



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:48 PM EDT

PDB ID : 3HCR / pdb_00003hcr
Title : Human Ferrochelatase with deuteroporphyrin and Ni Bound
Authors : Medlock, A.E.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2009-05-06
Resolution : 2.20 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 : 4-5-2 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

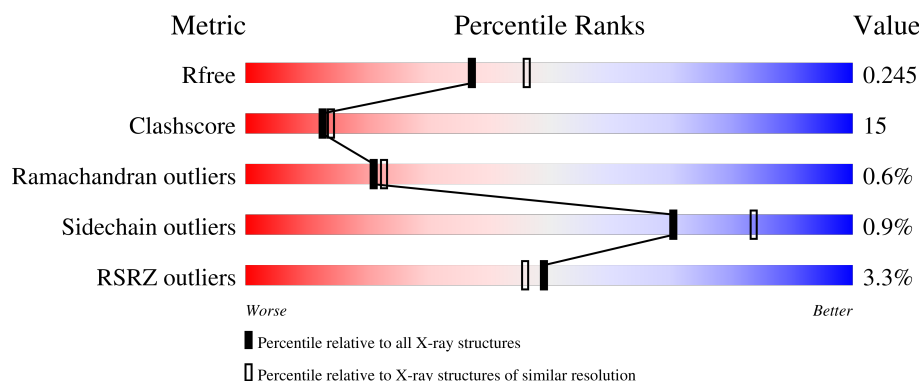
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	359	
1	B	359	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IMD	A	2	-	X	-	-
7	FDE	A	426	X	-	-	-
7	FDE	B	927	X	-	-	-

2 Entry composition [i](#)

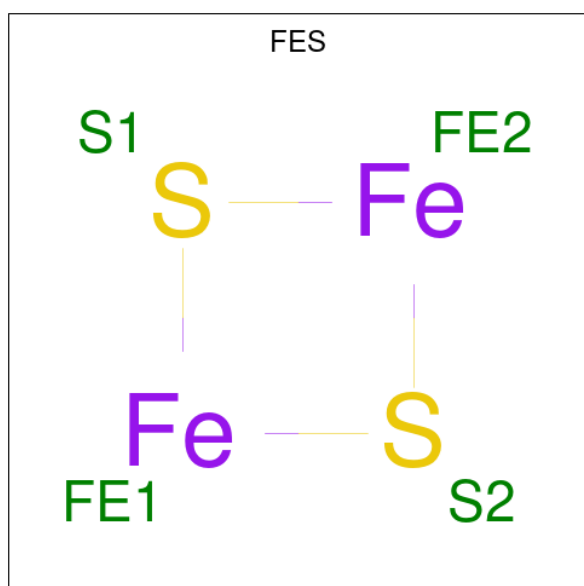
There are 10 unique types of molecules in this entry. The entry contains 6360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

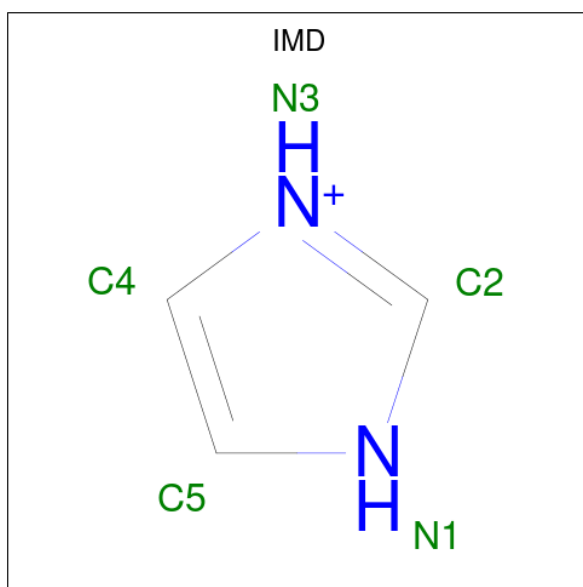
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2891	1841	503	529	18			
1	B	359	Total	C	N	O	S	0	1	0
			2900	1846	504	532	18			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



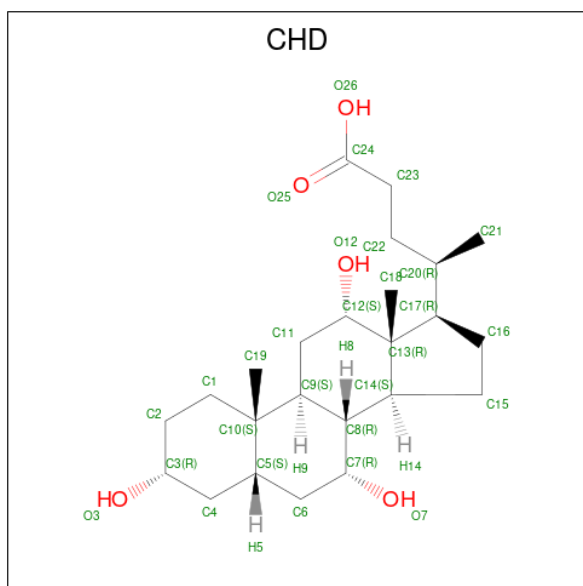
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $\text{C}_3\text{H}_5\text{N}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



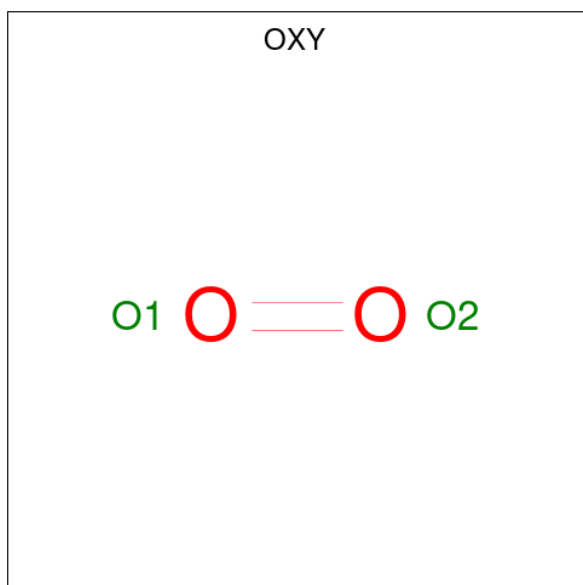
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	24	5		
4	A	1	Total	C	O	0	0
			29	24	5		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).

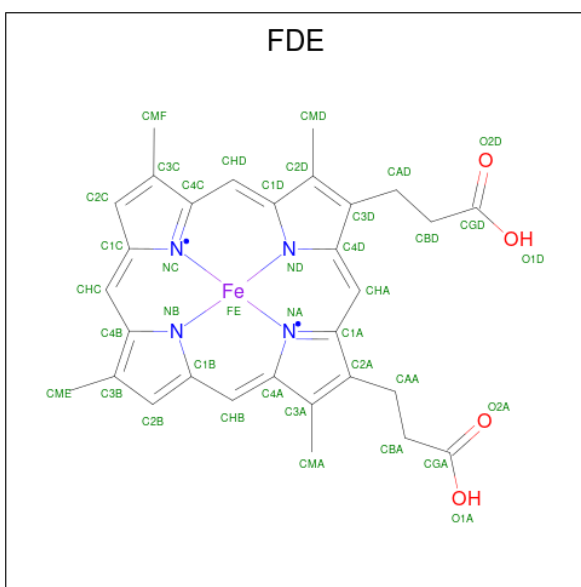


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

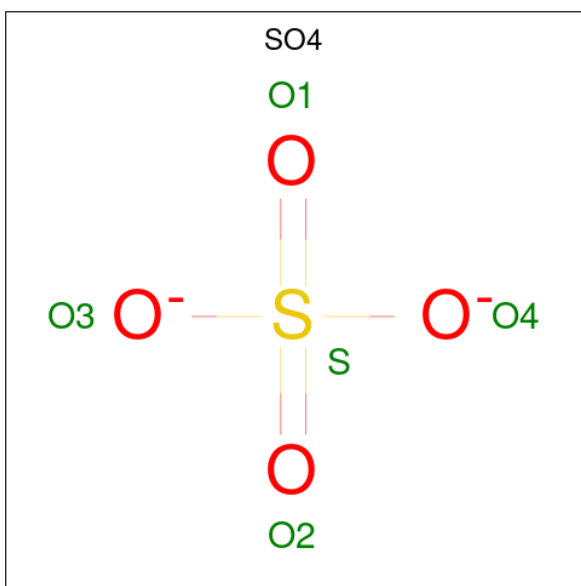
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is FE(III) DEUTEROPORPHYRIN IX (CCD ID: FDE) (formula: C₃₀H₂₈FeN₄O₄).



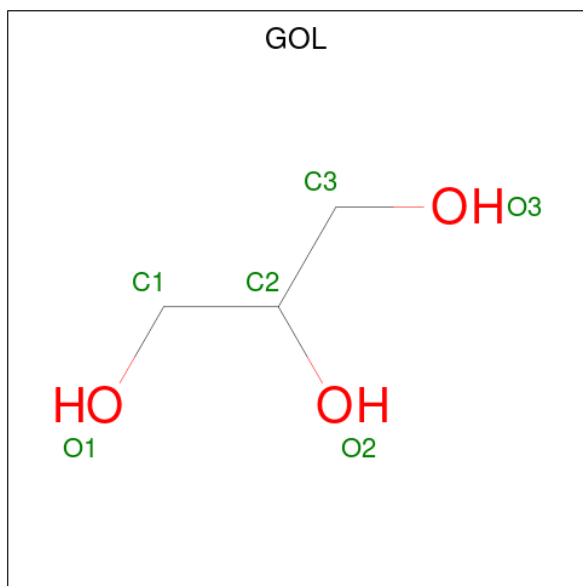
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 39	C 30	Fe 1	N 4	O 4	0	0
7	B	1	Total 39	C 30	Fe 1	N 4	O 4	0	0

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

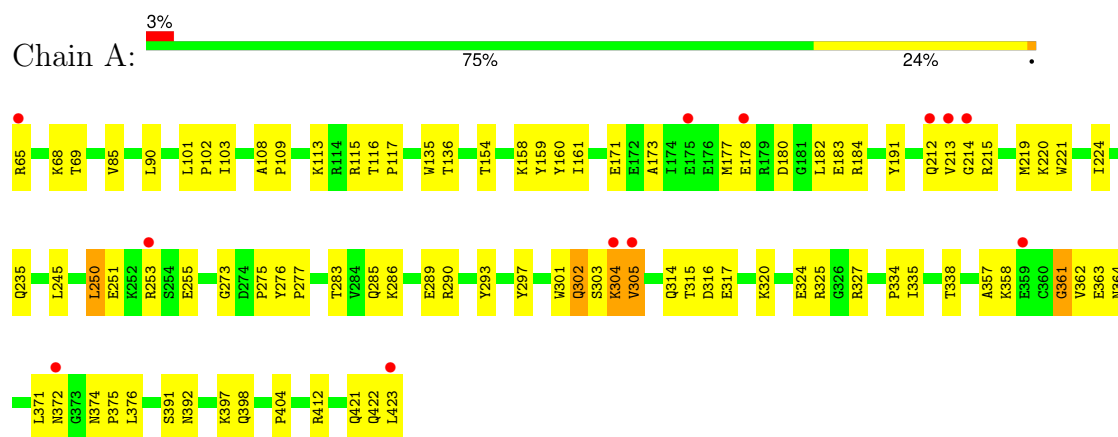
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	172	Total	O	0	0
			172	172		
10	B	164	Total	O	0	0
			164	164		

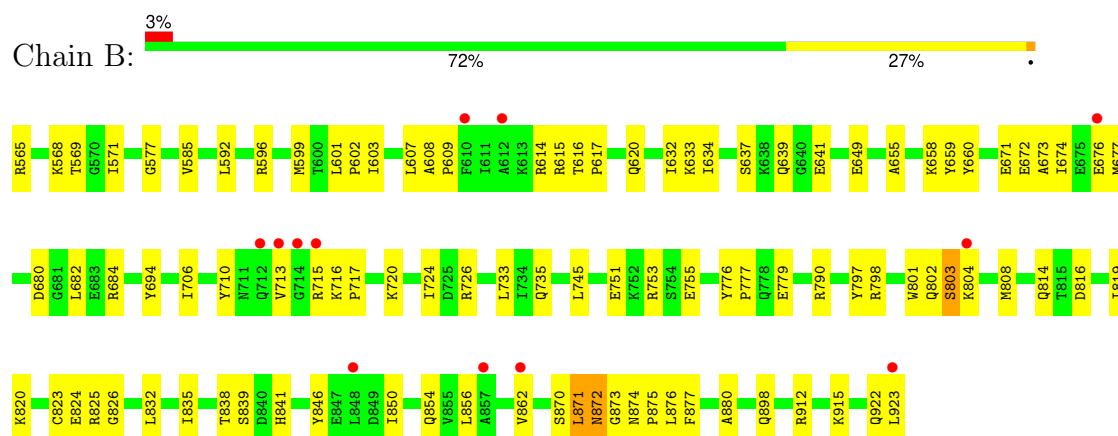
3 Residue-property plots

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: Ferrochelatase, mitochondrial



• Molecule 1: Ferrochelatase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.42Å 92.94Å 109.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 2.20 47.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (47.32-2.20) 92.1 (47.32-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.250 0.213 , 0.245	Depositor DCC
R_{free} test set	4205 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.889	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6360	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.94 % 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 1.6398e-04. 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: CHD, SO4, OXY, FDE, GOL, CL, IMD, FES

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	0.40	0/2961	0.89	4/4011 (0.1%)
1	B	0.39	0/2970	0.90	8/4023 (0.2%)
All	All	0.40	0/5931	0.89	12/8034 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	THR	N-CA-C	6.91	121.38	113.15
1	A	302	GLN	N-CA-C	6.90	119.89	109.95
1	B	838	THR	N-CA-C	6.55	121.12	113.20
1	A	224	ILE	N-CA-C	-6.30	96.23	109.34
1	B	585	VAL	N-CA-C	6.07	116.25	110.42
1	B	733	LEU	N-CA-C	-6.07	104.59	111.14
1	B	802	GLN	N-CA-C	6.06	119.04	110.14
1	B	724	ILE	N-CA-C	-5.87	97.12	109.34
1	B	803	SER	N-CA-C	5.32	119.05	112.24
1	A	85	VAL	N-CA-C	5.27	116.05	110.72
1	B	826	GLY	N-CA-C	5.18	121.95	115.21
1	B	694	TYR	N-CA-C	5.12	117.91	109.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2891	0	2899	95	0
1	B	2900	0	2904	92	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	5	0	4	2	0
3	B	5	0	4	1	0
4	A	58	0	78	2	0
4	B	58	0	78	5	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	1	0
7	A	39	0	22	0	0
7	B	39	0	22	0	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	B	6	0	8	3	0
10	A	172	0	0	14	0
10	B	164	0	0	14	0
All	All	6360	0	6019	183	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 15.

All (183) 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:304:LYS:HD3	1:A:304:LYS:H	1.16	1.04
1:A:297:TYR:H	1:B:898:GLN:HE22	1.03	0.94
1:A:250:LEU:H	1:A:250:LEU:HD23	1.38	0.87
1:B:682:LEU:HG	10:B:296:HOH:O	1.75	0.87
1:A:398:GLN:HE22	1:B:797:TYR:H	1.15	0.86
1:B:720:LYS:HE3	1:B:923:LEU:HD22	1.59	0.83
1:B:634:ILE:HG13	10:B:193:HOH:O	1.80	0.82
1:A:304:LYS:H	1:A:304:LYS:CD	1.94	0.80
1:B:615:ARG:HD2	4:B:924:CHD:H231	1.64	0.79
1:B:735:GLN:HG3	1:B:790:ARG:HH12	1.47	0.79
1:A:68:LYS:HE3	1:A:183:GLU:OE1	1.85	0.77
1:B:672:GLU:O	1:B:676[A]:GLU:HG2	1.85	0.76
1:B:808:MET:HB2	10:B:245:HOH:O	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TYR:N	1:B:898:GLN:HE22	1.84	0.74
1:A:250:LEU:HB2	10:A:514:HOH:O	1.85	0.74
1:B:637:SER:O	1:B:641:GLU:HG3	1.88	0.73
1:B:912:ARG:NH2	1:B:912:ARG:HB2	2.04	0.72
1:A:115:ARG:HD2	4:A:424:CHD:H231	1.72	0.72
1:A:357:ALA:O	1:A:361:GLY:HA2	1.90	0.71
1:A:177:MET:O	1:A:182:LEU:HD13	1.90	0.71
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.05	0.70
1:A:178:GLU:OE1	1:A:219:MET:HE2	1.92	0.69
1:B:639:GLN:HE21	1:B:873:GLY:HA2	1.58	0.68
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.08	0.66
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.78	0.65
1:B:720:LYS:CE	1:B:923:LEU:HD22	2.26	0.65
1:B:755:GLU:HB3	10:B:243:HOH:O	1.97	0.65
1:B:912:ARG:HB3	10:B:100:HOH:O	1.96	0.65
1:B:922:GLN:HG2	1:B:923:LEU:CD1	2.27	0.65
1:B:565:ARG:HH11	1:B:565:ARG:HB2	1.62	0.65
1:A:398:GLN:HE22	1:B:797:TYR:N	1.92	0.64
1:B:614:ARG:HH11	1:B:614:ARG:HG2	1.62	0.64
1:A:314:GLN:HG2	10:A:456:HOH:O	1.97	0.64
1:A:374:ASN:HD22	1:A:375:PRO:HD2	1.61	0.64
1:A:422:GLN:HG2	1:A:423:LEU:HD12	1.80	0.64
1:B:850:ILE:O	1:B:854:GLN:HG2	1.97	0.64
1:A:235:GLN:HG3	1:A:290:ARG:HH21	1.63	0.64
1:B:856:LEU:HG	1:B:862:VAL:HG21	1.79	0.63
1:A:314:GLN:HB2	1:A:317:GLU:HG2	1.80	0.62
1:A:220:LYS:HZ2	1:A:423:LEU:HD22	1.65	0.61
1:B:680:ASP:HB2	10:B:296:HOH:O	2.01	0.61
1:A:101:LEU:HD21	4:A:424:CHD:H7	1.82	0.61
1:A:173:ALA:O	1:A:177:MET:HG3	2.02	0.60
1:A:357:ALA:HA	1:A:362:VAL:HG12	1.84	0.60
1:B:874:ASN:HD22	1:B:875:PRO:CD	2.14	0.59
1:B:568:LYS:HD2	1:B:655:ALA:O	2.01	0.59
1:A:297:TYR:H	1:B:898:GLN:NE2	1.87	0.59
1:A:285:GLN:O	1:A:289:GLU:HG3	2.03	0.59
1:A:422:GLN:HG2	1:A:423:LEU:CD1	2.32	0.59
1:B:874:ASN:HD22	1:B:875:PRO:HD2	1.67	0.59
1:B:922:GLN:HG2	1:B:923:LEU:HD13	1.84	0.58
1:B:616:THR:O	1:B:620:GLN:HB2	2.04	0.57
1:A:358:LYS:HA	10:A:562:HOH:O	2.04	0.57
1:A:215:ARG:HH11	1:A:215:ARG:HB3	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:SER:C	1:B:872:ASN:H	2.12	0.56
1:B:816:ASP:HB2	10:B:227:HOH:O	2.04	0.56
1:A:212:GLN:C	1:A:214:GLY:H	2.12	0.56
1:A:69:THR:OG1	1:A:154:THR:HB	2.06	0.56
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.88	0.56
1:B:713:VAL:HG12	1:B:715:ARG:HG2	1.88	0.56
1:A:212:GLN:HA	1:A:212:GLN:OE1	2.05	0.55
1:A:213:VAL:HG23	1:A:215:ARG:HG2	1.88	0.55
1:B:716:LYS:N	1:B:716:LYS:HD2	2.21	0.55
1:A:304:LYS:HD3	1:A:304:LYS:N	2.01	0.55
1:B:671:GLU:OE1	1:B:671:GLU:N	2.27	0.55
1:B:745:LEU:HB3	1:B:753:ARG:NH1	2.21	0.55
1:B:777:PRO:HB3	9:B:925:GOL:H2	1.89	0.55
1:A:374:ASN:HD22	1:A:375:PRO:N	2.04	0.55
1:A:277:PRO:CB	9:B:925:GOL:H12	2.37	0.54
1:A:277:PRO:HB2	9:B:925:GOL:H12	1.88	0.54
1:A:316:ASP:HB2	10:A:516:HOH:O	2.07	0.53
1:B:565:ARG:HH11	1:B:565:ARG:CB	2.21	0.53
1:A:304:LYS:O	1:A:305:VAL:HG22	2.08	0.53
1:B:820:LYS:HE2	1:B:824:GLU:OE1	2.09	0.53
1:A:215:ARG:HD3	10:A:547:HOH:O	2.07	0.53
1:A:102:PRO:O	1:A:103:ILE:C	2.52	0.52
1:A:325:ARG:HH11	1:A:325:ARG:HG3	1.74	0.52
1:B:616:THR:HB	1:B:617:PRO:HD3	1.91	0.52
1:B:673:ALA:O	1:B:677:MET:HG3	2.10	0.52
1:B:823:CYS:SG	1:B:862:VAL:HG22	2.50	0.52
1:A:374:ASN:HD22	1:A:374:ASN:C	2.17	0.51
1:A:335:ILE:O	1:A:335:ILE:HG13	2.09	0.51
1:A:221:TRP:H	1:A:421:GLN:NE2	2.09	0.51
1:B:608:ALA:N	1:B:609:PRO:HD2	2.25	0.51
1:A:374:ASN:ND2	1:A:376:LEU:H	2.09	0.50
1:B:602:PRO:O	1:B:603:ILE:C	2.54	0.50
1:B:790:ARG:HG2	1:B:790:ARG:HH11	1.77	0.50
1:B:726:ARG:HD3	1:B:779:GLU:OE2	2.11	0.50
1:B:804:LYS:HD3	1:B:814:GLN:NE2	2.27	0.50
1:B:874:ASN:HD22	1:B:875:PRO:N	2.08	0.50
1:A:327:ARG:HD3	6:A:1:CL:CL	2.49	0.49
1:B:874:ASN:ND2	1:B:876:LEU:H	2.10	0.49
1:A:304:LYS:CD	1:A:304:LYS:N	2.71	0.49
1:A:304:LYS:HB2	10:A:550:HOH:O	2.11	0.49
1:B:839:SER:O	1:B:841:HIS:HD2	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LEU:C	10:A:537:HOH:O	2.56	0.48
1:B:874:ASN:HD22	1:B:874:ASN:C	2.21	0.48
1:A:245:LEU:HB3	1:A:253:ARG:NH1	2.29	0.48
1:A:334:PRO:HG2	10:A:567:HOH:O	2.12	0.48
1:B:912:ARG:HB2	1:B:912:ARG:HH21	1.75	0.48
1:A:184:ARG:HH11	1:A:184:ARG:HG3	1.79	0.48
1:A:286:LYS:NZ	10:A:511:HOH:O	2.46	0.48
1:B:649:GLU:HA	1:B:649:GLU:OE2	2.14	0.48
1:B:856:LEU:HG	1:B:862:VAL:CG2	2.41	0.48
4:B:924:CHD:H161	4:B:3:CHD:H151	1.96	0.48
1:A:363:GLU:C	1:A:364:ASN:HD22	2.21	0.47
1:B:565:ARG:CB	1:B:565:ARG:NH1	2.77	0.47
1:B:674:ILE:HD11	1:B:706:ILE:HG12	1.96	0.47
1:B:835:ILE:O	1:B:835:ILE:HG13	2.14	0.47
1:B:751:GLU:H	1:B:751:GLU:CD	2.22	0.47
1:B:633:LYS:HB3	10:B:193:HOH:O	2.15	0.47
1:B:603:ILE:HG13	1:B:607:LEU:HG	1.96	0.47
1:A:136:THR:CG2	1:A:161:ILE:HD12	2.45	0.47
1:A:212:GLN:C	1:A:214:GLY:N	2.73	0.47
1:A:220:LYS:NZ	1:A:423:LEU:HD22	2.28	0.47
1:B:803:SER:O	3:B:1:IMD:H4	2.15	0.47
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.95	0.47
1:B:854:GLN:NE2	1:B:854:GLN:HA	2.30	0.47
1:B:922:GLN:HG2	1:B:923:LEU:HD12	1.95	0.47
1:B:577:GLY:HA2	1:B:632:ILE:HD13	1.96	0.47
1:A:90:LEU:C	1:A:90:LEU:HD13	2.40	0.46
1:A:273:GLY:HA3	1:A:404:PRO:HD2	1.97	0.46
1:B:571:ILE:HD12	1:B:571:ILE:N	2.30	0.46
1:B:658:LYS:HD3	1:B:660:TYR:OH	2.15	0.46
1:B:596:ARG:HA	1:B:599:MET:O	2.16	0.46
1:A:135:TRP:CE2	1:A:372:ASN:HB3	2.51	0.46
1:A:158:LYS:NZ	1:A:180:ASP:OD2	2.43	0.46
1:B:912:ARG:HD2	10:B:100:HOH:O	2.15	0.46
1:A:180:ASP:HB2	1:A:182:LEU:CD1	2.45	0.46
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.15	0.46
1:A:305:VAL:HG23	1:A:305:VAL:O	2.16	0.46
1:A:136:THR:HG22	1:A:161:ILE:HD12	1.97	0.46
1:A:159:TYR:C	1:A:159:TYR:CD1	2.94	0.46
1:A:158:LYS:HD3	1:A:160:TYR:OH	2.17	0.45
1:B:720:LYS:HE2	10:B:140:HOH:O	2.16	0.45
1:B:715:ARG:NH2	10:B:295:HOH:O	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:TYR:CD2	1:B:856:LEU:HD22	2.52	0.45
1:B:684:ARG:HG3	10:B:182:HOH:O	2.16	0.45
1:A:302:GLN:HB3	1:A:315:THR:OG1	2.18	0.44
1:B:569:THR:HG23	1:B:684:ARG:HD2	1.99	0.44
1:A:304:LYS:HD3	10:A:34:HOH:O	2.17	0.44
1:A:325:ARG:HG3	1:A:325:ARG:NH1	2.32	0.44
1:A:171:GLU:H	1:A:171:GLU:CD	2.18	0.44
1:A:251:GLU:H	1:A:251:GLU:CD	2.26	0.44
1:B:659:TYR:C	1:B:659:TYR:CD1	2.95	0.44
10:A:543:HOH:O	1:B:825:ARG:HD3	2.17	0.44
1:A:320:LYS:O	1:A:324:GLU:HG3	2.18	0.43
1:A:103:ILE:HG13	1:A:103:ILE:O	2.17	0.43
1:A:250:LEU:H	1:A:250:LEU:CD2	2.17	0.43
1:A:283:THR:HG22	1:A:335:ILE:HD11	2.00	0.43
1:A:301:TRP:O	1:A:314:GLN:HA	2.18	0.43
1:A:372:ASN:HA	10:A:509:HOH:O	2.18	0.43
1:A:158:LYS:HD3	1:A:160:TYR:CZ	2.53	0.43
1:A:304:LYS:O	1:A:305:VAL:CG2	2.66	0.43
1:B:710:TYR:CE2	1:B:717:PRO:HA	2.54	0.43
1:B:915:LYS:HD3	10:B:197:HOH:O	2.19	0.43
1:A:65:ARG:HB3	10:A:517:HOH:O	2.17	0.43
1:A:215:ARG:HH11	1:A:215:ARG:CB	2.31	0.43
1:B:601:LEU:HD21	4:B:924:CHD:H151	2.01	0.43
1:B:825:ARG:HH11	1:B:825:ARG:HG3	1.83	0.43
1:B:870:SER:C	1:B:872:ASN:N	2.76	0.42
1:B:639:GLN:NE2	1:B:873:GLY:HA2	2.27	0.42
1:B:912:ARG:HH21	1:B:912:ARG:CB	2.33	0.42
1:B:601:LEU:HD21	4:B:924:CHD:H7	2.01	0.42
1:A:303:SER:HB2	3:A:2:IMD:HN3	1.83	0.42
1:A:363:GLU:C	1:A:364:ASN:ND2	2.78	0.42
4:B:924:CHD:H112	10:B:245:HOH:O	2.19	0.42
1:A:391:SER:O	1:A:392:ASN:HB2	2.19	0.42
1:B:592:LEU:HD23	1:B:592:LEU:C	2.45	0.42
1:A:191:TYR:HE1	10:A:533:HOH:O	2.02	0.42
1:B:819:ILE:HD11	1:B:832:LEU:HD21	2.00	0.42
1:A:116:THR:HB	1:A:117:PRO:HD3	2.02	0.41
1:A:374:ASN:ND2	1:A:375:PRO:HD2	2.31	0.41
1:B:877:PHE:O	1:B:880:ALA:HB3	2.20	0.41
1:B:614:ARG:HG2	1:B:614:ARG:NH1	2.33	0.41
1:A:275:PRO:HD3	1:B:798:ARG:NH2	2.36	0.41
1:A:303:SER:CB	3:A:2:IMD:HN3	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:LEU:O	1:B:872:ASN:C	2.63	0.41
1:B:922:GLN:O	1:B:923:LEU:HB2	2.21	0.41
1:A:215:ARG:CB	1:A:215:ARG:NH1	2.84	0.41
1:B:801:TRP:O	1:B:814:GLN:HA	2.21	0.40
1:A:102:PRO:C	1:A:103:ILE:HG12	2.47	0.40
1:B:912:ARG:HB2	1:B:912:ARG:CZ	2.51	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	357/359 (99%)	335 (94%)	20 (6%)	2 (1%)	21	23
1	B	358/359 (100%)	339 (95%)	17 (5%)	2 (1%)	21	23
All	All	715/718 (100%)	674 (94%)	37 (5%)	4 (1%)	21	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	872	ASN
1	A	361	GLY
1	A	305	VAL
1	B	871	LEU

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	324/324 (100%)	318 (98%)	6 (2%)	50	66
1	B	325/324 (100%)	325 (100%)	0	100	100
All	All	649/648 (100%)	643 (99%)	6 (1%)	70	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LYS
1	A	250	LEU
1	A	255	GLU
1	A	304	LYS
1	A	397	LYS
1	A	412	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	120	GLN
1	A	231	HIS
1	A	235	GLN
1	A	329	ASN
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	386	HIS
1	A	390	GLN
1	A	398	GLN
1	A	421	GLN
1	B	622	GLN
1	B	639	GLN
1	B	653	ASN
1	B	735	GLN
1	B	795	ASN
1	B	802	GLN
1	B	814	GLN
1	B	829	ASN
1	B	841	HIS
1	B	854	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	864	ASN
1	B	874	ASN
1	B	886	HIS
1	B	898	GLN
1	B	921	GLN
1	B	922	GLN

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, 1 is monoatomic - leaving 15 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	CHD	B	924	-	32,32,32	1.52	9 (28%)	51,51,51	1.38	6 (11%)
3	IMD	A	2	7	5,5,5	3.30	4 (80%)	5,5,5	2.37	3 (60%)
4	CHD	A	424	-	32,32,32	1.46	7 (21%)	51,51,51	1.41	8 (15%)
2	FES	B	502	1	0,4,4	-	-	-	-	-
4	CHD	B	3	-	32,32,32	1.48	6 (18%)	51,51,51	1.42	9 (17%)
8	SO4	A	427	-	4,4,4	0.37	0	6,6,6	0.07	0
3	IMD	B	1	7	5,5,5	0.78	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OXY	A	425	-	1,1,1	0.05	0	-		
7	FDE	B	927	3	46,46,46	3.39	27 (58%)	60,76,76	4.60	37 (61%)
9	GOL	B	925	-	5,5,5	0.25	0	5,5,5	0.34	0
7	FDE	A	426	3	46,46,46	3.19	26 (56%)	60,76,76	4.55	37 (61%)
2	FES	A	501	1	0,4,4	-	-	-		
8	SO4	B	2	-	4,4,4	0.37	0	6,6,6	0.09	0
4	CHD	A	4	-	32,32,32	1.51	6 (18%)	51,51,51	1.44	8 (15%)
5	OXY	B	926	-	1,1,1	0.06	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHD	B	924	-	-	0/9/74/74	0/4/4/4
3	IMD	A	2	7	-	-	0/1/1/1
4	CHD	A	424	-	-	0/9/74/74	0/4/4/4
2	FES	B	502	1	-	-	0/1/1/1
4	CHD	B	3	-	-	0/9/74/74	0/4/4/4
3	IMD	B	1	7	-	-	0/1/1/1
7	FDE	B	927	3	1/1/3/7	3/10/50/50	-
9	GOL	B	925	-	-	0/4/4/4	-
7	FDE	A	426	3	1/1/3/7	3/10/50/50	-
2	FES	A	501	1	-	-	0/1/1/1
4	CHD	A	4	-	-	0/9/74/74	0/4/4/4

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	927	FDE	CBA-CGA	-8.35	1.31	1.50
7	A	426	FDE	CBA-CGA	-8.34	1.31	1.50
7	A	426	FDE	C2A-C3A	7.75	1.53	1.36
7	B	927	FDE	CHC-C1C	6.75	1.51	1.38
7	B	927	FDE	C3D-C2D	6.71	1.51	1.36
7	B	927	FDE	C2A-C3A	6.27	1.50	1.36
7	A	426	FDE	C3D-C2D	5.65	1.49	1.36
7	A	426	FDE	CHC-C1C	5.52	1.49	1.38
7	A	426	FDE	FE-ND	5.31	2.12	1.95
7	B	927	FDE	C4A-C3A	5.10	1.54	1.44
7	A	426	FDE	CHC-C4B	5.07	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	927	FDE	CHB-C4A	-5.06	1.28	1.38
7	B	927	FDE	C1B-NB	-4.97	1.32	1.39
7	B	927	FDE	FE-NB	4.88	2.11	1.95
7	A	426	FDE	FE-NB	4.86	2.11	1.95
7	B	927	FDE	FE-ND	4.75	2.10	1.95
7	B	927	FDE	C4B-C3B	4.50	1.48	1.41
7	B	927	FDE	FE-NC	4.50	2.08	1.94
3	A	2	IMD	C5-N1	4.31	1.50	1.35
7	B	927	FDE	CHC-C4B	4.30	1.49	1.39
3	A	2	IMD	C2-N1	4.22	1.50	1.34
7	A	426	FDE	FE-NC	4.20	2.07	1.94
7	A	426	FDE	CHB-C4A	-3.82	1.30	1.38
7	A	426	FDE	C4C-C3C	-3.71	1.36	1.42
7	A	426	FDE	C4B-NB	-3.64	1.32	1.39
7	B	927	FDE	CHA-C4D	3.61	1.45	1.38
7	B	927	FDE	C1A-C2A	3.60	1.51	1.45
7	A	426	FDE	CHA-C4D	3.58	1.45	1.38
7	A	426	FDE	C4A-C3A	3.51	1.51	1.44
7	B	927	FDE	C4B-NB	-3.50	1.33	1.39
7	B	927	FDE	C4D-ND	-3.34	1.33	1.39
7	A	426	FDE	C1D-ND	-3.34	1.33	1.39
7	B	927	FDE	C1D-ND	-3.30	1.33	1.39
7	A	426	FDE	C1B-NB	-3.19	1.35	1.39
7	B	927	FDE	CHA-C1A	-3.17	1.32	1.39
7	A	426	FDE	CAA-C2A	3.11	1.59	1.51
3	A	2	IMD	C2-N3	2.99	1.45	1.32
7	B	927	FDE	C4C-C3C	-2.98	1.37	1.42
7	A	426	FDE	C4B-C3B	2.82	1.46	1.41
7	A	426	FDE	CMA-C3A	2.81	1.56	1.50
7	B	927	FDE	CHB-C1B	-2.78	1.32	1.39
4	A	4	CHD	C18-C13	2.68	1.58	1.54
7	A	426	FDE	CHB-C1B	-2.68	1.32	1.39
4	B	924	CHD	C11-C9	2.68	1.58	1.53
7	A	426	FDE	C4A-NA	-2.67	1.35	1.40
7	B	927	FDE	C1C-NC	-2.66	1.34	1.40
4	B	3	CHD	C18-C13	2.65	1.58	1.54
7	B	927	FDE	CMA-C3A	2.61	1.56	1.50
3	A	2	IMD	C5-C4	2.58	1.44	1.35
4	A	424	CHD	C18-C13	2.55	1.58	1.54
7	B	927	FDE	CHD-C4C	-2.53	1.33	1.39
7	A	426	FDE	CHD-C4C	-2.52	1.33	1.39
4	A	4	CHD	C20-C17	2.51	1.58	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	924	CHD	C18-C13	2.49	1.58	1.54
4	B	3	CHD	C20-C17	2.47	1.58	1.54
4	A	4	CHD	C11-C9	2.47	1.57	1.53
7	A	426	FDE	O1D-CGD	-2.46	1.22	1.30
4	B	924	CHD	C6-C5	2.42	1.57	1.53
4	A	424	CHD	C20-C17	2.42	1.58	1.54
4	A	424	CHD	C11-C9	2.39	1.57	1.53
4	B	3	CHD	C11-C9	2.37	1.57	1.53
7	B	927	FDE	CAA-C2A	2.35	1.57	1.51
7	B	927	FDE	O1D-CGD	-2.34	1.23	1.30
7	A	426	FDE	C1C-NC	-2.31	1.35	1.40
7	A	426	FDE	C1A-C2A	2.27	1.48	1.45
7	A	426	FDE	C4D-C3D	2.25	1.49	1.45
4	B	3	CHD	C6-C5	2.22	1.57	1.53
4	B	924	CHD	C4-C3	2.21	1.55	1.52
4	B	924	CHD	C6-C7	2.20	1.56	1.52
7	A	426	FDE	C4D-ND	-2.17	1.35	1.39
4	B	924	CHD	C20-C17	2.16	1.58	1.54
4	B	924	CHD	C8-C9	2.15	1.58	1.53
4	B	924	CHD	C4-C5	2.13	1.57	1.53
4	A	424	CHD	C6-C5	2.12	1.57	1.53
4	A	424	CHD	C4-C3	2.11	1.55	1.52
4	B	3	CHD	C8-C9	2.11	1.57	1.53
7	B	927	FDE	C4A-NA	-2.10	1.36	1.40
4	A	4	CHD	C8-C9	2.08	1.57	1.53
7	B	927	FDE	CHD-C1D	-2.07	1.34	1.38
4	B	924	CHD	C10-C9	2.07	1.59	1.56
4	A	4	CHD	C6-C7	2.06	1.56	1.52
4	A	4	CHD	C6-C5	2.05	1.57	1.53
4	A	424	CHD	C6-C7	2.05	1.56	1.52
4	B	3	CHD	C4-C3	2.04	1.55	1.52
4	A	424	CHD	C8-C9	2.01	1.57	1.53

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	426	FDE	CHD-C1D-ND	-14.82	108.31	124.45
7	B	927	FDE	CHD-C1D-ND	-13.62	109.62	124.45
7	B	927	FDE	C1D-CHD-C4C	13.19	154.06	126.02
7	A	426	FDE	C1D-CHD-C4C	12.47	152.52	126.02
7	B	927	FDE	CHD-C4C-NC	-10.70	112.91	124.42
7	B	927	FDE	C1B-CHB-C4A	8.94	152.93	125.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	426	FDE	CHD-C4C-NC	-8.89	114.86	124.42
7	B	927	FDE	C2B-C1B-NB	8.85	117.21	109.71
7	A	426	FDE	CAA-CBA-CGA	8.72	136.80	113.67
7	B	927	FDE	CMF-C3C-C4C	8.58	137.55	125.57
7	B	927	FDE	CHB-C4A-NA	-7.85	114.66	124.37
7	A	426	FDE	C1B-CHB-C4A	7.79	149.37	125.21
7	A	426	FDE	CMF-C3C-C4C	7.43	135.94	125.57
7	A	426	FDE	CMA-C3A-C4A	-6.66	114.62	125.03
7	B	927	FDE	CAA-CBA-CGA	6.45	130.78	113.67
7	A	426	FDE	C2B-C1B-NB	6.25	115.00	109.71
7	A	426	FDE	C1A-C2A-C3A	-6.24	97.81	106.89
7	B	927	FDE	CHD-C4C-C3C	5.73	134.05	125.03
7	A	426	FDE	CBA-CAA-C2A	-5.51	97.29	112.53
7	A	426	FDE	C1B-C2B-C3B	-5.49	101.05	108.58
7	A	426	FDE	CHA-C1A-C2A	-5.39	116.92	124.77
7	B	927	FDE	O2A-CGA-CBA	-5.34	106.16	123.09
7	B	927	FDE	C4A-C3A-C2A	-5.19	101.53	106.98
7	B	927	FDE	CBA-CAA-C2A	-5.16	98.27	112.53
7	A	426	FDE	CHB-C4A-NA	-5.14	118.01	124.37
7	B	927	FDE	C1B-C2B-C3B	-5.05	101.66	108.58
7	B	927	FDE	C1A-C2A-C3A	-4.93	99.72	106.89
7	A	426	FDE	CHC-C4B-NB	4.86	132.68	123.86
7	A	426	FDE	CHC-C4B-C3B	-4.82	120.31	130.51
7	A	426	FDE	CHD-C4C-C3C	4.81	132.60	125.03
7	A	426	FDE	C3D-C4D-ND	4.80	114.95	110.32
7	A	426	FDE	C2D-C1D-ND	4.65	118.23	109.64
7	A	426	FDE	CHA-C1A-NA	4.57	129.34	124.42
7	B	927	FDE	CHA-C1A-C2A	-4.53	118.17	124.77
7	B	927	FDE	C2A-C1A-NA	4.34	114.55	110.35
7	B	927	FDE	CME-C3B-C4B	4.32	130.24	125.94
7	A	426	FDE	CAA-C2A-C1A	-4.28	117.25	124.70
7	A	426	FDE	C4D-C3D-C2D	-4.22	101.55	107.11
7	B	927	FDE	C3D-C4D-ND	4.06	114.24	110.32
7	B	927	FDE	C4D-C3D-C2D	-4.04	101.78	107.11
7	B	927	FDE	C2D-C1D-ND	4.02	117.08	109.64
4	B	924	CHD	C9-C11-C12	-3.98	109.09	114.29
7	B	927	FDE	CAD-C3D-C2D	3.97	135.31	127.87
7	A	426	FDE	CHA-C4D-ND	-3.93	120.17	124.45
7	A	426	FDE	CHD-C1D-C2D	3.82	133.42	125.49
7	B	927	FDE	O1A-CGA-CBA	3.80	126.00	114.00
4	A	424	CHD	C9-C11-C12	-3.76	109.37	114.29
7	B	927	FDE	CHD-C1D-C2D	3.75	133.29	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	927	FDE	CHC-C4B-C3B	-3.73	122.61	130.51
7	A	426	FDE	CAD-C3D-C2D	3.66	134.72	127.87
4	B	3	CHD	C9-C11-C12	-3.51	109.70	114.29
4	A	4	CHD	C9-C11-C12	-3.48	109.74	114.29
7	B	927	FDE	CAA-C2A-C1A	-3.44	118.69	124.70
7	A	426	FDE	CMF-C3C-C2C	-3.41	117.84	125.57
7	A	426	FDE	C4A-C3A-C2A	-3.41	103.40	106.98
7	B	927	FDE	CMF-C3C-C2C	-3.36	117.96	125.57
7	B	927	FDE	C1D-C2D-C3D	-3.34	102.02	106.97
3	A	2	IMD	C4-C5-N1	3.22	115.05	106.79
7	A	426	FDE	C2B-C3B-C4B	3.20	109.76	106.17
7	A	426	FDE	C1C-CHC-C4B	-3.19	116.00	124.97
7	A	426	FDE	C2A-C1A-NA	3.14	113.39	110.35
7	B	927	FDE	CHA-C4D-ND	-3.14	121.04	124.45
7	A	426	FDE	C1D-C2D-C3D	-3.06	102.43	106.97
7	A	426	FDE	CAD-CBD-CGD	-3.04	105.61	113.67
3	A	2	IMD	C5-N1-C2	-3.04	100.64	107.19
4	A	4	CHD	C17-C13-C12	3.03	120.40	117.67
7	B	927	FDE	CHC-C4B-NB	2.99	129.28	123.86
7	A	426	FDE	C4A-NA-C1A	2.94	108.69	105.21
4	B	924	CHD	C16-C15-C14	-2.86	99.55	105.14
4	B	3	CHD	C17-C13-C12	2.83	120.21	117.67
7	B	927	FDE	CMA-C3A-C4A	-2.77	120.70	125.03
7	B	927	FDE	C3C-C4C-NC	2.76	113.00	109.88
4	A	424	CHD	C16-C15-C14	-2.71	99.83	105.14
7	B	927	FDE	CAD-CBD-CGD	-2.71	106.48	113.67
4	A	4	CHD	C11-C9-C10	-2.64	111.02	113.70
4	A	4	CHD	C13-C14-C8	-2.60	111.43	114.72
4	B	3	CHD	C11-C9-C10	-2.60	111.07	113.70
4	A	424	CHD	C11-C9-C10	-2.55	111.12	113.70
4	B	3	CHD	C16-C15-C14	-2.54	100.17	105.14
4	A	4	CHD	C16-C15-C14	-2.52	100.22	105.14
7	B	927	FDE	CHB-C4A-C3A	2.51	134.08	126.95
4	B	3	CHD	C13-C14-C8	-2.50	111.55	114.72
4	A	4	CHD	C13-C17-C20	-2.50	116.46	119.48
7	B	927	FDE	C1C-CHC-C4B	-2.43	118.12	124.97
4	B	924	CHD	C6-C5-C10	-2.40	110.11	112.66
4	A	424	CHD	C13-C14-C8	-2.39	111.69	114.72
7	B	927	FDE	CMA-C3A-C2A	-2.37	119.73	126.15
7	A	426	FDE	CHB-C4A-C3A	2.35	133.61	126.95
4	A	4	CHD	C6-C5-C10	-2.32	110.19	112.66
4	A	424	CHD	C17-C13-C12	2.32	119.75	117.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	426	FDE	O1D-CGD-CBD	2.31	121.30	114.00
7	B	927	FDE	CHA-C1A-NA	2.29	126.89	124.42
4	B	3	CHD	C18-C13-C14	-2.26	107.67	111.20
4	B	924	CHD	C10-C9-C8	-2.25	109.33	111.84
4	B	3	CHD	C13-C17-C20	-2.25	116.76	119.48
4	A	424	CHD	C6-C5-C10	-2.25	110.27	112.66
4	A	4	CHD	C18-C13-C14	-2.24	107.69	111.20
4	B	3	CHD	C6-C5-C10	-2.22	110.30	112.66
7	A	426	FDE	C3C-C4C-NC	2.20	112.37	109.88
3	A	2	IMD	C5-C4-N3	-2.17	102.42	109.11
7	B	927	FDE	CBD-CAD-C3D	-2.13	106.63	112.53
4	A	424	CHD	C10-C9-C8	-2.12	109.47	111.84
4	B	924	CHD	C11-C9-C10	-2.11	111.56	113.70
4	B	924	CHD	C18-C13-C14	-2.10	107.91	111.20
7	A	426	FDE	CMD-C2D-C1D	2.09	128.40	124.73
4	B	3	CHD	C10-C9-C8	-2.06	109.54	111.84
7	A	426	FDE	C3B-C4B-NB	-2.05	106.89	110.13
4	A	424	CHD	C18-C13-C14	-2.03	108.02	111.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	426	FDE	ND
7	B	927	FDE	ND

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	426	FDE	C3A-C2A-CAA-CBA
7	B	927	FDE	C3A-C2A-CAA-CBA
7	A	426	FDE	C2A-CAA-CBA-CGA
7	B	927	FDE	C2A-CAA-CBA-CGA
7	A	426	FDE	C3D-CAD-CBD-CGD
7	B	927	FDE	C3D-CAD-CBD-CGD

There are no ring outliers.

6 monomers are involved in 13 short contacts:

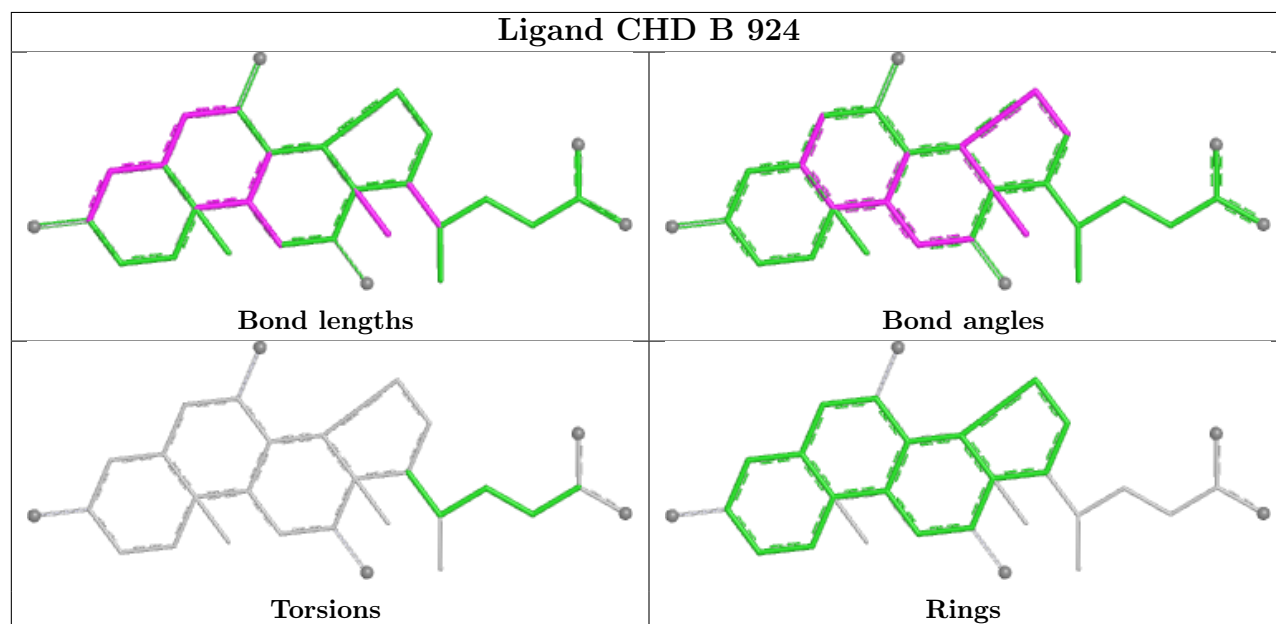
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	924	CHD	5	0
3	A	2	IMD	2	0

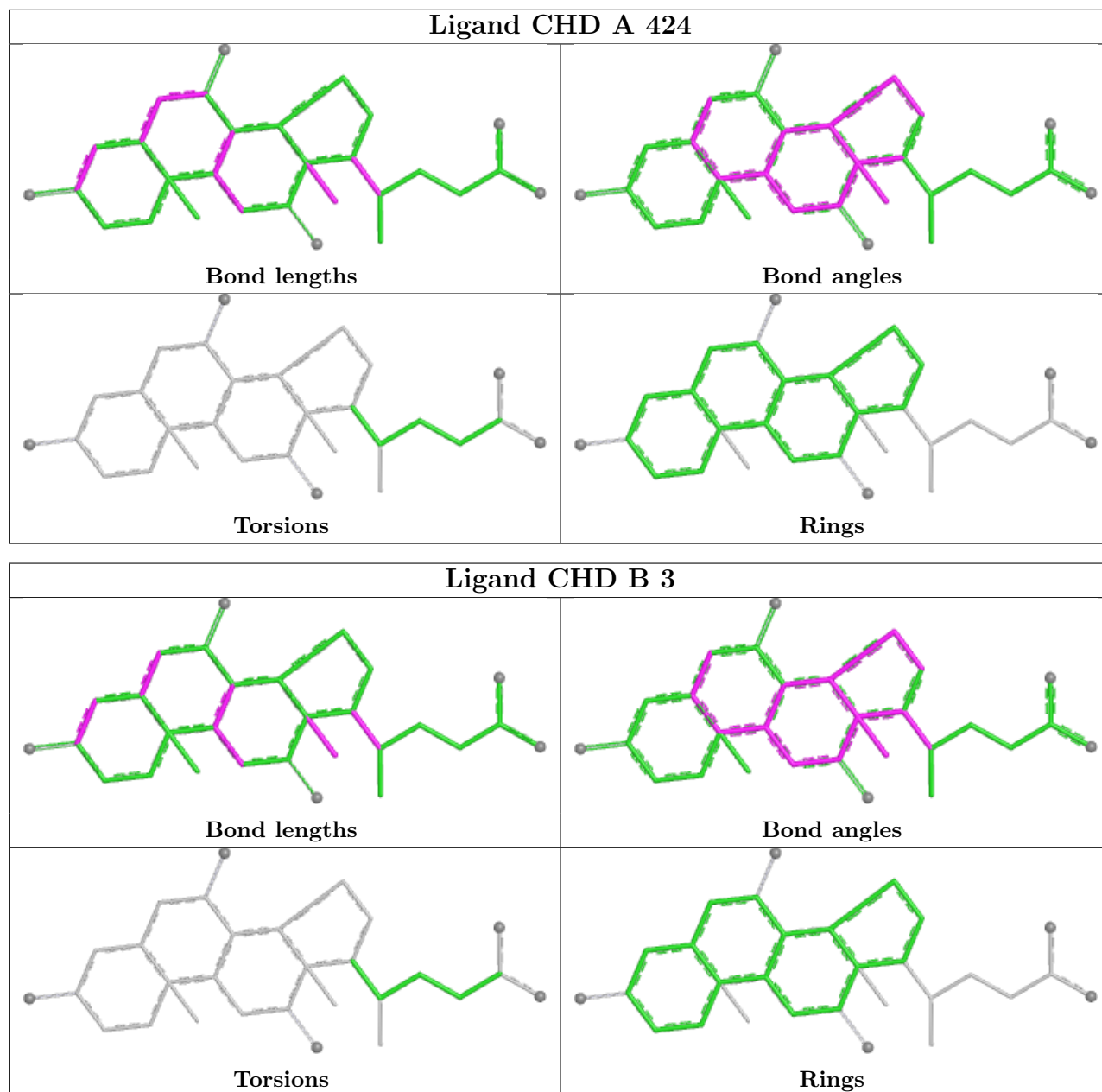
Continued on next page...

Continued from previous page...

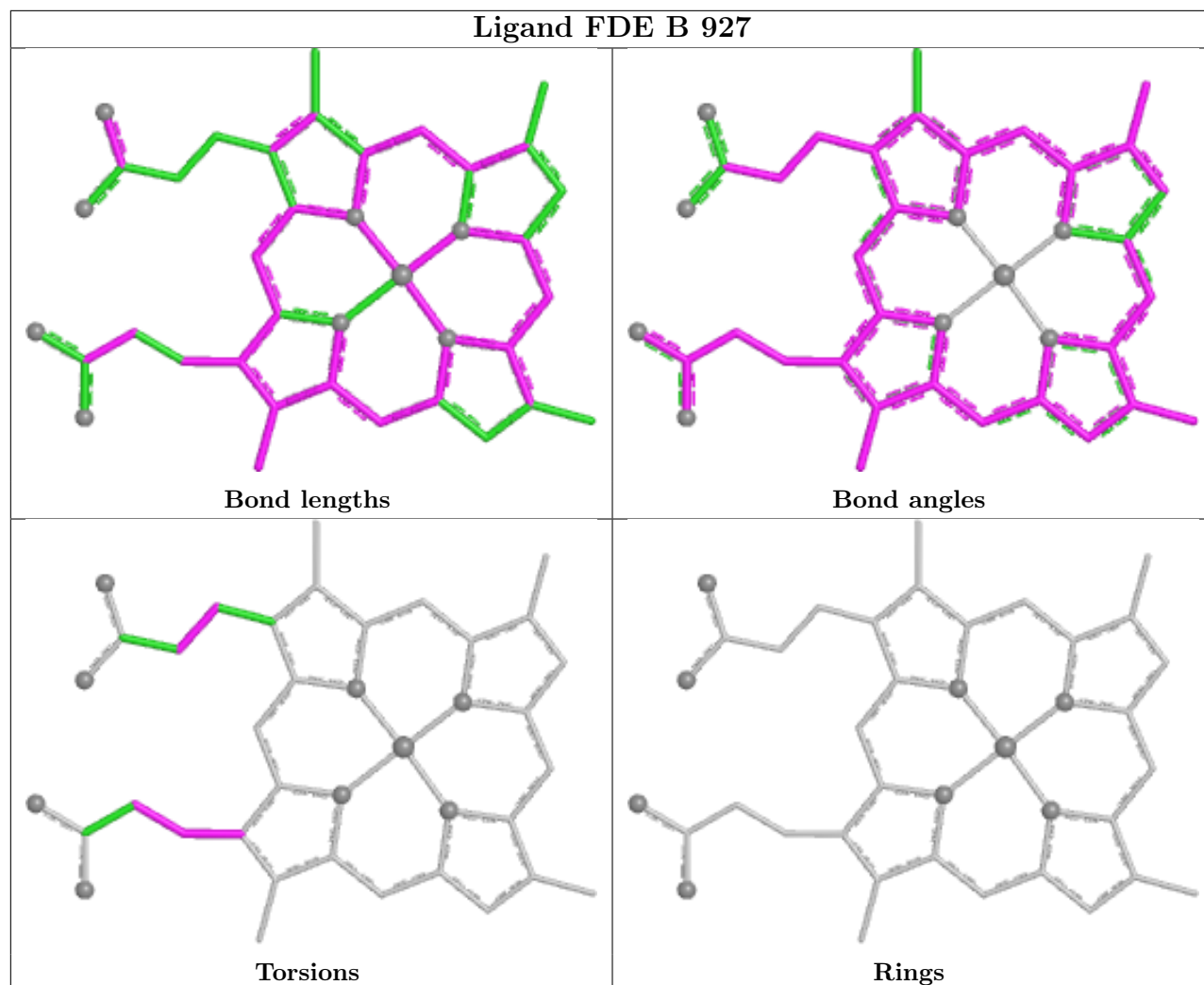
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	424	CHD	2	0
4	B	3	CHD	1	0
3	B	1	IMD	1	0
9	B	925	GOL	3	0

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.

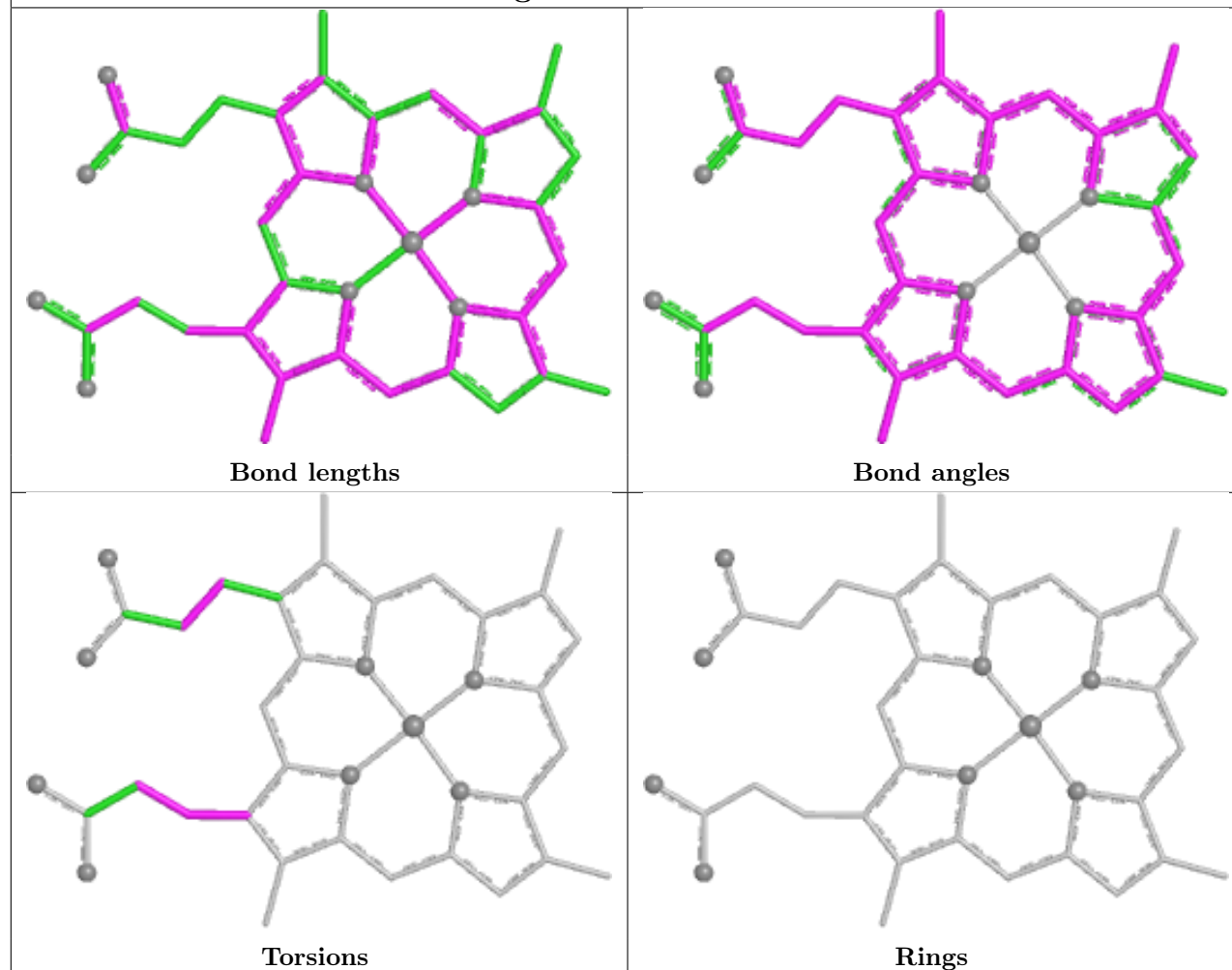




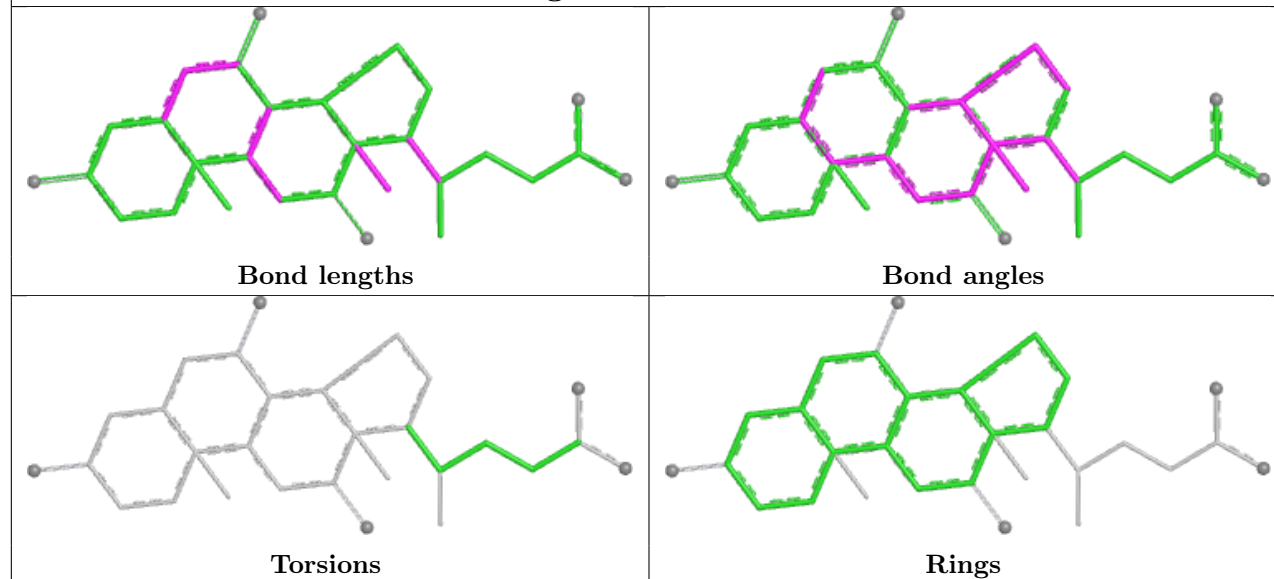
Ligand FDE B 927



Ligand FDE A 426



Ligand CHD A 4



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

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	359/359 (100%)	0.41	12 (3%)	49	46	8, 33, 56, 72	3 (0%)
1	B	359/359 (100%)	0.50	12 (3%)	49	46	9, 35, 59, 68	3 (0%)
All	All	718/718 (100%)	0.46	24 (3%)	49	46	8, 34, 58, 72	6 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	676[A]	GLU	6.9
1	A	178	GLU	4.7
1	A	304	LYS	4.6
1	B	712	GLN	4.0
1	A	305	VAL	3.9
1	A	423	LEU	3.8
1	B	923	LEU	3.5
1	A	359	GLU	3.5
1	B	713	VAL	3.4
1	A	372	ASN	3.4
1	A	213	VAL	3.3
1	A	212	GLN	2.8
1	A	253	ARG	2.7
1	B	715	ARG	2.6
1	B	610	PHE	2.6
1	A	65	ARG	2.3
1	B	857	ALA	2.3
1	B	862	VAL	2.3
1	B	714	GLY	2.2
1	A	214	GLY	2.2
1	B	612	ALA	2.2
1	B	804	LYS	2.1
1	A	175	GLU	2.1
1	B	848	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

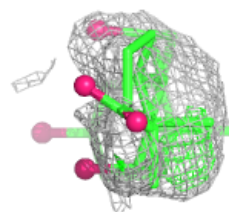
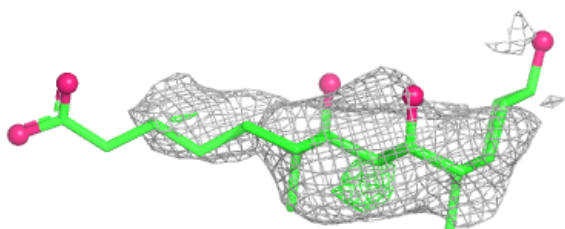
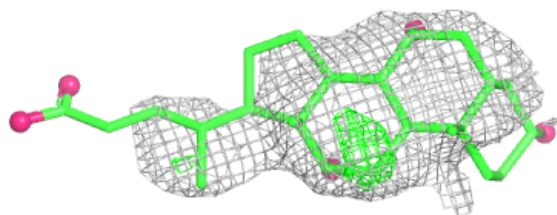
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CHD	A	4	29/29	0.75	0.24	117,118,120,120	0
8	SO4	A	427	5/5	0.75	0.13	92,92,93,93	0
5	OXY	A	425	2/2	0.77	0.21	44,44,44,46	0
4	CHD	A	424	29/29	0.78	0.25	76,78,87,88	0
4	CHD	B	924	29/29	0.80	0.19	53,58,71,72	0
4	CHD	B	3	29/29	0.81	0.19	73,74,83,85	0
8	SO4	B	2	5/5	0.81	0.11	85,85,86,86	0
5	OXY	B	926	2/2	0.85	0.20	44,44,44,44	0
9	GOL	B	925	6/6	0.85	0.17	35,36,38,39	0
3	IMD	B	1	5/5	0.95	0.08	28,29,30,31	0
3	IMD	A	2	5/5	0.95	0.10	26,27,28,28	0
7	FDE	A	426	39/39	0.97	0.07	21,26,36,39	0
7	FDE	B	927	39/39	0.97	0.08	17,26,37,41	0
2	FES	A	501	4/4	0.97	0.06	26,27,28,29	0
2	FES	B	502	4/4	0.97	0.07	26,27,28,28	0
6	CL	A	1	1/1	0.97	0.07	59,59,59,59	0

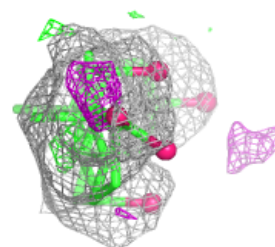
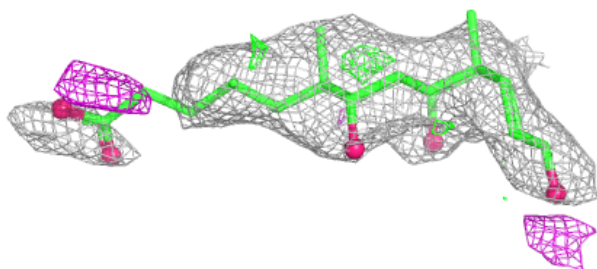
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD A 4:

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

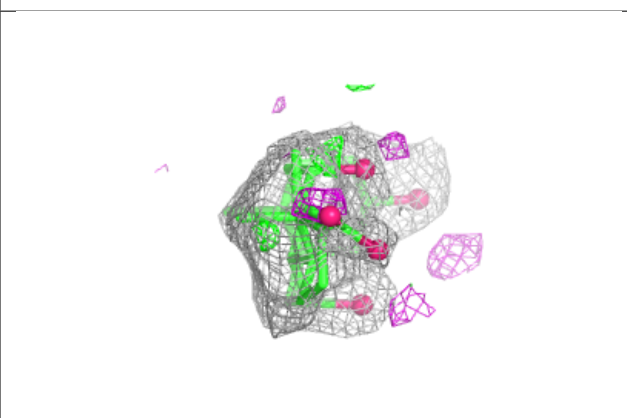
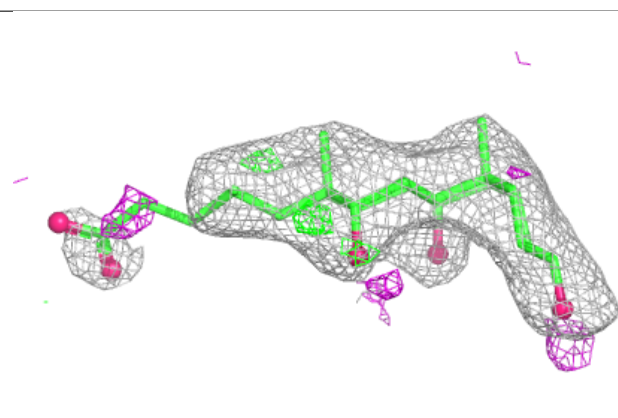
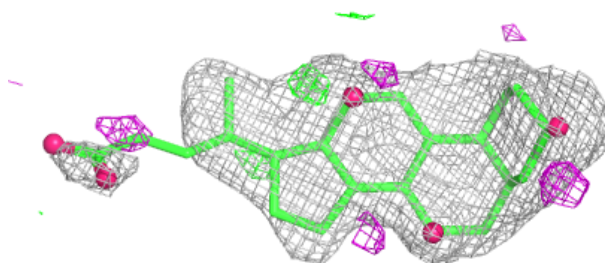
**Electron density around CHD A 424:**

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

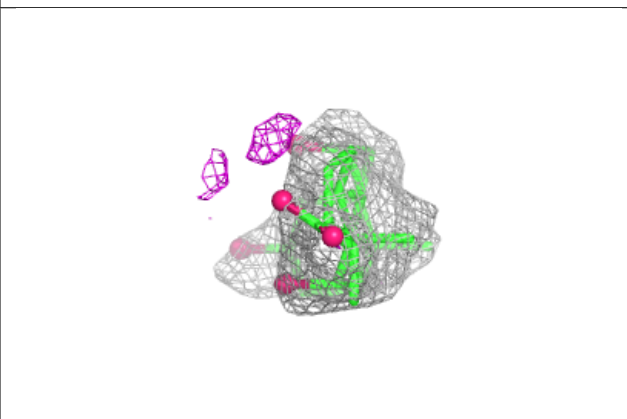
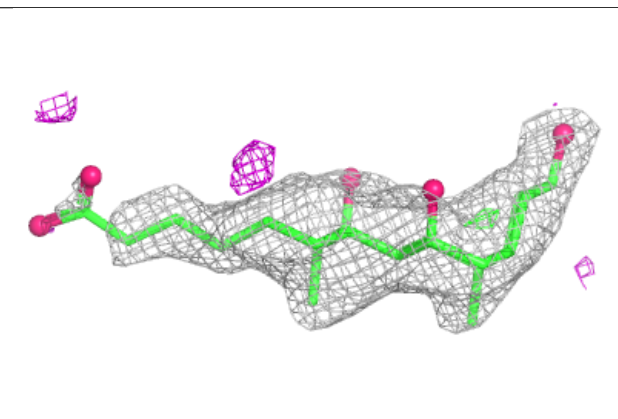
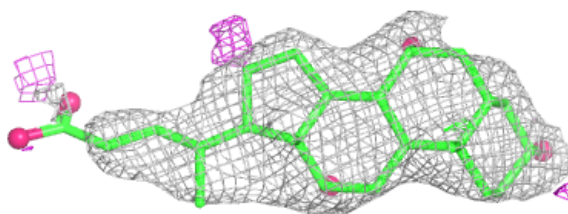


Electron density around CHD B 924:

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

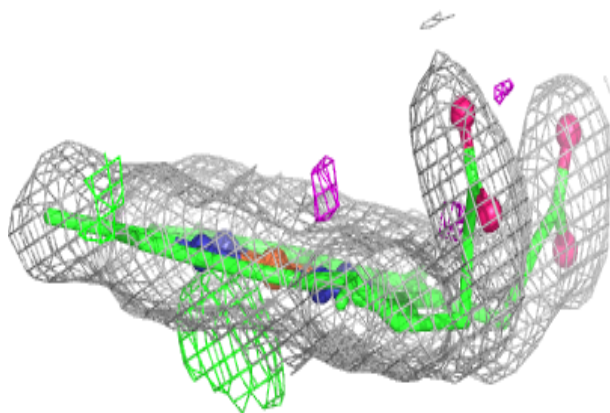
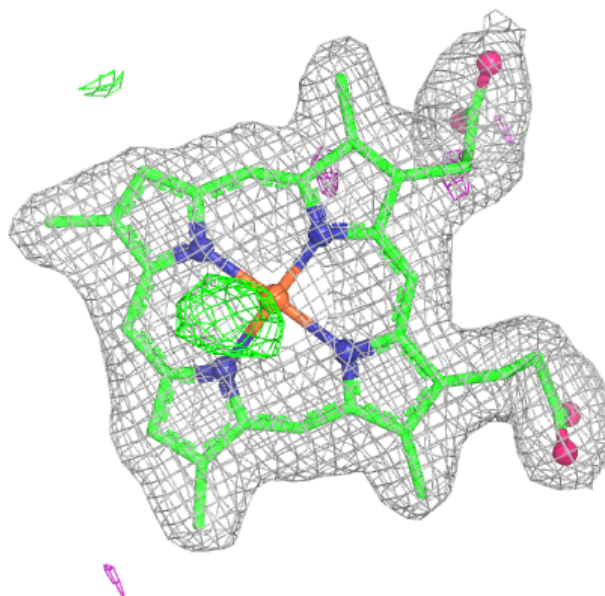
**Electron density around CHD B 3:**

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



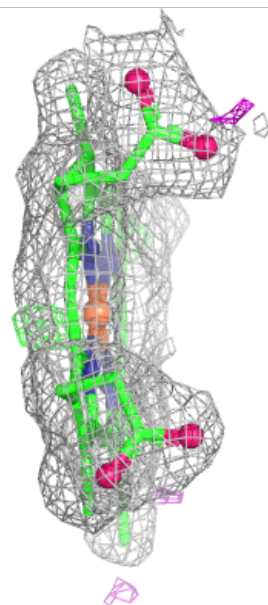
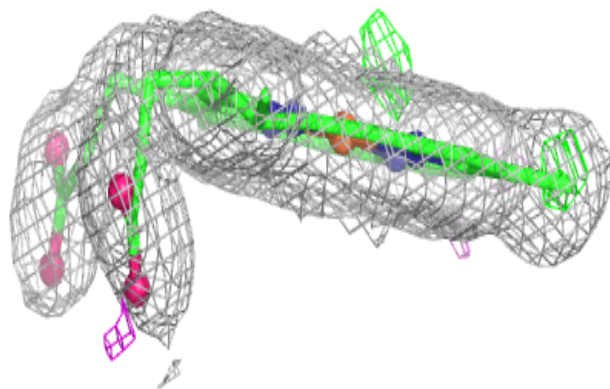
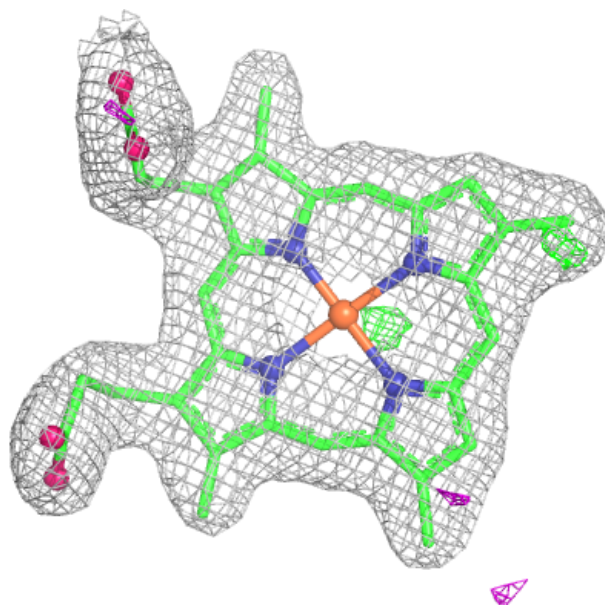
Electron density around FDE A 426:

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



Electron density around FDE B 927:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.