52	LEU
1	C	66	SER
1	C	95	CYS
1	C	96	ARG
1	C	104	LEU
1	C	105	TYR
1	C	107	PHE
1	C	110	ILE
1	C	113	SER
1	C	114	LYS
1	C	132	VAL
1	C	146	THR
1	C	156	LEU
1	C	166	LEU
1	C	173	ARG
1	C	179	LEU

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Mol	Chain	Res	Type
1	C	182	SER
1	C	187	GLN
1	C	192	LEU
1	C	196	VAL
1	C	225	ARG
1	C	233	ARG
1	C	238	ASP
1	C	239	VAL
1	C	244	ARG
1	C	245	VAL
1	C	248	ASN
1	C	260	ASN
1	C	263	ARG
1	C	284	LEU
1	C	285	GLN
1	C	292	VAL
1	D	52	LEU
1	D	61	ASP
1	D	72	ASN
1	D	86	THR
1	D	91	SER
1	D	98	LEU
1	D	107	PHE
1	D	110	ILE
1	D	115	VAL
1	D	136	LEU
1	D	140	SER
1	D	156	LEU
1	D	166	LEU
1	D	170	ILE
1	D	179	LEU
1	D	189	ILE
1	D	192	LEU
1	D	200	ILE
1	D	221	THR
1	D	231	ARG
1	D	232	LEU
1	D	233	ARG
1	D	235	THR
1	D	238	ASP
1	D	242	VAL
1	D	252	ASN

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Mol	Chain	Res	Type
1	D	260	ASN
1	D	263	ARG
1	D	265	ASP
1	D	271	VAL
1	D	284	LEU
1	D	285	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	187	GLN
1	A	274	HIS
1	A	285	GLN
1	A	286	ASN
1	B	153	ASN
1	B	248	ASN
1	B	269	HIS
1	B	274	HIS
1	B	285	GLN
1	B	286	ASN
1	C	72	ASN
1	C	153	ASN
1	C	248	ASN
1	C	260	ASN
1	C	273	ASN
1	C	285	GLN
1	D	81	ASN
1	D	187	GLN
1	D	260	ASN
1	D	273	ASN
1	D	274	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 16 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 4 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	CHW	A	504	-	23,24,24	1.53	3 (13%)	30,33,33	1.91	6 (20%)
4	CHW	D	504	-	23,24,24	1.51	3 (13%)	30,33,33	1.68	4 (13%)
4	CHW	C	504	-	23,24,24	1.72	3 (13%)	30,33,33	1.35	4 (13%)
4	CHW	B	504	-	23,24,24	1.54	1 (4%)	30,33,33	1.31	4 (13%)

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	CHW	A	504	-	-	4/17/17/17	0/1/1/1
4	CHW	D	504	-	-	4/17/17/17	0/1/1/1
4	CHW	C	504	-	-	8/17/17/17	0/1/1/1
4	CHW	B	504	-	-	3/17/17/17	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	CHW	CAO-CAU	6.82	1.50	1.41
4	D	504	CHW	CAO-CAU	6.08	1.49	1.41
4	B	504	CHW	CAO-CAU	6.05	1.49	1.41
4	A	504	CHW	CAO-CAU	5.06	1.47	1.41
4	C	504	CHW	CAI-CAJ	2.76	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	CHW	CAV-CLAW	2.65	1.78	1.72
4	D	504	CHW	CAV-CLAW	2.45	1.78	1.72
4	A	504	CHW	CAP-CAC	-2.20	1.36	1.40
4	D	504	CHW	CAI-CAJ	2.11	1.35	1.33
4	C	504	CHW	CAV-CLAW	2.07	1.77	1.72

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	CHW	CAC-CAD-CAE	-6.09	102.53	112.17
4	D	504	CHW	CAH-CAI-CAJ	-4.48	122.21	127.41
4	A	504	CHW	OAM-CAN-CAO	-4.46	115.19	124.91
4	A	504	CHW	CAC-CAD-CAE	-4.32	105.32	112.17
4	A	504	CHW	CAD-CAE-CAF	-4.16	120.78	127.24
4	A	504	CHW	CAH-CAI-CAJ	-4.09	122.66	127.41
4	D	504	CHW	OAM-CAN-CAO	-3.03	118.31	124.91
4	C	504	CHW	CAX-CAU-CAO	3.01	125.09	120.62
4	B	504	CHW	CAH-CAI-CAJ	-2.86	124.09	127.41
4	C	504	CHW	OAM-CAN-CAO	-2.85	118.69	124.91
4	C	504	CHW	CAS-CAJ-CAI	-2.55	117.59	123.33
4	A	504	CHW	CAU-CAO-CAN	2.39	125.00	121.61
4	B	504	CHW	CAP-CAV-CAU	2.39	124.31	122.79
4	C	504	CHW	CAR-CAF-CAG	2.35	119.22	115.27
4	D	504	CHW	CAR-CAF-CAG	2.23	119.03	115.27
4	A	504	CHW	CAB-CAO-CAN	-2.16	116.83	119.90
4	B	504	CHW	CAB-CAO-CAN	2.15	122.94	119.90
4	B	504	CHW	CAX-CAU-CAO	2.07	123.71	120.62

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	CHW	CAI-CAJ-CAK-OAL
4	A	504	CHW	CAS-CAJ-CAK-OAL
4	C	504	CHW	CAI-CAJ-CAK-OAL
4	C	504	CHW	CAI-CAJ-CAK-CAT
4	C	504	CHW	CAS-CAJ-CAK-OAL
4	C	504	CHW	CAS-CAJ-CAK-CAT
4	C	504	CHW	CAF-CAG-CAH-CAI
4	B	504	CHW	CAB-CAC-CAD-CAE
4	B	504	CHW	CAP-CAC-CAD-CAE
4	D	504	CHW	CAS-CAJ-CAK-OAL

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Mol	Chain	Res	Type	Atoms
4	D	504	CHW	CAI-CAJ-CAK-OAL
4	C	504	CHW	CAC-CAD-CAE-CAF
4	A	504	CHW	CAS-CAJ-CAK-CAT
4	D	504	CHW	CAS-CAJ-CAK-CAT
4	C	504	CHW	CAB-CAC-CAD-CAE
4	A	504	CHW	CAI-CAJ-CAK-CAT
4	D	504	CHW	CAI-CAJ-CAK-CAT
4	B	504	CHW	CAR-CAF-CAG-CAH
4	C	504	CHW	CAP-CAC-CAD-CAE

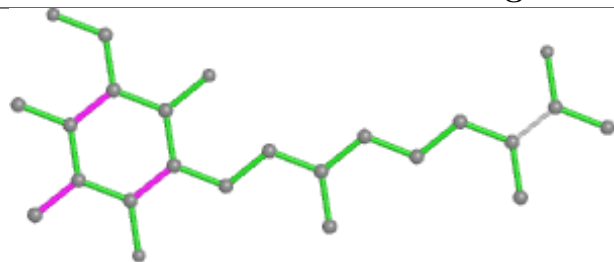
There are no ring outliers.

4 monomers are involved in 9 short contacts:

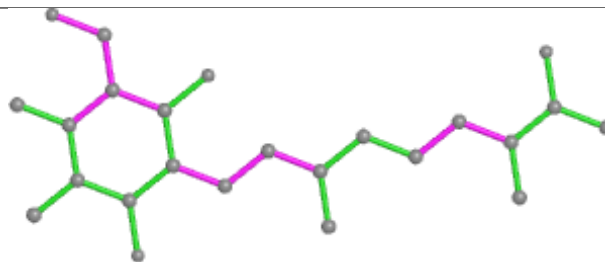
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	CHW	1	0
4	D	504	CHW	1	0
4	C	504	CHW	5	0
4	B	504	CHW	2	0

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.

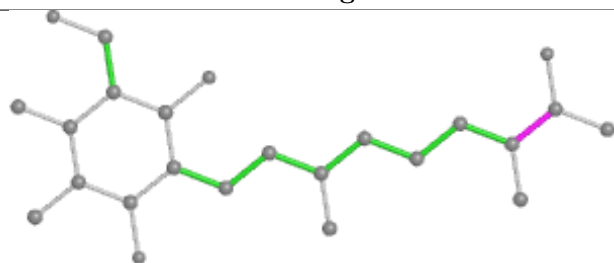
Ligand CHW A 504



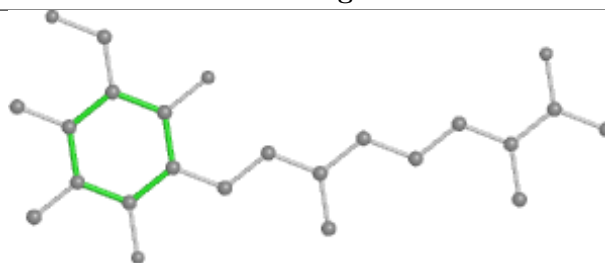
Bond lengths



Bond angles

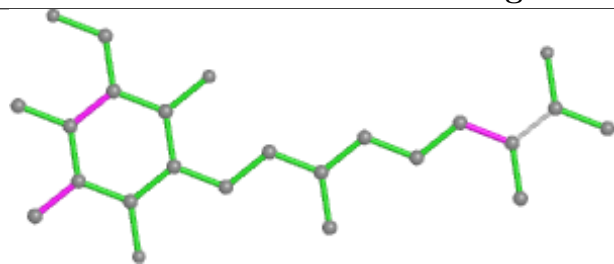


Torsions

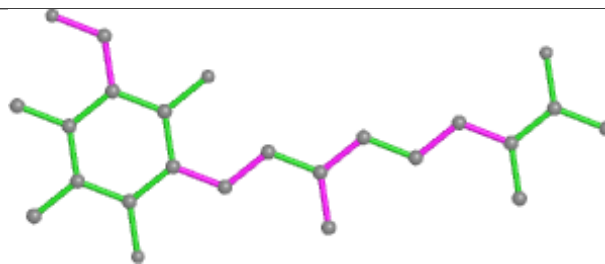


Rings

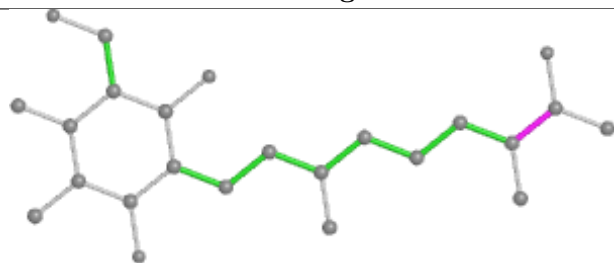
Ligand CHW D 504



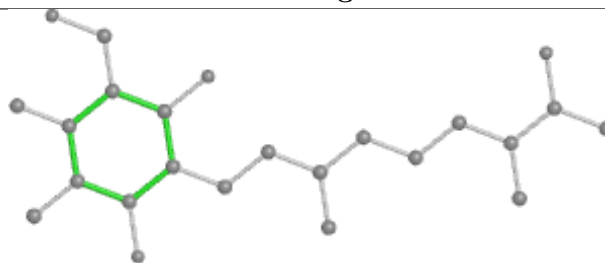
Bond lengths



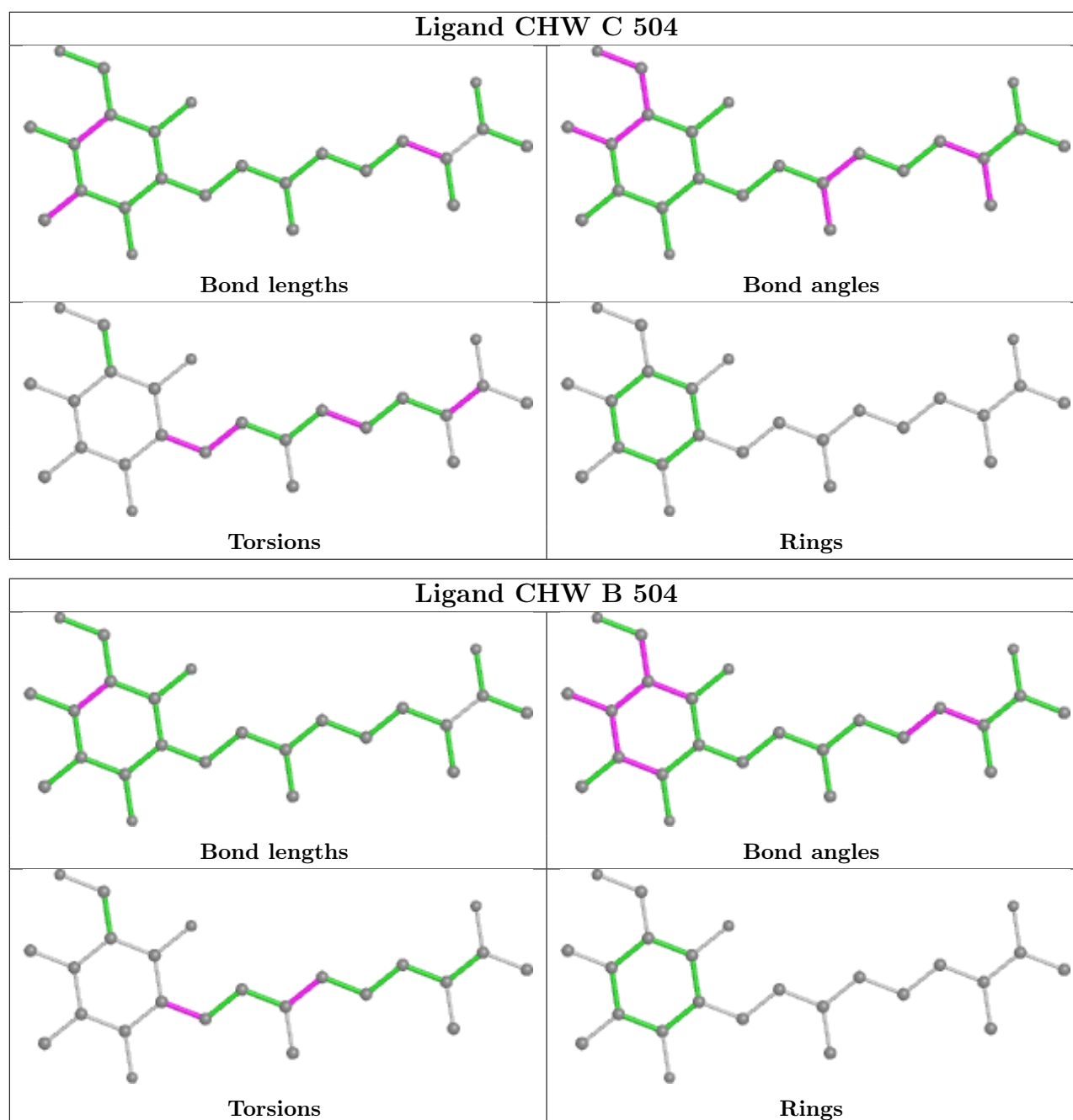
Bond angles



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	266/329 (80%)	-1.14	0 100 100	23, 37, 58, 102	0
1	B	265/329 (80%)	-1.20	0 100 100	22, 37, 53, 67	0
1	C	266/329 (80%)	-0.97	0 100 100	25, 46, 75, 120	0
1	D	266/329 (80%)	-0.96	0 100 100	26, 45, 78, 111	0
All	All	1063/1316 (80%)	-1.07	0 100 100	22, 40, 67, 120	0

There are no RSRZ outliers to report.

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.

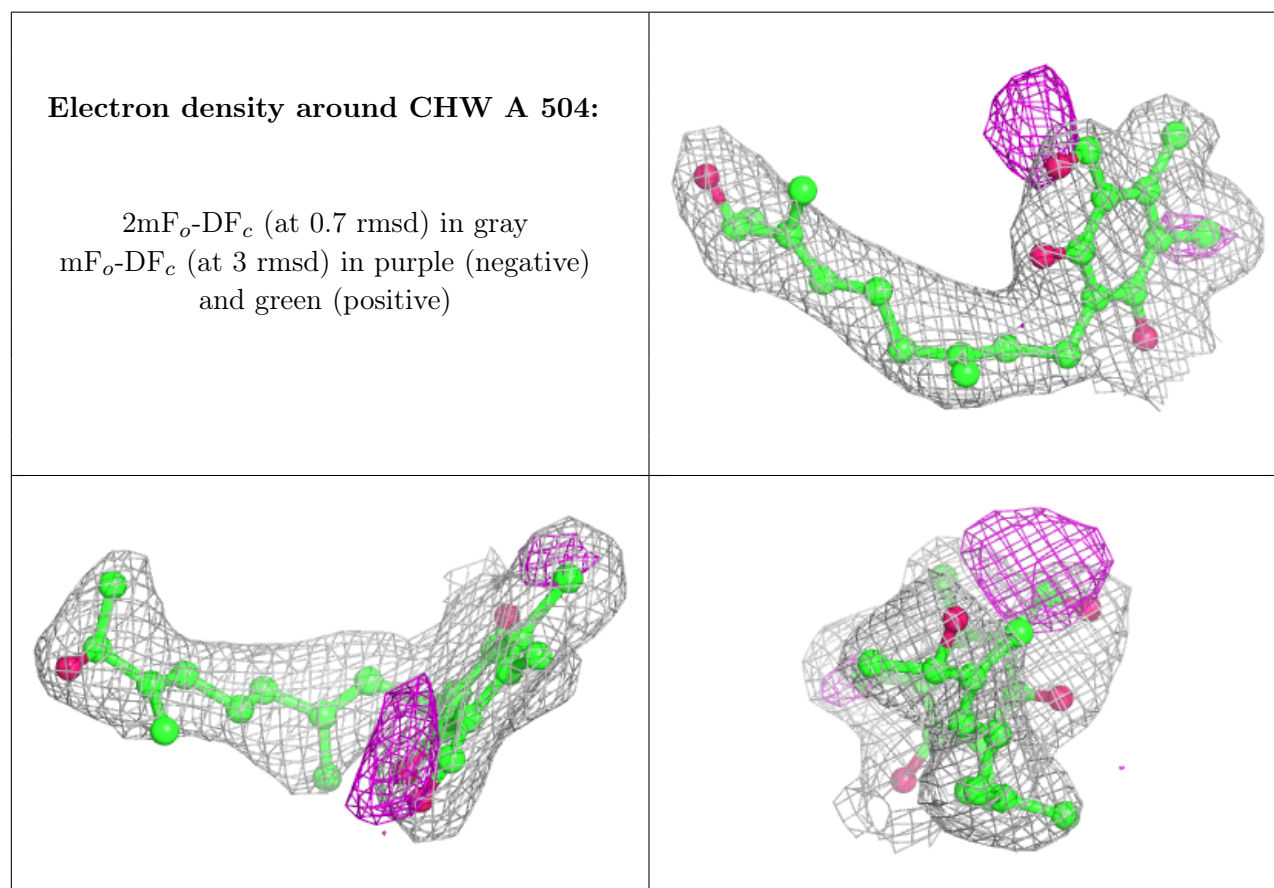
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CHW	A	504	24/24	0.98	0.07	23,32,48,52	0
4	CHW	C	504	24/24	0.98	0.07	44,54,61,64	0
4	CHW	D	504	24/24	0.98	0.07	50,56,64,66	0
3	OH	B	503	1/1	0.99	0.06	14,14,14,14	0

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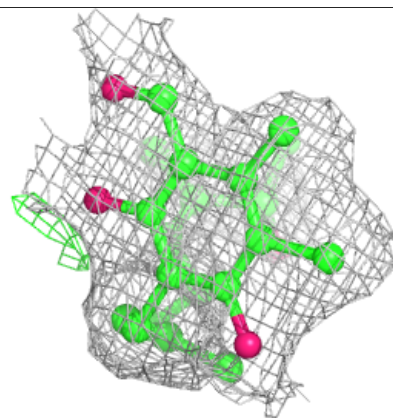
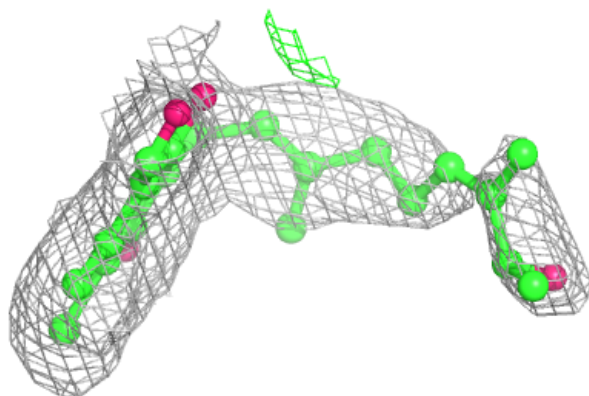
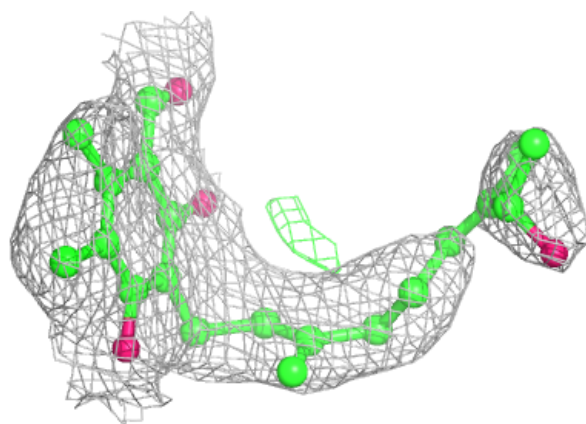
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CHW	B	504	24/24	0.99	0.05	31,47,67,69	0
2	FE	C	502	1/1	1.00	0.01	35,35,35,35	0
2	FE	D	501	1/1	1.00	0.02	44,44,44,44	0
2	FE	D	502	1/1	1.00	0.01	33,33,33,33	0
3	OH	A	503	1/1	1.00	0.01	14,14,14,14	0
2	FE	A	501	1/1	1.00	0.01	31,31,31,31	0
3	OH	C	503	1/1	1.00	0.01	11,11,11,11	0
3	OH	D	503	1/1	1.00	0.02	9,9,9,9	0
2	FE	A	502	1/1	1.00	0.01	29,29,29,29	0
2	FE	B	501	1/1	1.00	0.02	29,29,29,29	0
2	FE	B	502	1/1	1.00	0.01	30,30,30,30	0
2	FE	C	501	1/1	1.00	0.01	43,43,43,43	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.

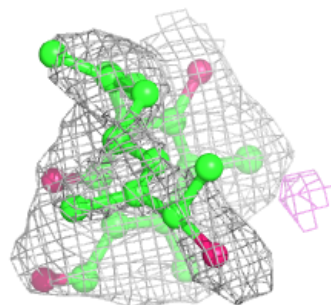
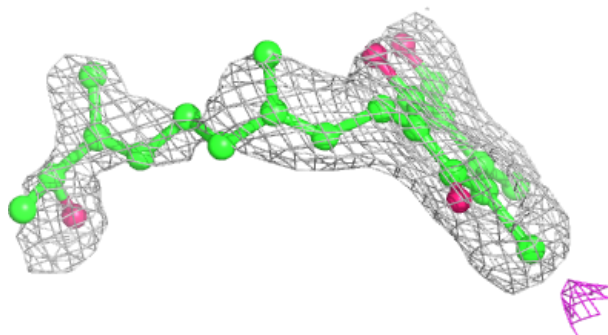
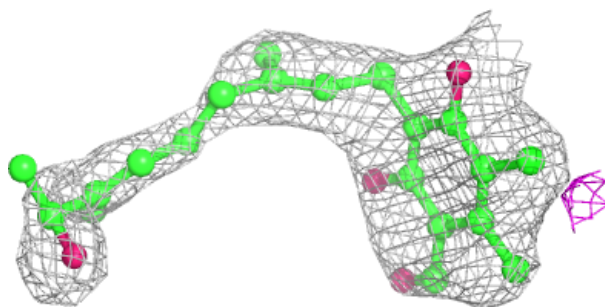


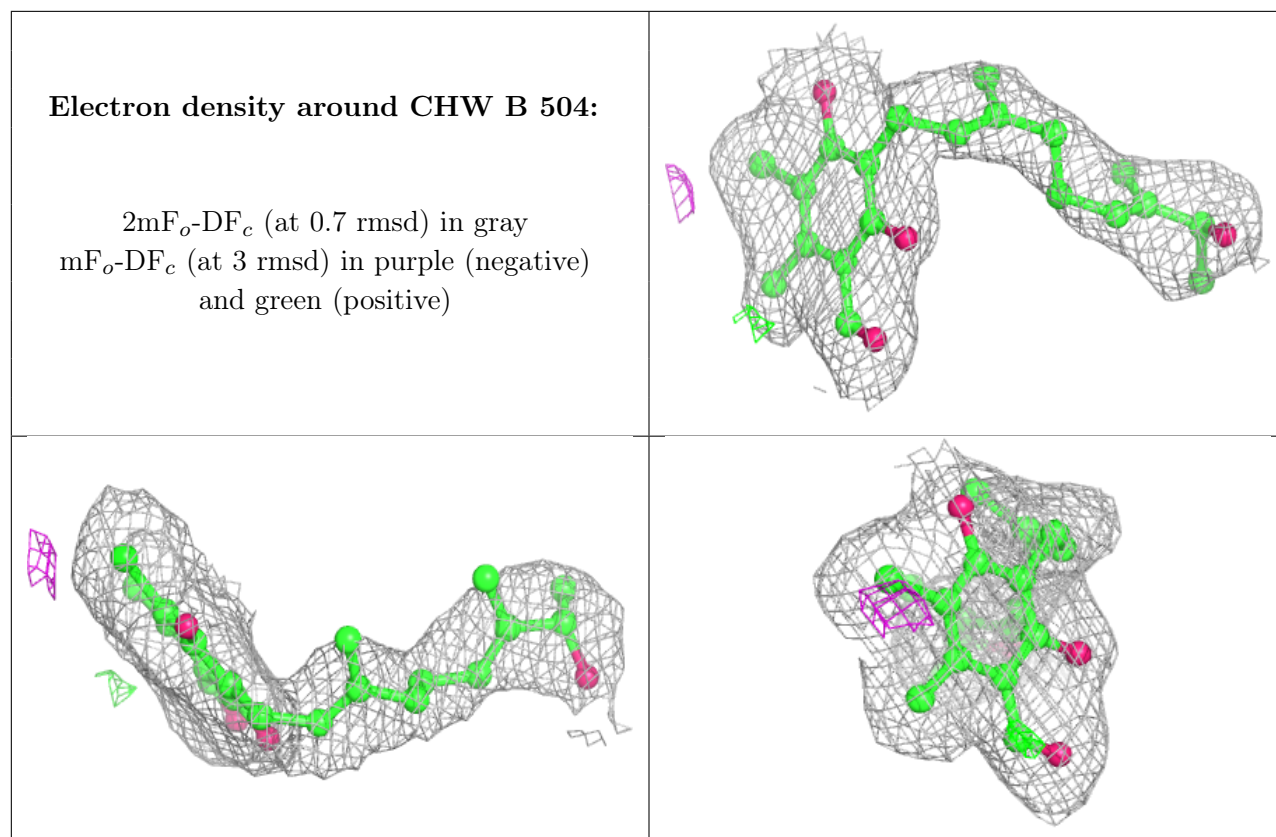
Electron density around CHW C 504:

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

**Electron density around CHW 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.