



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 02:12 PM EDT

PDB ID : 2PNJ
Title : Crystal structure of human ferrochelatase mutant with Phe 337 replaced by Ala
Authors : Dailey, H.A.; Wu, C.-K.; Horanyi, P.; Medlock, A.E.; Najahi-Missaoui, W.; Burden, A.E.; Dailey, T.A.; Rose, J.P.
Deposited on : 2007-04-24
Resolution : 2.35 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

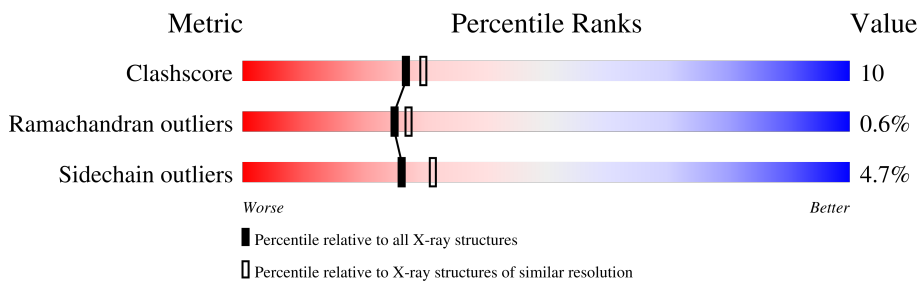
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	359	79% 16% ..
1	B	359	78% 18% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6166 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.

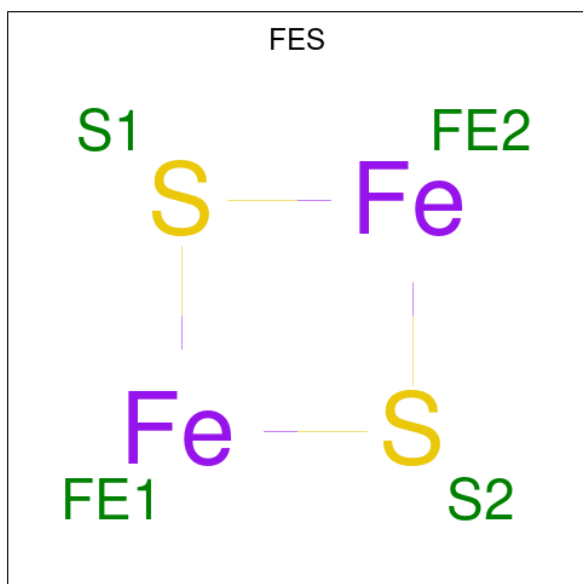
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	355	2815	1794	481	522	18	0	0	0
1	B	356	2827	1803	484	522	18	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

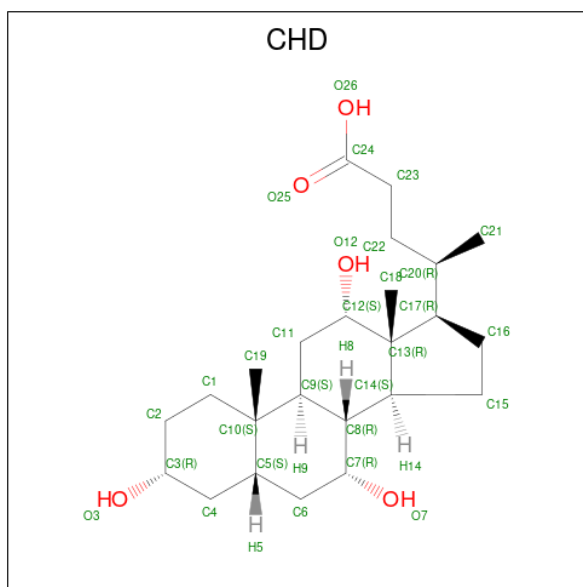
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	engineered mutation	UNP P22830
A	337	ALA	PHE	engineered mutation	UNP P22830
B	115	LEU	ARG	engineered mutation	UNP P22830
B	337	ALA	PHE	engineered mutation	UNP P22830

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 4 2 2	0	0
2	B	1	Total Fe S 4 2 2	0	0

- Molecule 3 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0
3	B	1	Total C O 29 24 5	0	0


- Molecule 4 is water.

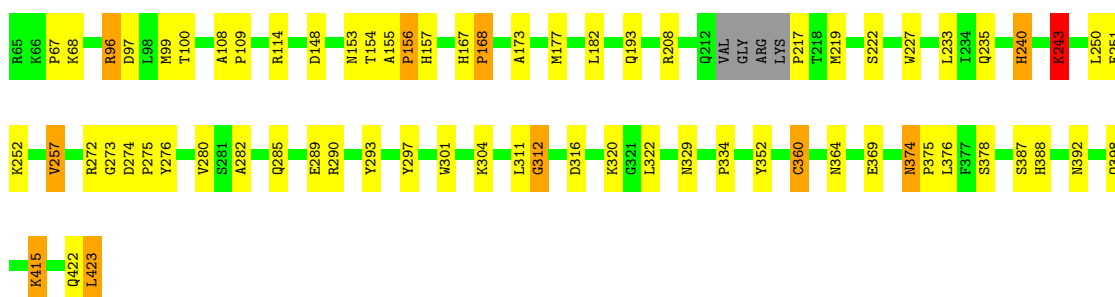
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	172	Total O 172 172	0	0
4	B	170	Total O 170 170	0	0

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. 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. 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.

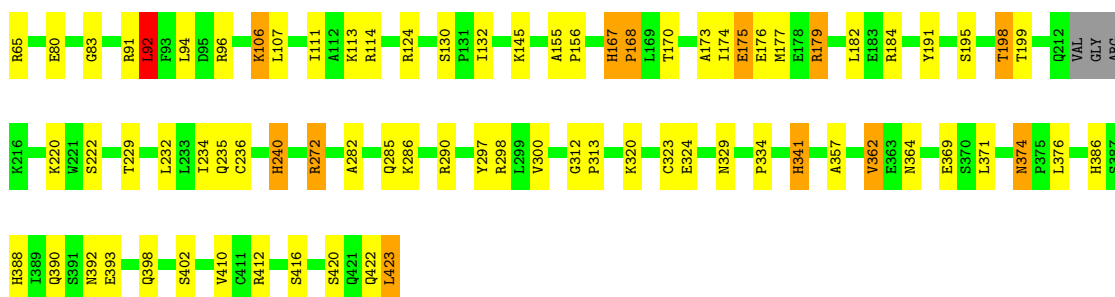
- Molecule 1: Ferrochelatase, mitochondrial

Chain A: 



- Molecule 1: Ferrochelatase, mitochondrial

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.69Å 94.05Å 113.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 2.35 48.52 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.44-2.35) 80.5 (48.52-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.192 , 0.253 0.401 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtrriage
Anisotropy	0.511	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	6166	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5269e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FES, CHD

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	0.76	1/2883 (0.0%)	0.78	2/3916 (0.1%)
1	B	0.77	0/2895	0.81	4/3931 (0.1%)
All	All	0.76	1/5778 (0.0%)	0.80	6/7847 (0.1%)

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	A	0	4
1	B	0	5
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	GLY	CA-C	-5.00	1.43	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	HIS	C-N-CD	-9.73	99.19	120.60
1	B	92	LEU	CA-CB-CG	7.40	132.33	115.30
1	A	312	GLY	N-CA-C	-6.72	96.29	113.10
1	B	91	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	243	LYS	CD-CE-NZ	5.49	124.32	111.70
1	B	167	HIS	C-N-CA	5.03	143.13	122.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ALA	Peptide
1	A	167	HIS	Mainchain,Peptide
1	A	311	LEU	Peptide
1	B	155	ALA	Mainchain,Peptide
1	B	167	HIS	Peptide
1	B	312	GLY	Mainchain,Peptide

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	2815	0	2769	56	8
1	B	2827	0	2790	64	5
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	87	0	117	2	0
3	B	87	0	117	4	0
4	A	172	0	0	13	2
4	B	170	0	0	19	7
All	All	6166	0	5793	118	11

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 10.

All (118) 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:243:LYS:HD2	4:A:616:HOH:O	1.28	1.31
1:B:410:VAL:HB	4:B:633:HOH:O	1.43	1.18
1:B:323:CYS:HB3	4:B:602:HOH:O	1.47	1.13
1:A:398:GLN:HE22	1:B:297:TYR:H	1.15	0.94
1:B:272:ARG:NH1	4:B:673:HOH:O	2.01	0.93
1:B:323:CYS:CB	4:B:602:HOH:O	2.09	0.86
1:A:240:HIS:O	1:A:243:LYS:HE3	1.75	0.85
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:CYS:SG	4:B:602:HOH:O	2.35	0.83
1:B:198:THR:HG22	1:B:199:THR:H	1.42	0.83
1:A:67:PRO:HA	1:A:156:PRO:HB2	1.60	0.82
1:A:388:HIS:HD2	4:A:561:HOH:O	1.69	0.76
1:B:300:VAL:HG12	1:B:313:PRO:HG2	1.70	0.74
1:B:198:THR:HG21	4:B:517:HOH:O	1.87	0.74
1:B:176:GLU:HG3	4:B:609:HOH:O	1.87	0.73
1:A:297:TYR:H	1:B:398:GLN:HE22	1.33	0.73
1:B:334:PRO:CG	4:B:564:HOH:O	2.37	0.72
1:A:222:SER:OG	1:A:388:HIS:HE1	1.73	0.71
1:A:217:PRO:N	4:A:504:HOH:O	2.23	0.70
1:B:222:SER:OG	1:B:388:HIS:HE1	1.75	0.70
1:B:334:PRO:HG3	4:B:564:HOH:O	1.90	0.70
1:B:402:SER:CB	4:B:551:HOH:O	2.40	0.70
1:A:392:ASN:ND2	4:A:605:HOH:O	2.26	0.68
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.59	0.67
1:B:298:ARG:HG2	4:B:565:HOH:O	1.95	0.65
1:A:240:HIS:HD2	1:A:369:GLU:O	1.79	0.64
1:B:422:GLN:O	1:B:423:LEU:HB2	1.98	0.64
1:B:402:SER:HB3	4:B:551:HOH:O	1.98	0.63
1:A:329:ASN:ND2	1:A:364:ASN:HB2	2.12	0.63
1:B:175:GLU:O	1:B:179:ARG:HG2	1.99	0.62
1:A:114:ARG:HG3	4:A:585:HOH:O	2.00	0.61
1:B:240:HIS:HD2	1:B:369:GLU:O	1.83	0.61
1:A:422:GLN:O	1:A:423:LEU:HB2	2.01	0.61
1:A:398:GLN:HE22	1:B:297:TYR:N	1.93	0.60
1:B:168:PRO:HD3	4:B:639:HOH:O	2.00	0.60
1:B:198:THR:CG2	1:B:199:THR:H	2.16	0.58
1:B:388:HIS:HD2	1:B:393:GLU:OE1	1.86	0.58
1:B:386:HIS:O	1:B:390:GLN:HG3	2.04	0.57
1:A:273:GLY:O	1:B:298:ARG:HD3	2.04	0.57
1:B:191:TYR:CD1	1:B:198:THR:HG23	2.40	0.57
1:B:402:SER:HB2	4:B:551:HOH:O	2.04	0.56
1:A:240:HIS:HA	1:A:243:LYS:HE3	1.87	0.56
1:B:195:SER:HB3	1:B:198:THR:HB	1.87	0.56
1:B:229:THR:HB	1:B:286:LYS:HE2	1.87	0.55
1:A:334:PRO:HG2	4:A:578:HOH:O	2.05	0.54
1:B:173:ALA:O	1:B:177:MET:HG3	2.08	0.54
1:A:97:ASP:CG	1:A:208:ARG:HH22	2.11	0.53
1:A:97:ASP:OD1	1:A:208:ARG:NH2	2.41	0.53
1:A:243:LYS:CD	4:A:616:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:NZ	1:A:153:ASN:O	2.41	0.52
1:A:168:PRO:HD3	4:A:626:HOH:O	2.08	0.52
1:B:222:SER:OG	1:B:388:HIS:CE1	2.60	0.52
1:A:240:HIS:HA	1:A:243:LYS:CE	2.40	0.52
1:B:232:LEU:HD22	1:B:376:LEU:HD11	1.92	0.52
1:B:392:ASN:HB2	4:B:660:HOH:O	2.09	0.52
1:B:229:THR:HB	1:B:286:LYS:CE	2.40	0.51
1:A:154:THR:OG1	1:A:157:HIS:HE1	1.94	0.51
1:B:106:LYS:HB2	1:B:106:LYS:NZ	2.26	0.51
1:A:374:ASN:HD22	1:A:375:PRO:N	2.09	0.50
1:B:416:SER:O	1:B:420:SER:HB2	2.10	0.50
1:B:235:GLN:HG3	1:B:290:ARG:CZ	2.42	0.49
1:A:243:LYS:CE	4:A:616:HOH:O	2.50	0.49
1:B:198:THR:HG22	1:B:199:THR:N	2.19	0.49
1:B:92:LEU:HD11	3:B:501:CHD:H62	1.95	0.49
1:A:240:HIS:CA	1:A:243:LYS:HE3	2.42	0.49
1:B:320:LYS:O	1:B:324:GLU:HG3	2.13	0.49
1:A:148:ASP:OD1	1:A:157:HIS:HD2	1.94	0.49
1:B:94:LEU:O	1:B:96:ARG:NH1	2.44	0.48
1:A:374:ASN:ND2	1:A:376:LEU:H	2.11	0.48
1:A:222:SER:OG	1:A:388:HIS:CE1	2.61	0.48
1:A:374:ASN:HD22	1:A:374:ASN:C	2.16	0.48
1:A:320:LYS:HG3	1:A:360:CYS:SG	2.53	0.47
1:B:198:THR:CG2	1:B:199:THR:N	2.74	0.47
1:A:154:THR:OG1	1:A:157:HIS:CE1	2.68	0.47
1:A:240:HIS:C	1:A:243:LYS:HE3	2.34	0.47
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.95	0.47
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.48	0.47
1:A:301:TRP:CD1	1:A:312:GLY:HA3	2.50	0.47
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.77	0.46
1:B:130:SER:OG	1:B:132:ILE:HG13	2.16	0.46
1:A:97:ASP:HB2	4:A:665:HOH:O	2.15	0.46
1:B:65:ARG:N	4:B:601:HOH:O	2.49	0.46
1:B:113:LYS:HG2	4:B:661:HOH:O	2.15	0.46
1:B:235:GLN:HG3	1:B:290:ARG:NH1	2.30	0.46
1:A:285:GLN:HG2	1:B:282:ALA:HB1	1.98	0.46
1:B:334:PRO:HG2	4:B:564:HOH:O	2.07	0.46
1:A:415:LYS:CE	4:A:563:HOH:O	2.64	0.45
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.17	0.45
1:A:257:VAL:HG21	1:A:322:LEU:HD13	1.99	0.45
1:B:398:GLN:NE2	1:B:398:GLN:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:HG2	1:A:280:VAL:HA	1.99	0.43
1:A:173:ALA:O	1:A:177:MET:HG3	2.17	0.43
1:B:234:ILE:HG13	1:B:286:LYS:HE3	2.00	0.43
1:A:282:ALA:HB1	1:B:285:GLN:HG2	1.99	0.42
3:A:501:CHD:H222	3:A:501:CHD:C18	2.50	0.42
1:B:374:ASN:HD22	1:B:376:LEU:H	1.67	0.42
1:B:329:ASN:ND2	1:B:364:ASN:HB2	2.30	0.42
3:B:501:CHD:H212	3:B:501:CHD:H12	2.01	0.42
1:A:177:MET:HB3	1:A:182:LEU:HD12	2.01	0.42
1:A:285:GLN:O	1:A:289:GLU:HG3	2.20	0.42
1:B:170:THR:O	1:B:174:ILE:HG13	2.20	0.42
1:A:374:ASN:HD22	1:A:376:LEU:H	1.67	0.42
1:A:304:LYS:HE2	4:A:635:HOH:O	2.19	0.42
1:A:227:TRP:CZ3	1:A:233:LEU:HD13	2.55	0.41
1:A:96:ARG:HA	1:A:99:MET:O	2.19	0.41
1:B:412:ARG:HH11	1:B:412:ARG:HG2	1.85	0.41
1:A:276:TYR:O	1:A:280:VAL:HG23	2.20	0.41
3:B:501:CHD:H183	3:B:501:CHD:H20	1.92	0.41
1:A:235:GLN:HG3	1:A:290:ARG:CZ	2.51	0.41
3:B:503:CHD:H162	3:B:503:CHD:H222	1.79	0.41
1:B:107:LEU:O	1:B:111:ILE:HG13	2.20	0.41
1:B:145:LYS:NZ	1:B:145:LYS:HB3	2.36	0.41
1:B:357:ALA:HB1	1:B:362:VAL:HG11	2.03	0.40
1:B:236:CYS:HB3	1:B:371:LEU:HD22	2.03	0.40
3:A:502:CHD:H112	3:A:502:CHD:H12A	1.90	0.40
4:A:624:HOH:O	1:B:286:LYS:HD3	2.20	0.40
1:B:341:HIS:HE1	4:B:563:HOH:O	2.03	0.40
1:A:273:GLY:HA2	1:B:313:PRO:HG3	2.04	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:645:HOH:O	4:B:628:HOH:O[3_655]	0.89	1.31
1:B:80:GLU:OE1	4:A:620:HOH:O[3_645]	1.08	1.12
1:A:252:LYS:CE	4:B:599:HOH:O[3_655]	1.09	1.11
1:A:252:LYS:CD	4:B:599:HOH:O[3_655]	1.66	0.54
1:A:251:GLU:CB	1:B:83:GLY:O[3_655]	1.75	0.45
1:B:124:ARG:O	4:B:521:HOH:O[3_645]	1.79	0.41
1:A:251:GLU:CA	1:B:83:GLY:O[3_655]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:OE1	4:B:567:HOH:O[3_655]	2.00	0.20
1:A:251:GLU:CG	4:B:567:HOH:O[3_655]	2.01	0.19
1:A:251:GLU:O	1:B:83:GLY:CA[3_655]	2.03	0.17
1:A:251:GLU:CD	4:B:567:HOH:O[3_655]	2.05	0.15

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	351/359 (98%)	338 (96%)	11 (3%)	2 (1%)	25	27
1	B	352/359 (98%)	340 (97%)	10 (3%)	2 (1%)	25	27
All	All	703/718 (98%)	678 (96%)	21 (3%)	4 (1%)	25	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	B	168	PRO
1	A	168	PRO
1	B	156	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/323 (96%)	296 (96%)	14 (4%)	27	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	311/323 (96%)	296 (95%)	15 (5%)	25	30
All	All	621/646 (96%)	592 (95%)	29 (5%)	26	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	100	THR
1	A	219	MET
1	A	240	HIS
1	A	243	LYS
1	A	250	LEU
1	A	257	VAL
1	A	272	ARG
1	A	360	CYS
1	A	374	ASN
1	A	378	SER
1	A	387	SER
1	A	415	LYS
1	A	423	LEU
1	B	92	LEU
1	B	106	LYS
1	B	114	ARG
1	B	175	GLU
1	B	179	ARG
1	B	182	LEU
1	B	184	ARG
1	B	198	THR
1	B	220	LYS
1	B	240	HIS
1	B	272	ARG
1	B	341	HIS
1	B	362	VAL
1	B	374	ASN
1	B	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	235	GLN

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Mol	Chain	Res	Type
1	A	240	HIS
1	A	314	GLN
1	A	329	ASN
1	A	341	HIS
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	388	HIS
1	A	390	GLN
1	A	392	ASN
1	A	398	GLN
1	A	421	GLN
1	B	167	HIS
1	B	235	GLN
1	B	240	HIS
1	B	314	GLN
1	B	329	ASN
1	B	341	HIS
1	B	374	ASN
1	B	388	HIS
1	B	398	GLN
1	B	421	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CHD	A	502	-	32,32,32	0.60	0	51,51,51	1.85	15 (29%)
3	CHD	B	502	-	32,32,32	0.57	0	51,51,51	1.82	12 (23%)
3	CHD	B	501	-	32,32,32	0.75	0	51,51,51	1.90	12 (23%)
3	CHD	B	503	-	32,32,32	0.62	0	51,51,51	1.51	11 (21%)
2	FES	A	499	1	0,4,4	-	-	-	-	-
3	CHD	A	503	-	32,32,32	0.64	0	51,51,51	1.46	9 (17%)
2	FES	B	499	1	0,4,4	-	-	-	-	-
3	CHD	A	501	-	32,32,32	0.64	0	51,51,51	1.82	14 (27%)

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
3	CHD	A	502	-	-	6/9/74/74	0/4/4/4
3	CHD	B	502	-	-	5/9/74/74	0/4/4/4
3	CHD	B	501	-	-	9/9/74/74	0/4/4/4
3	CHD	B	503	-	-	7/9/74/74	0/4/4/4
2	FES	A	499	1	-	-	0/1/1/1
3	CHD	A	503	-	-	3/9/74/74	0/4/4/4
2	FES	B	499	1	-	-	0/1/1/1
3	CHD	A	501	-	-	7/9/74/74	0/4/4/4

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CHD	C13-C17-C20	-4.70	113.89	119.50
3	A	501	CHD	C6-C5-C4	-4.58	105.91	111.19
3	A	501	CHD	C16-C17-C20	4.53	119.16	112.15
3	B	501	CHD	C23-C22-C20	-4.50	106.29	114.52
3	A	502	CHD	C6-C5-C4	-4.46	106.05	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CHD	C6-C5-C4	-4.44	106.08	111.19
3	B	502	CHD	C17-C13-C14	-4.40	95.65	100.09
3	B	502	CHD	C15-C14-C13	4.40	107.87	103.55
3	A	503	CHD	C15-C14-C13	4.04	107.52	103.55
3	B	501	CHD	C16-C17-C20	3.86	118.12	112.15
3	A	502	CHD	C21-C20-C17	3.62	118.46	112.92
3	B	502	CHD	C1-C10-C5	3.56	113.03	107.77
3	B	501	CHD	C14-C13-C12	3.53	110.69	107.40
3	A	501	CHD	C14-C13-C12	3.53	110.69	107.40
3	B	502	CHD	C6-C5-C4	-3.51	107.15	111.19
3	B	503	CHD	C15-C14-C13	3.50	106.99	103.55
3	A	502	CHD	C13-C17-C20	3.43	123.59	119.50
3	A	501	CHD	C22-C23-C24	-3.42	103.42	112.51
3	B	502	CHD	C13-C17-C20	3.36	123.50	119.50
3	B	503	CHD	C16-C17-C13	3.29	106.78	103.55
3	B	501	CHD	C11-C9-C10	-3.28	110.34	113.73
3	B	502	CHD	C19-C10-C5	-3.28	104.80	110.36
3	A	502	CHD	C9-C10-C5	3.25	113.14	108.58
3	B	503	CHD	C9-C10-C5	3.25	113.14	108.58
3	A	502	CHD	C17-C13-C14	-3.22	96.84	100.09
3	A	501	CHD	C13-C17-C20	-3.14	115.75	119.50
3	B	502	CHD	C22-C20-C17	-3.12	103.84	110.28
3	A	503	CHD	C10-C9-C8	3.01	115.05	111.82
3	B	503	CHD	C4-C5-C10	2.97	115.81	112.66
3	A	501	CHD	C15-C14-C13	2.95	106.45	103.55
3	A	501	CHD	C21-C20-C17	-2.94	108.42	112.92
3	A	503	CHD	C6-C7-C8	2.93	114.61	111.48
3	A	501	CHD	C9-C11-C12	2.92	118.16	114.30
3	A	501	CHD	C9-C8-C7	-2.86	108.45	111.88
3	A	502	CHD	C1-C10-C5	2.79	111.89	107.77
3	A	501	CHD	C11-C9-C8	2.79	114.96	110.88
3	A	502	CHD	C22-C20-C17	-2.76	104.59	110.28
3	A	502	CHD	C2-C1-C10	2.71	117.43	112.78
3	B	501	CHD	C22-C23-C24	-2.69	105.38	112.51
3	A	502	CHD	C6-C5-C10	2.66	115.48	112.66
3	B	502	CHD	C21-C20-C17	2.66	116.99	112.92
3	B	501	CHD	C11-C9-C8	2.66	114.76	110.88
3	A	503	CHD	C9-C10-C5	2.64	112.29	108.58
3	B	503	CHD	C11-C12-C13	2.63	113.94	111.24
3	B	501	CHD	C17-C13-C12	-2.60	115.29	117.67
3	A	503	CHD	C14-C8-C9	-2.55	106.21	109.71
3	A	502	CHD	C19-C10-C1	-2.51	104.21	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CHD	C15-C14-C13	2.51	106.01	103.55
3	A	501	CHD	C16-C17-C13	2.50	106.00	103.55
3	B	503	CHD	C17-C13-C14	-2.49	97.58	100.09
3	B	501	CHD	O3-C3-C4	-2.46	104.96	109.85
3	B	502	CHD	C11-C9-C8	2.41	114.41	110.88
3	A	503	CHD	C4-C5-C10	2.39	115.19	112.66
3	B	501	CHD	C18-C13-C12	2.39	111.50	109.07
3	A	503	CHD	C14-C8-C7	2.35	114.93	111.81
3	A	502	CHD	C21-C20-C22	-2.34	106.69	110.36
3	B	503	CHD	C14-C8-C9	-2.31	106.55	109.71
3	A	501	CHD	C17-C13-C14	-2.26	97.82	100.09
3	A	502	CHD	C5-C4-C3	2.21	116.01	112.76
3	B	502	CHD	C16-C17-C20	-2.18	108.78	112.15
3	B	503	CHD	C14-C13-C12	2.17	109.42	107.40
3	B	503	CHD	C10-C9-C8	2.16	114.14	111.82
3	A	503	CHD	C9-C8-C7	2.15	114.45	111.88
3	B	501	CHD	C13-C14-C8	-2.09	112.06	114.74
3	B	502	CHD	C16-C15-C14	-2.09	101.00	105.13
3	A	503	CHD	C19-C10-C5	-2.07	106.85	110.36
3	B	502	CHD	C16-C17-C13	2.07	105.58	103.55
3	A	501	CHD	C11-C12-C13	2.07	113.37	111.24
3	A	501	CHD	C1-C2-C3	-2.06	107.82	110.47
3	B	503	CHD	C11-C9-C8	2.06	113.89	110.88
3	A	502	CHD	C11-C9-C8	2.06	113.89	110.88
3	A	502	CHD	C4-C3-C2	2.02	112.97	110.55
3	B	503	CHD	C6-C5-C4	-2.00	108.88	111.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CHD	C20-C22-C23-C24
3	A	502	CHD	C13-C17-C20-C21
3	B	501	CHD	C21-C20-C22-C23
3	B	501	CHD	C17-C20-C22-C23
3	A	501	CHD	C13-C17-C20-C22
3	B	501	CHD	C20-C22-C23-C24
3	B	503	CHD	C16-C17-C20-C21
3	B	503	CHD	C16-C17-C20-C22
3	A	501	CHD	C16-C17-C20-C21
3	A	501	CHD	C13-C17-C20-C21
3	A	502	CHD	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
3	B	503	CHD	C13-C17-C20-C22
3	B	503	CHD	C20-C22-C23-C24
3	B	502	CHD	C13-C17-C20-C21
3	A	502	CHD	C13-C17-C20-C22
3	B	503	CHD	C13-C17-C20-C21
3	B	502	CHD	C20-C22-C23-C24
3	B	501	CHD	C13-C17-C20-C22
3	A	503	CHD	C20-C22-C23-C24
3	B	501	CHD	C13-C17-C20-C21
3	B	501	CHD	C16-C17-C20-C22
3	B	501	CHD	C16-C17-C20-C21
3	B	501	CHD	C22-C23-C24-O25
3	A	503	CHD	C22-C23-C24-O25
3	B	501	CHD	C22-C23-C24-O26
3	A	501	CHD	C22-C23-C24-O26
3	A	501	CHD	C22-C23-C24-O25
3	A	503	CHD	C22-C23-C24-O26
3	B	502	CHD	C22-C23-C24-O25
3	B	502	CHD	C22-C23-C24-O26
3	A	502	CHD	C22-C23-C24-O26
3	A	502	CHD	C22-C23-C24-O25
3	B	502	CHD	C16-C17-C20-C22
3	A	501	CHD	C16-C17-C20-C22
3	B	503	CHD	C22-C23-C24-O26
3	A	502	CHD	C16-C17-C20-C21
3	B	503	CHD	C22-C23-C24-O25

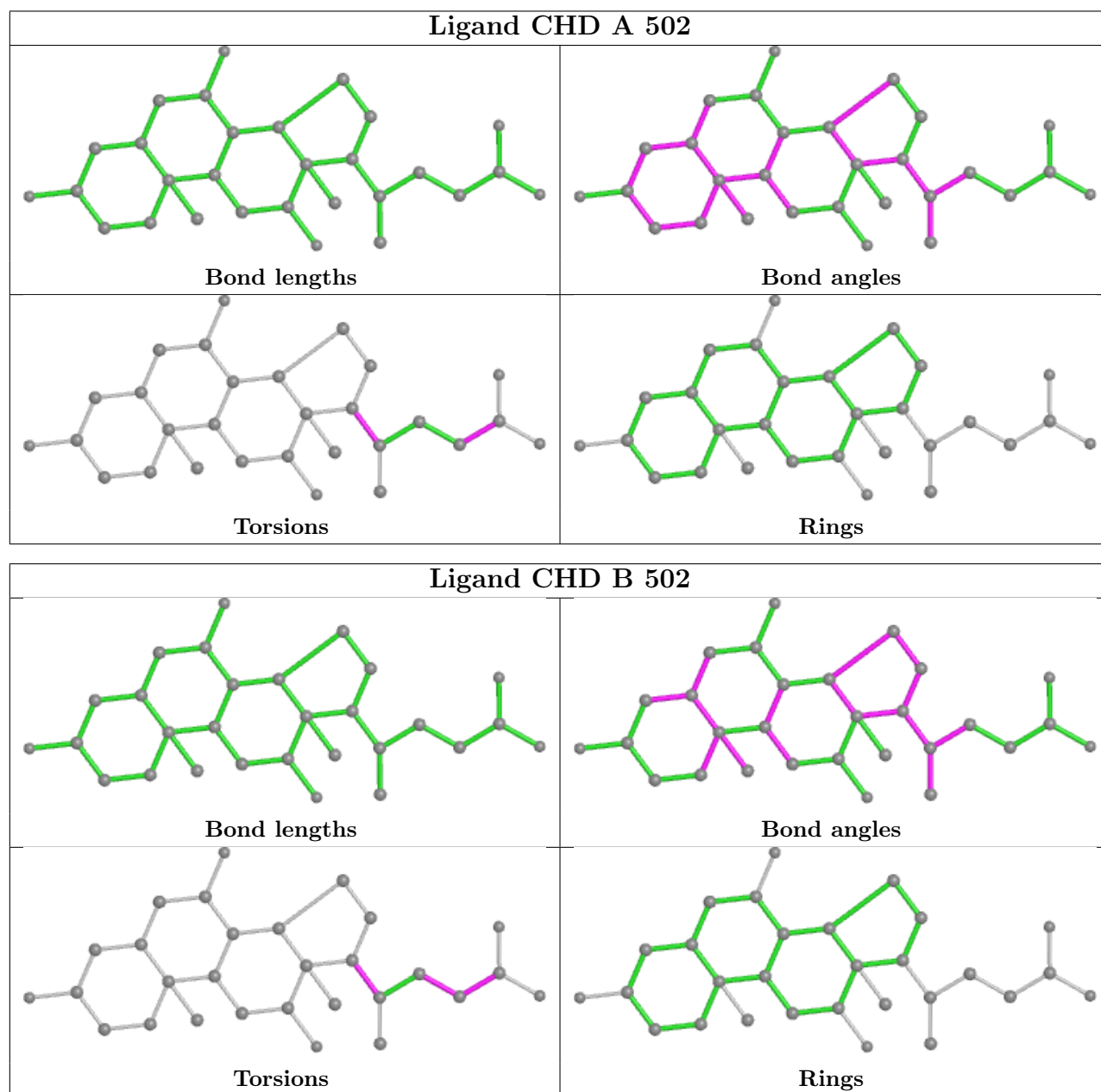
There are no ring outliers.

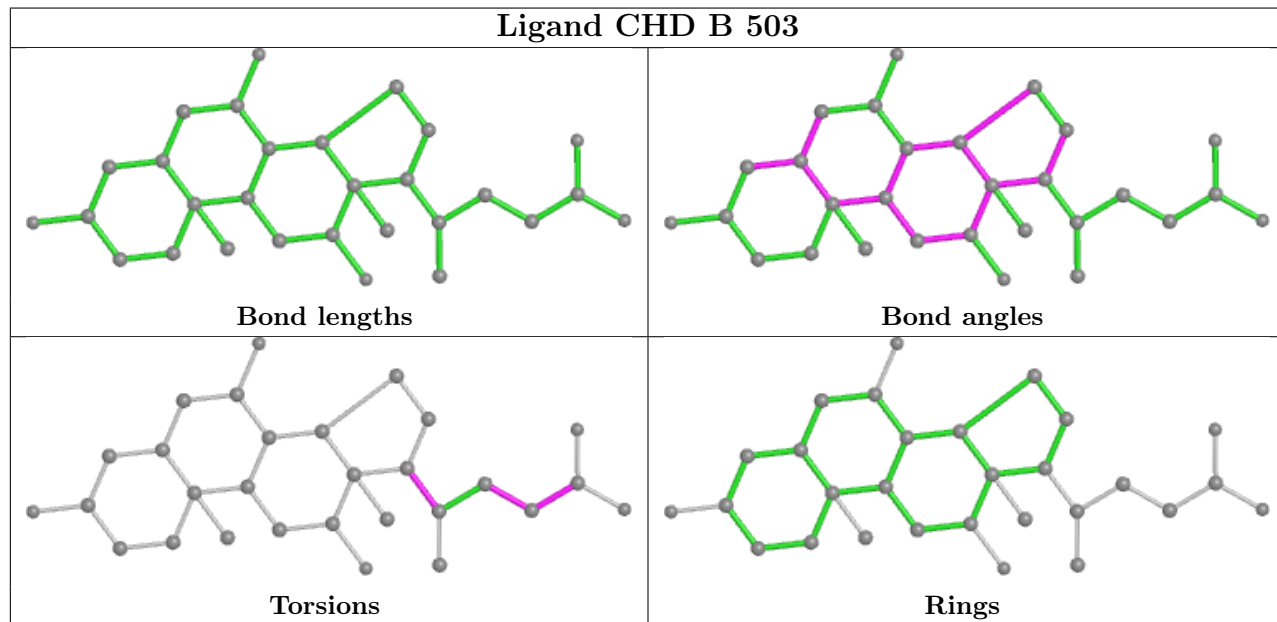
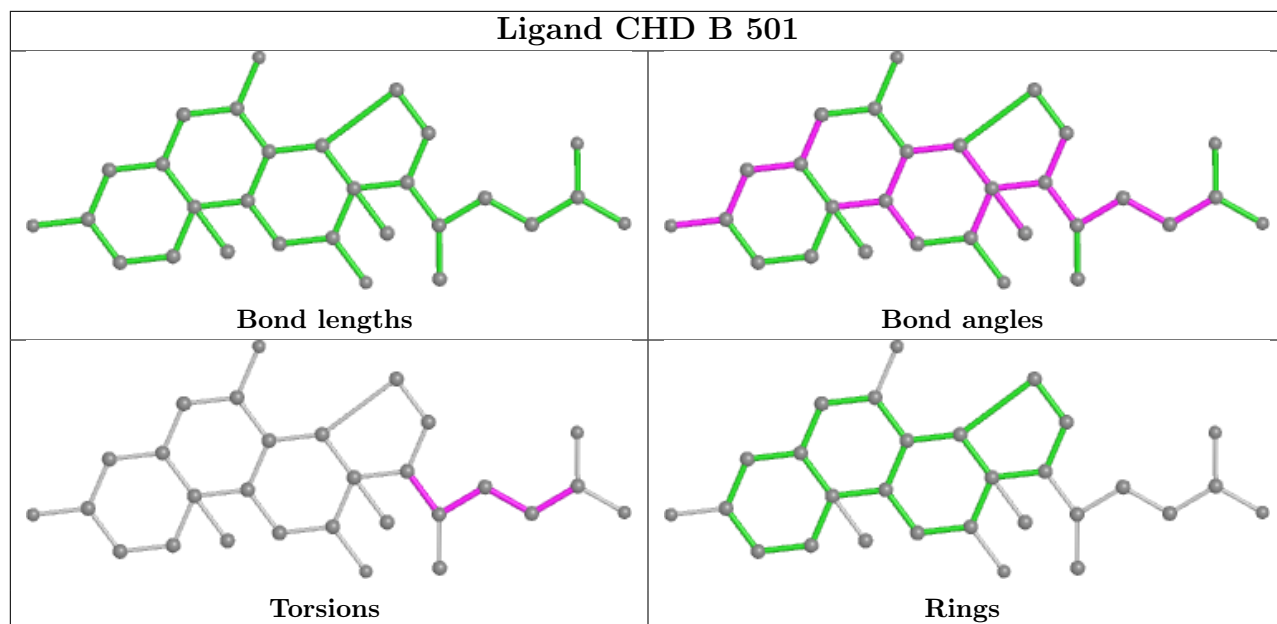
4 monomers are involved in 6 short contacts:

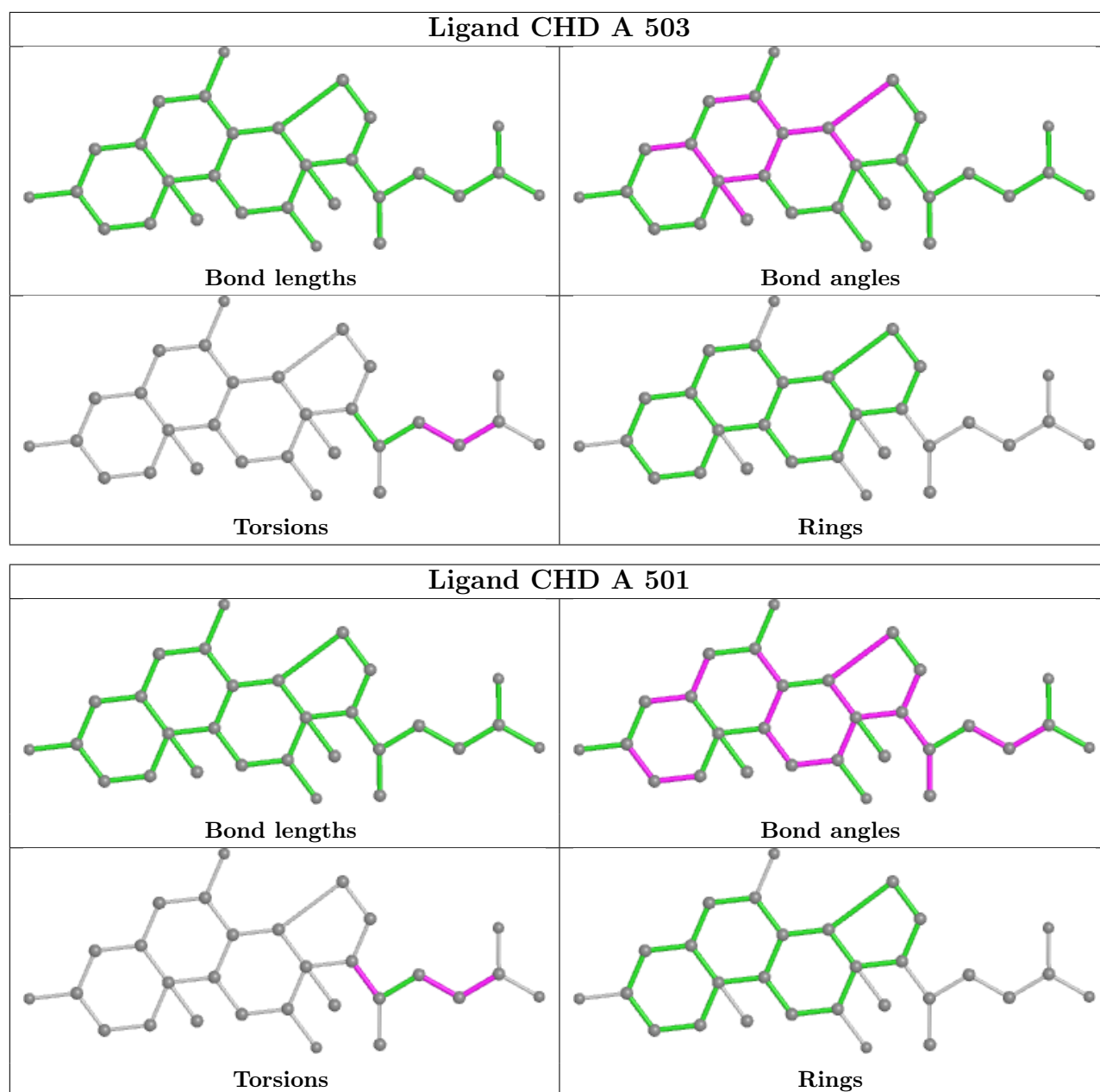
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	CHD	1	0
3	B	501	CHD	3	0
3	B	503	CHD	1	0
3	A	501	CHD	1	0

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 [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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

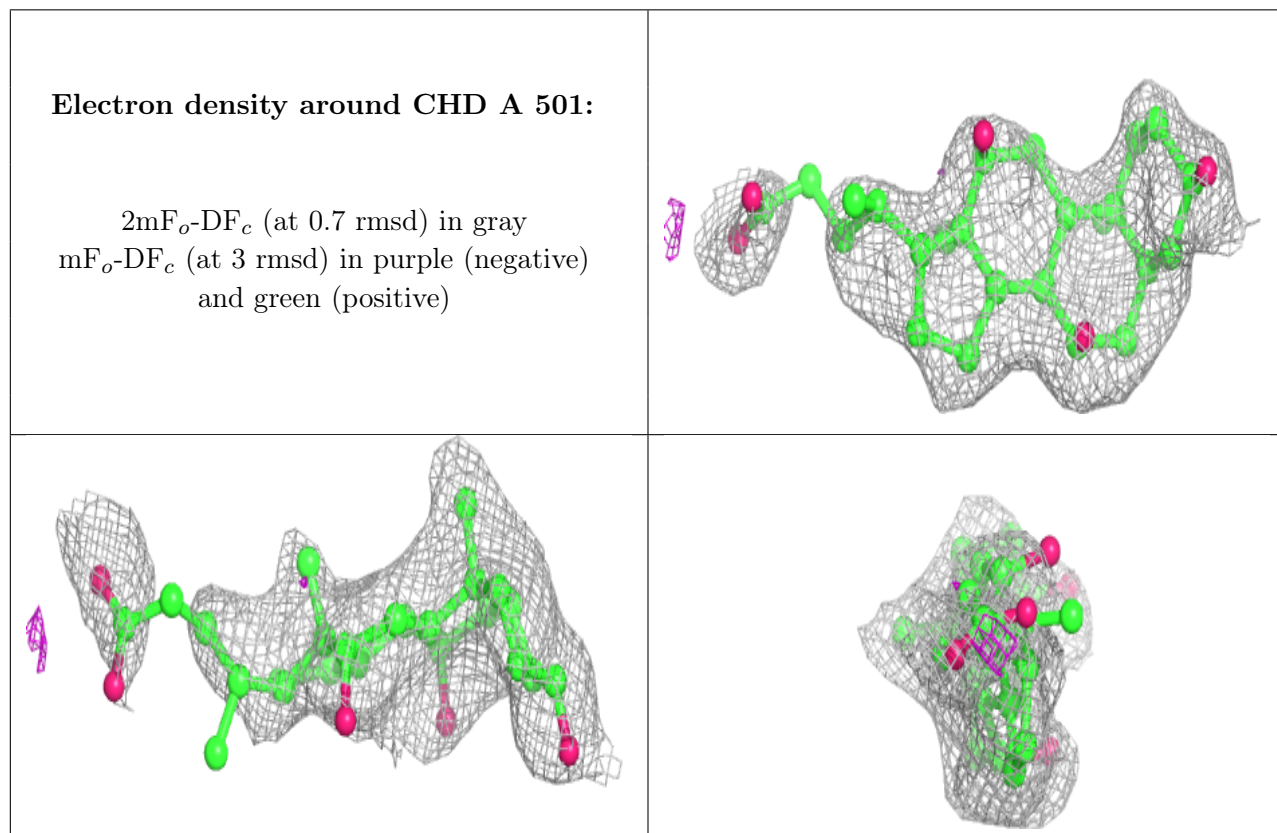
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

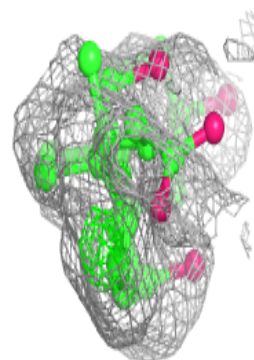
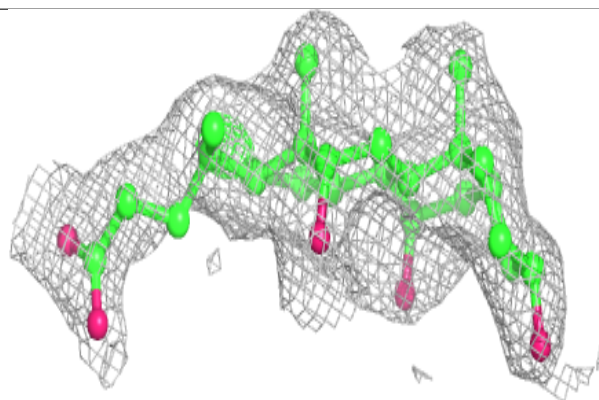
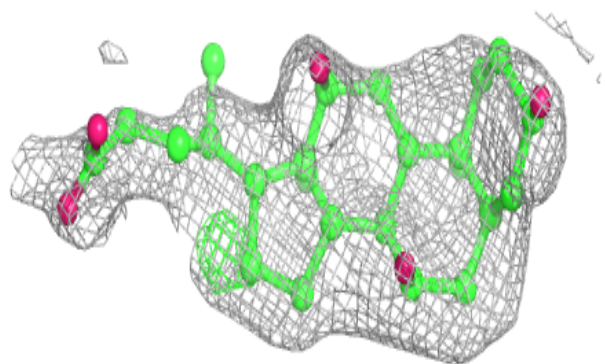
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

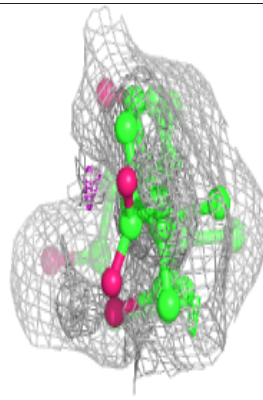
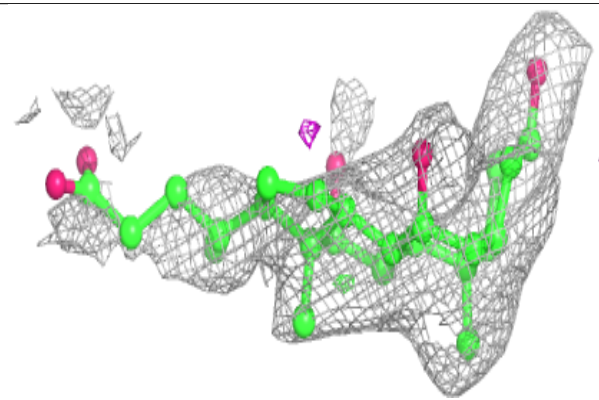
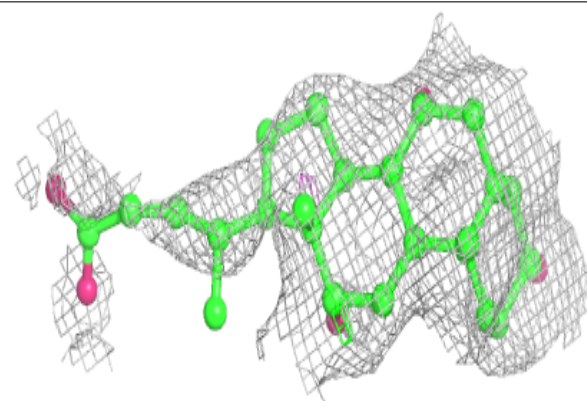


Electron density around CHD A 502:

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

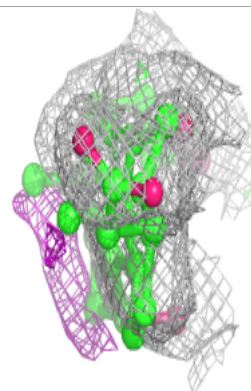
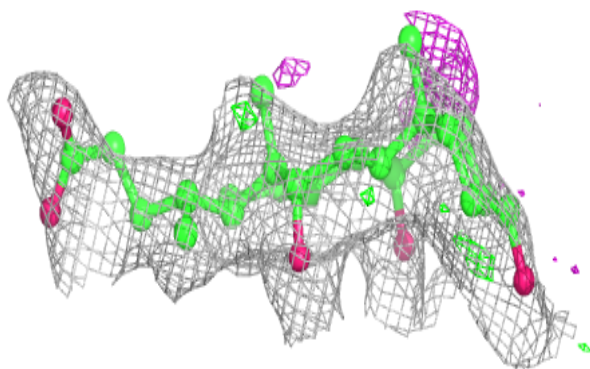
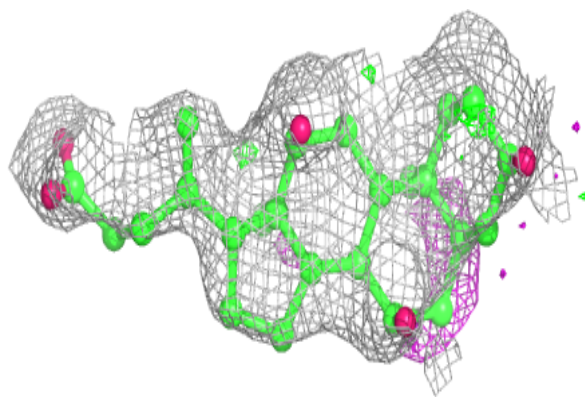
**Electron density around CHD A 503:**

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

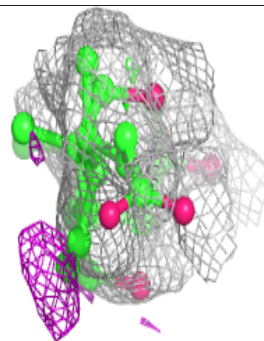
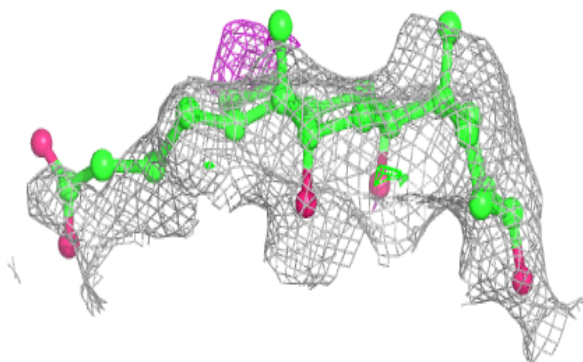
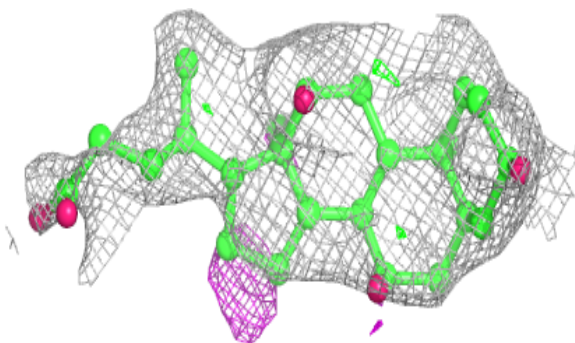


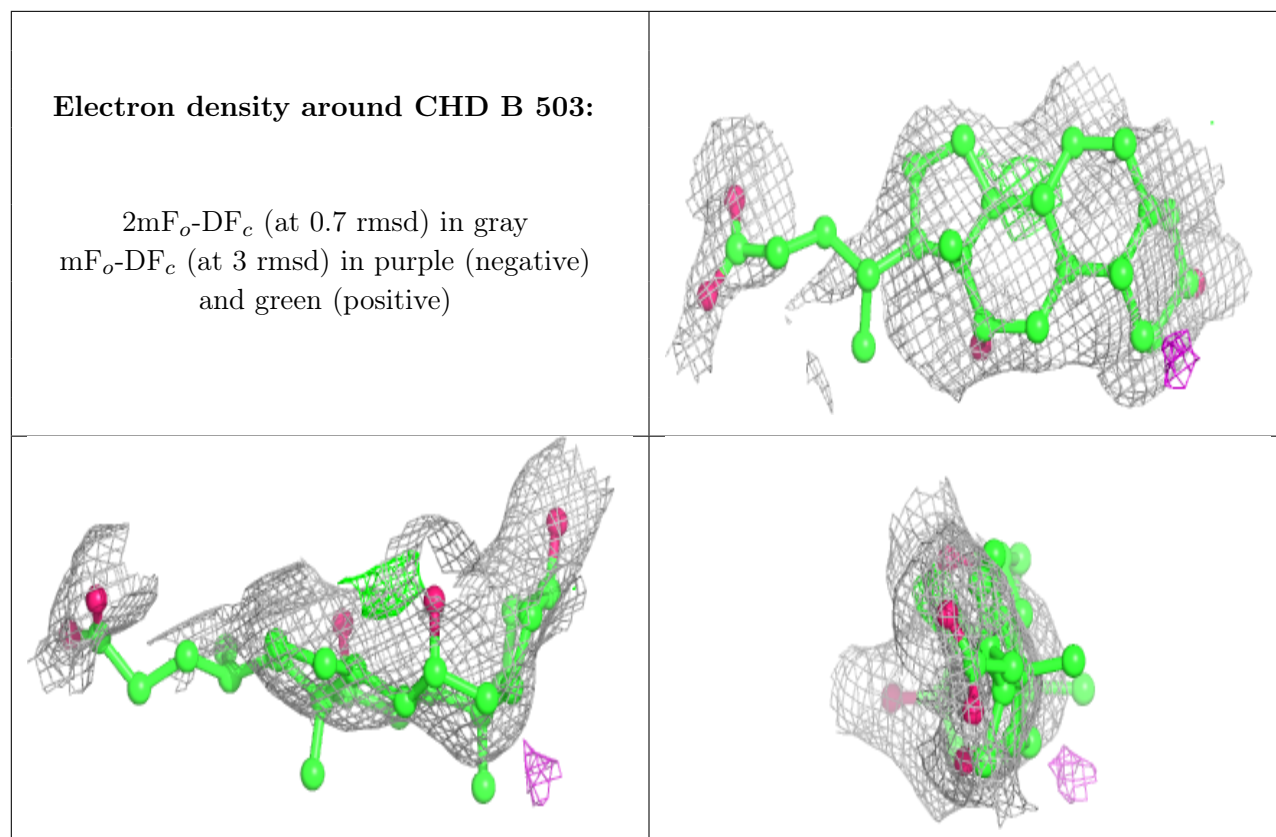
Electron density around CHD B 501:

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

**Electron density around CHD B 502:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.