Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:12 pm BST

PDB ID	:	2QD5
Title	:	Structure of wild type human ferrochelatase in complex with a lead-porphyrin compound
Authors	:	Meldock, A.E.; Dailey, T.A.; Ross, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on	:	2007-06-20
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

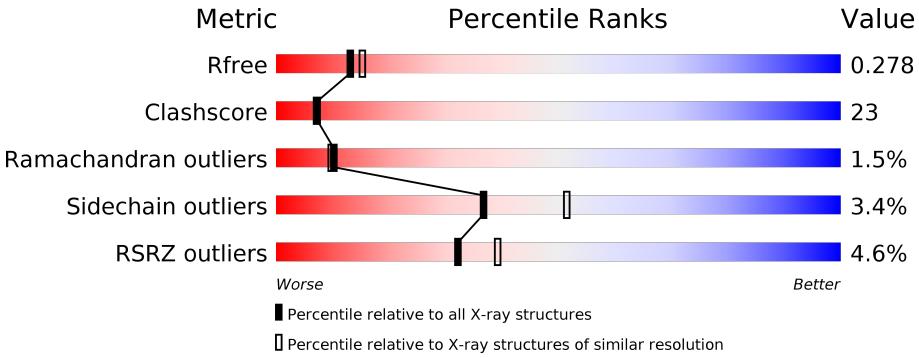
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% 60% 36% .
1	B	359	4% 67% 29% .

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
7	ACY	A	803	-	-	X	-
7	ACY	B	1106	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6253 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.

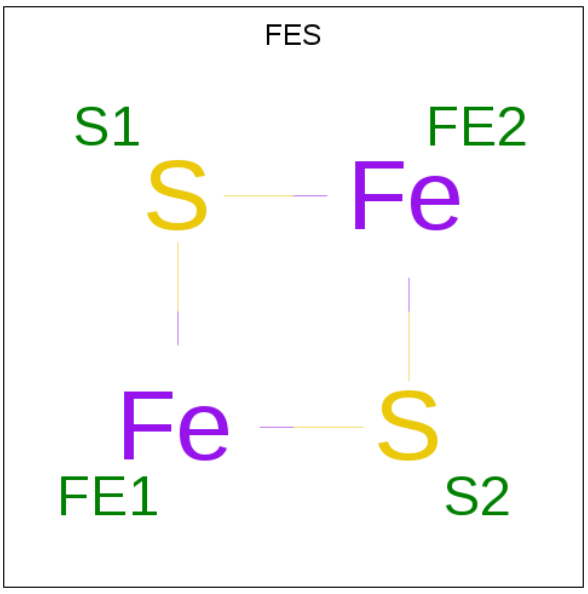
- Molecule 1 is a protein called Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	4	0
			2925	1861	508	537	19			
1	B	359	Total	C	N	O	S	0	3	0
			2917	1856	506	536	19			

- Molecule 2 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

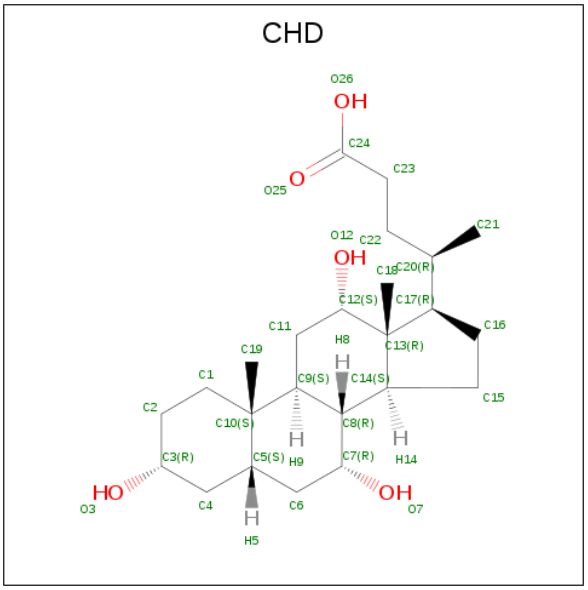
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Pb	0	1
			2	2		
2	A	1	Total	Pb	0	1
			2	2		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



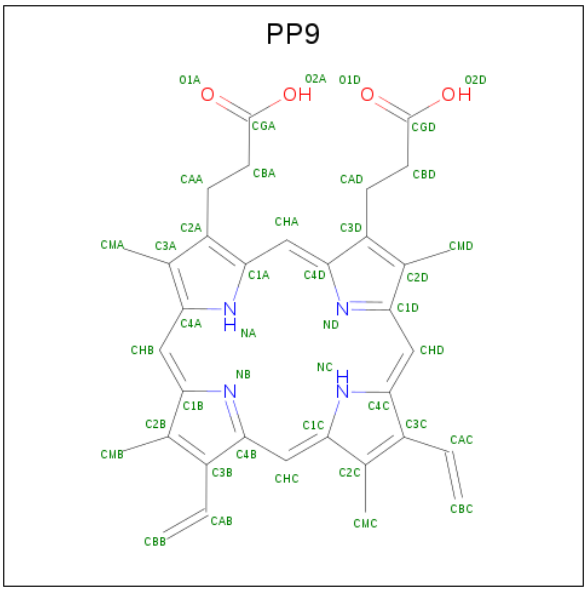
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0

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



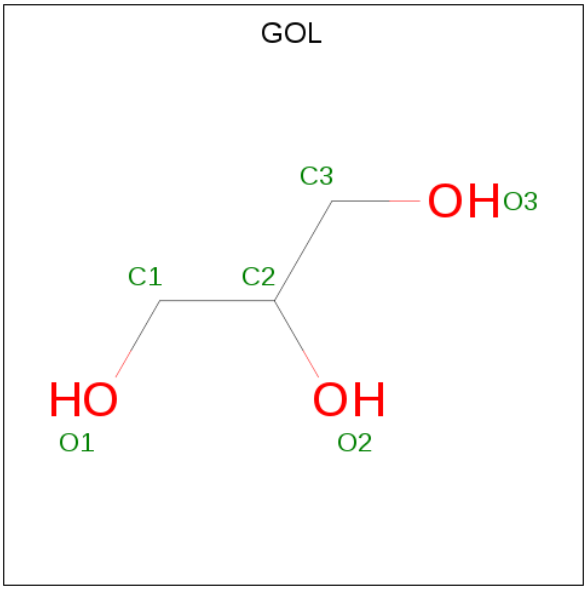
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 29 24 5	0	0
4	A	1	Total C O 29 24 5	0	0
4	B	1	Total C O 29 24 5	0	0
4	B	1	Total C O 29 24 5	0	0

- Molecule 5 is PROTOPORPHYRIN IX (three-letter code: PP9) (formula: $C_{34}H_{34}N_4O_4$).



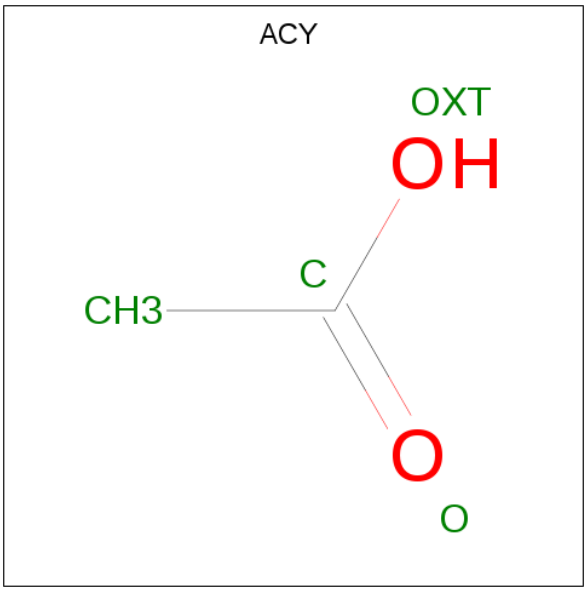
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			42	34	4	4		
5	B	1	Total	C	N	O	0	0
			42	34	4	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



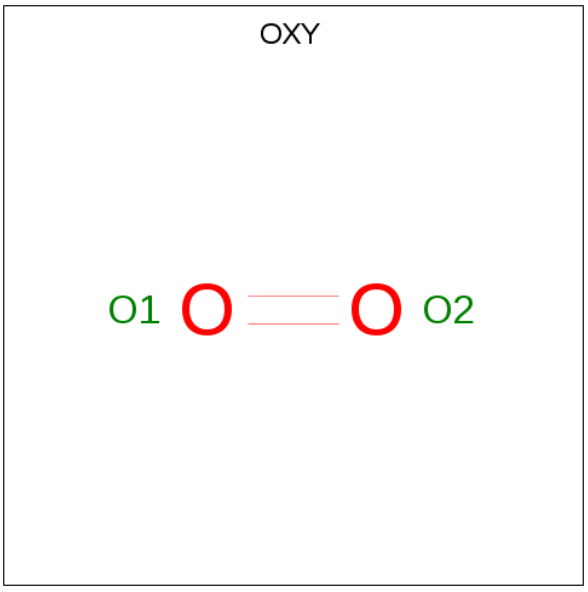
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



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

- Molecule 9 is water.

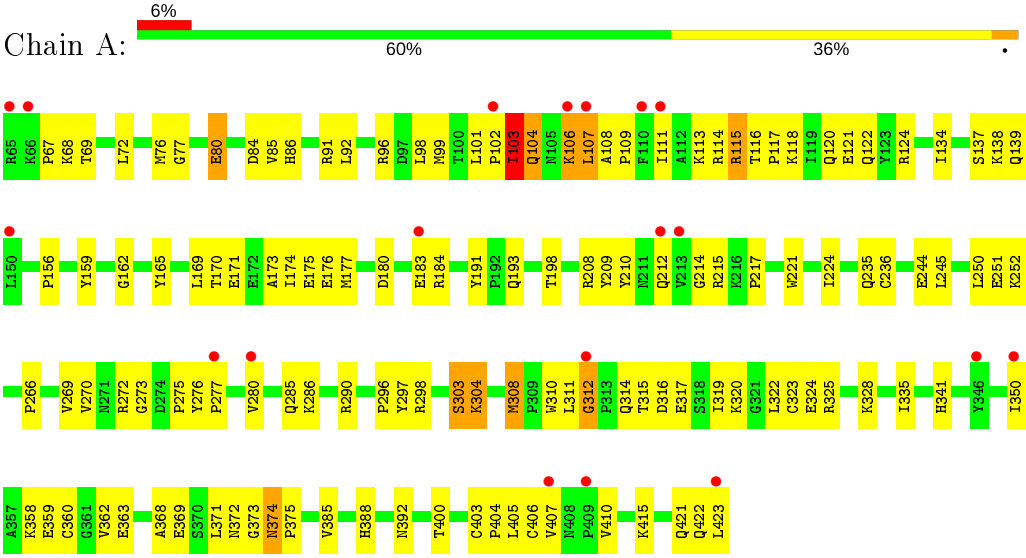
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	94	Total O 94 94	0	0
9	B	85	Total O 85 85	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

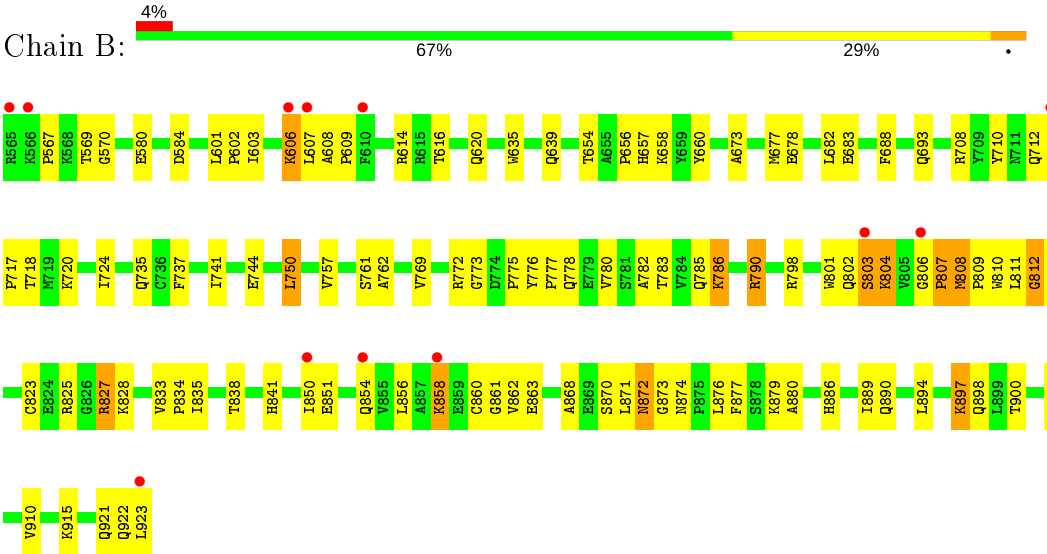
- Molecule 1: Ferrochelatase

Chain A:



- Molecule 1: Ferrochelatase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.22Å 92.81Å 109.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 2.30 47.25 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.26-2.30) 94.0 (47.25-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.280 0.238 , 0.278	Depositor DCC
R_{free} test set	4105 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6253	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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 51.84 % 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 5.2967e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CHD, OXY, PB, FES, PP9, ACY

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	0.37	0/2995	0.61	2/4056 (0.0%)
1	B	0.37	0/2987	0.60	1/4046 (0.0%)
All	All	0.37	0/5982	0.61	3/8102 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	ILE	N-CA-C	-5.32	96.64	111.00
1	A	103	ILE	N-CA-C	-5.23	96.89	111.00
1	B	724	ILE	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2925	0	2928	156	0
1	B	2917	0	2918	129	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	58	0	78	7	0
4	B	58	0	78	3	0
5	A	42	0	31	1	0
5	B	42	0	30	4	0
6	A	6	0	8	2	0
7	A	8	0	6	5	0
7	B	4	0	3	4	0
8	B	2	0	0	0	0
9	A	94	0	0	9	0
9	B	85	0	0	2	0
All	All	6253	0	6080	274	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 23.

All (274) 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)
5:B:1105:PP9:O1D	5:B:1105:PP9:CGD	1.64	1.46
5:B:1105:PP9:C2C	5:B:1105:PP9:C1C	1.74	1.38
1:A:311:LEU:HD12	1:A:312:GLY:H	1.16	1.04
1:B:811:LEU:HD12	1:B:812:GLY:H	1.23	1.01
1:A:285:GLN:HG2	1:B:778:GLN:HE22	1.31	0.95
1:A:285:GLN:HG3	1:B:782:ALA:HB2	1.50	0.93
1:A:297:TYR:H	1:B:898:GLN:HE22	1.17	0.91
1:A:115:ARG:HH12	4:A:701:CHD:H222	1.36	0.90
1:B:750:LEU:H	1:B:750:LEU:HD12	1.37	0.89
1:A:308[A]:MET:SD	4:A:701:CHD:H21	2.12	0.89
2:A:1101[A]:PB:PB	7:A:803:ACY:OXT	1.34	0.88
1:A:250:LEU:HD12	1:A:250:LEU:H	1.40	0.85
1:A:107:LEU:HD23	1:A:108:ALA:N	1.91	0.85
1:A:67:PRO:HA	1:A:156:PRO:HG2	1.58	0.84
1:A:303:SER:CB	7:A:803:ACY:H2	2.08	0.83
1:A:303:SER:HB2	7:A:803:ACY:H2	1.59	0.83
1:A:272:ARG:HD2	9:A:1130:HOH:O	1.77	0.82
1:A:311:LEU:HD12	1:A:312:GLY:N	1.94	0.81
1:B:757:VAL:HG21	1:B:827:ARG:HG2	1.60	0.81
1:B:708:ARG:NH2	1:B:910:VAL:HG21	1.96	0.80
1:B:790:ARG:HH11	1:B:790:ARG:HG2	1.44	0.80
1:B:814:GLN:HE21	1:B:816:ASP:HB2	1.45	0.80
1:B:601:LEU:HD21	4:B:1103:CHD:H151	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:O	1:A:141:GLU:HG3	1.83	0.79
1:A:350:ILE:O	1:A:354:GLN:HG3	1.84	0.78
1:B:811:LEU:CD1	1:B:812:GLY:H	1.97	0.78
1:B:806:GLY:HA3	9:B:1108:HOH:O	1.83	0.77
1:A:314:GLN:HB3	1:A:317:GLU:HG2	1.67	0.76
4:A:701:CHD:H151	4:A:702:CHD:H151	1.66	0.76
1:A:244:GLU:HG3	1:A:368:ALA:HA	1.68	0.74
1:A:103:ILE:O	1:A:107:LEU:HD22	1.88	0.74
1:A:311:LEU:CD1	1:A:312:GLY:H	1.99	0.74
1:A:171:GLU:O	1:A:175:GLU:HG3	1.88	0.73
1:B:744:GLU:HG3	1:B:868:ALA:HA	1.68	0.73
1:A:356:LEU:HD12	1:A:362:VAL:HG21	1.69	0.72
1:B:903:CYS:HB2	1:B:906:CYS:HB2	1.71	0.72
1:A:103:ILE:HD13	1:A:103:ILE:H	1.55	0.71
1:A:208:ARG:NH2	1:A:410:VAL:HG21	2.04	0.71
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.06	0.70
1:A:68:LYS:HD2	1:A:183:GLU:HB2	1.73	0.70
1:B:639:GLN:HE21	1:B:873:GLY:HA2	1.56	0.70
1:A:285:GLN:HG3	1:B:782:ALA:CB	2.22	0.70
1:A:208:ARG:HH22	1:A:410:VAL:HG21	1.56	0.70
1:B:757:VAL:CG2	1:B:827:ARG:HG2	2.22	0.70
1:B:750:LEU:CD1	1:B:750:LEU:H	2.05	0.69
1:B:735:GLN:HG3	1:B:790:ARG:NH2	2.07	0.69
1:A:351:GLU:H	1:A:351:GLU:CD	1.95	0.69
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.05	0.69
1:B:856:LEU:HG	1:B:862:VAL:HG21	1.75	0.69
1:B:897:LYS:HB2	1:B:897:LYS:NZ	2.07	0.69
1:B:811:LEU:HD12	1:B:812:GLY:N	2.04	0.69
1:A:107:LEU:HD23	1:A:108:ALA:H	1.59	0.68
1:B:735:GLN:HG3	1:B:790:ARG:HH22	1.59	0.67
1:B:823:CYS:SG	1:B:862:VAL:HG22	2.34	0.67
1:B:608:ALA:HB3	1:B:609:PRO:HD3	1.77	0.67
1:B:673:ALA:O	1:B:677:MET:HG3	1.95	0.66
1:B:850:ILE:O	1:B:854:GLN:HG3	1.95	0.66
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.76	0.66
1:A:139:GLN:HE21	1:A:373:GLY:HA2	1.61	0.66
5:B:1105:PP9:C2C	5:B:1105:PP9:CHC	2.67	0.64
1:B:683:GLU:O	1:B:720:LYS:HG2	1.97	0.64
1:B:804:LYS:HZ3	1:B:814:GLN:HB2	1.62	0.64
1:A:374:ASN:HD22	1:A:375:PRO:HD2	1.62	0.64
1:A:85:VAL:HG21	1:A:120:GLN:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:NE2	1:A:373:GLY:HA2	2.13	0.63
1:A:314:GLN:HE21	1:A:316:ASP:HB2	1.63	0.63
1:B:710:TYR:HA	1:B:713:VAL:HG12	1.81	0.63
1:A:208:ARG:NH1	1:A:410:VAL:HG11	2.14	0.63
1:B:713:VAL:O	1:B:715:ARG:HG2	1.98	0.63
1:B:603:ILE:HG13	1:B:603:ILE:O	1.98	0.62
1:A:374:ASN:HD22	1:A:375:PRO:N	1.96	0.62
1:A:86:HIS:NE2	1:A:113:LYS:HG2	2.14	0.62
1:B:803:SER:C	1:B:804:LYS:HG3	2.19	0.62
1:B:841:HIS:HB2	5:B:1105:PP9:O2D	1.98	0.62
1:B:804:LYS:HD2	1:B:814:GLN:HG3	1.81	0.61
1:A:277:PRO:HB3	6:A:601:GOL:H2	1.82	0.61
1:B:811:LEU:CG	1:B:812:GLY:N	2.63	0.61
1:A:298:ARG:NH1	1:B:773:GLY:O	2.33	0.61
1:B:735:GLN:HA	1:B:790:ARG:NH1	2.15	0.61
1:A:311:LEU:CD1	1:A:312:GLY:N	2.61	0.61
1:A:320:LYS:HG3	1:A:356:LEU:HD21	1.84	0.60
1:A:303:SER:HB3	7:A:803:ACY:H2	1.81	0.60
1:B:639:GLN:NE2	1:B:873:GLY:HA2	2.16	0.60
1:B:811:LEU:O	1:B:812:GLY:O	2.19	0.60
1:A:80:GLU:HG3	1:A:84:ASP:OD2	2.02	0.60
1:B:808[A]:MET:HB2	1:B:809:PRO:HD2	1.82	0.60
1:A:115:ARG:HA	9:A:1120:HOH:O	2.01	0.60
1:B:858:LYS:HE2	1:B:858:LYS:HA	1.83	0.60
1:A:403:CYS:HB2	1:A:406:CYS:HB2	1.83	0.59
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.85	0.59
1:B:790:ARG:NH1	1:B:790:ARG:HG2	2.14	0.58
1:B:874:ASN:ND2	1:B:876:LEU:HB3	2.19	0.58
1:A:145:LYS:HB3	9:A:1142:HOH:O	2.02	0.58
1:B:900:THR:O	1:B:915:LYS:HE2	2.04	0.58
1:A:69:THR:HG23	1:A:184:ARG:HD2	1.86	0.58
1:B:811:LEU:HG	1:B:812:GLY:N	2.17	0.58
1:A:103:ILE:O	1:A:107:LEU:CD2	2.53	0.57
1:B:886:HIS:O	1:B:890:GLN:HG2	2.05	0.57
1:A:244:GLU:CG	1:A:368:ALA:HA	2.34	0.57
1:A:170:THR:O	1:A:174:ILE:HG13	2.04	0.57
1:B:811:LEU:CD1	1:B:812:GLY:N	2.65	0.57
1:B:804:LYS:H	7:B:1106:ACY:H1	1.69	0.57
1:A:115:ARG:HH11	1:A:115:ARG:HG2	1.69	0.56
1:A:356:LEU:O	1:A:362:VAL:HG23	2.04	0.56
1:A:285:GLN:HG2	1:B:778:GLN:NE2	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:CG	1:A:312:GLY:N	2.68	0.56
1:B:922:GLN:HG2	1:B:923:LEU:HD22	1.87	0.56
1:B:823:CYS:HB3	1:B:860:CYS:HB3	1.88	0.56
1:B:851[A]:GLU:H	1:B:851[A]:GLU:CD	2.08	0.55
1:A:191:TYR:CZ	1:A:198:THR:HB	2.41	0.55
1:A:255:GLU:O	1:A:255:GLU:HG2	2.07	0.55
1:A:116:THR:N	1:A:117:PRO:CD	2.69	0.55
1:B:803:SER:HB3	7:B:1106:ACY:OXT	2.06	0.55
1:A:311:LEU:O	1:A:312:GLY:O	2.24	0.55
1:B:580[B]:GLU:HG3	1:B:584:ASP:OD2	2.07	0.55
1:A:296:PRO:HD3	1:B:897:LYS:HD2	1.89	0.55
1:A:275:PRO:HD3	1:B:798:ARG:HH12	1.70	0.55
1:A:323:CYS:SG	1:A:362:VAL:HG22	2.46	0.55
1:A:85:VAL:HG12	1:A:116:THR:HG23	1.89	0.55
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.88	0.54
1:B:828:LYS:HB3	1:B:863:GLU:H	1.73	0.54
1:A:308[A]:MET:HE3	1:A:310:TRP:NE1	2.22	0.54
1:A:245:LEU:HB3	1:A:253:ARG:NH1	2.22	0.54
1:B:606:LYS:HB3	1:B:606:LYS:NZ	2.21	0.54
1:B:804:LYS:CD	1:B:814:GLN:HG3	2.37	0.54
1:B:750:LEU:N	1:B:750:LEU:HD12	2.16	0.54
1:A:99:MET:HB2	4:A:701:CHD:C19	2.37	0.54
1:B:922:GLN:HG2	1:B:923:LEU:CD2	2.37	0.54
1:A:173:ALA:O	1:A:177:MET:HG3	2.07	0.53
1:A:96:ARG:HA	1:A:99:MET:O	2.07	0.53
1:A:297:TYR:N	1:B:898:GLN:HE22	1.95	0.53
1:A:212:GLN:OE1	1:A:212:GLN:HA	2.08	0.53
1:A:308[A]:MET:CE	1:A:310:TRP:HE1	2.22	0.53
1:A:358:LYS:O	1:A:358:LYS:HD3	2.09	0.53
1:A:98:LEU:HD13	7:A:801:ACY:H3	1.91	0.53
1:B:922:GLN:O	1:B:923:LEU:HB2	2.09	0.53
1:B:874:ASN:HD22	1:B:876:LEU:HB3	1.73	0.53
1:B:616:THR:O	1:B:620:GLN:HG3	2.09	0.52
1:A:253:ARG:HD2	9:A:1115:HOH:O	2.09	0.52
1:B:783:THR:HG22	1:B:835:ILE:HD11	1.91	0.52
1:A:328:LYS:HB3	1:A:363:GLU:HG2	1.91	0.52
1:A:400:THR:O	1:A:415:LYS:HE2	2.09	0.52
1:A:250:LEU:CD1	1:A:250:LEU:H	2.16	0.51
1:A:266:PRO:HB3	1:A:308[A]:MET:HE3	1.91	0.51
1:A:114:ARG:HH12	4:A:702:CHD:H42	1.75	0.51
1:A:350:ILE:HG13	1:A:351:GLU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:PRO:HA	1:B:656:PRO:HG2	1.91	0.51
1:A:422:GLN:O	1:A:423:LEU:HB2	2.10	0.51
1:B:744:GLU:CG	1:B:868:ALA:HA	2.39	0.51
1:B:897:LYS:HB2	1:B:897:LYS:HZ3	1.75	0.50
1:B:602:PRO:O	1:B:607:LEU:HD12	2.12	0.50
1:A:114:ARG:NH1	4:A:702:CHD:H42	2.26	0.50
1:B:735:GLN:HG3	1:B:790:ARG:CZ	2.42	0.50
1:A:374:ASN:ND2	1:A:375:PRO:HD2	2.26	0.49
1:B:804:LYS:NZ	1:B:814:GLN:HB2	2.27	0.49
1:B:870:SER:HB2	1:B:872:ASN:ND2	2.27	0.49
1:A:116:THR:O	1:A:120:GLN:HG3	2.13	0.49
1:A:273:GLY:HA3	1:A:404:PRO:HD2	1.94	0.49
1:A:221:TRP:O	1:A:421:GLN:HG3	2.12	0.49
1:A:422:GLN:HG2	1:A:423:LEU:HD22	1.95	0.49
1:A:208:ARG:HH12	1:A:410:VAL:HG11	1.78	0.48
1:A:285:GLN:CG	1:B:778:GLN:HE22	2.13	0.48
1:A:308[A]:MET:HE2	1:A:310:TRP:HE1	1.78	0.48
1:B:762:ALA:O	1:B:801:TRP:HA	2.13	0.48
1:A:304:LYS:HE2	1:A:310:TRP:HB2	1.95	0.48
1:B:856:LEU:HG	1:B:862:VAL:CG2	2.44	0.48
1:B:737:PHE:O	1:B:741:ILE:HG13	2.13	0.48
1:B:894:LEU:HD22	1:B:921:GLN:HB2	1.96	0.48
1:A:106:LYS:O	1:A:109:PRO:HD2	2.13	0.48
1:B:801:TRP:N	1:B:801:TRP:CD1	2.81	0.48
1:A:103:ILE:HG12	1:A:103:ILE:O	2.13	0.47
1:B:790:ARG:NH1	1:B:790:ARG:CG	2.77	0.47
1:B:803:SER:CB	7:B:1106:ACY:OXT	2.62	0.47
1:B:772:ARG:HA	1:B:905:LEU:HB2	1.96	0.47
1:A:355:VAL:HG13	1:A:359:GLU:OE2	2.13	0.47
1:A:236:CYS:HB3	1:A:371:LEU:HD22	1.96	0.47
1:A:298:ARG:HH12	1:B:775:PRO:HD3	1.78	0.47
1:A:175:GLU:HG2	1:A:209:TYR:OH	2.14	0.47
1:A:252:LYS:HA	1:A:255:GLU:OE2	2.15	0.47
1:A:335:ILE:O	1:A:335:ILE:HG13	2.15	0.47
1:A:72:LEU:HD11	1:A:162:GLY:HA3	1.97	0.47
1:A:275:PRO:HD3	1:B:798:ARG:NH1	2.29	0.46
1:A:351:GLU:HA	1:A:354:GLN:CD	2.35	0.46
1:A:176:GLU:HG2	1:A:180:ASP:OD2	2.16	0.46
1:A:212:GLN:C	1:A:214:GLY:N	2.67	0.46
1:A:341:HIS:HB2	5:A:901:PP9:O2D	2.16	0.46
1:B:735:GLN:HG3	1:B:790:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:HG3	1:A:77:GLY:O	2.15	0.46
1:B:838:THR:HG22	1:B:871:LEU:HD12	1.96	0.46
1:A:374:ASN:C	1:A:374:ASN:HD22	2.17	0.46
1:A:99:MET:HB2	4:A:701:CHD:H191	1.96	0.46
1:A:191:TYR:CE1	1:A:198:THR:HB	2.51	0.46
1:B:769:VAL:O	1:B:772:ARG:HG2	2.16	0.46
1:A:210:TYR:CE2	1:A:217:PRO:HA	2.52	0.46
1:A:311:LEU:HG	1:A:312:GLY:N	2.29	0.46
1:B:677:MET:HB3	1:B:682:LEU:HD12	1.97	0.46
1:B:827:ARG:HG3	9:B:1157:HOH:O	2.16	0.45
1:A:103:ILE:N	1:A:103:ILE:HD13	2.26	0.45
1:A:92:LEU:HD23	1:A:92:LEU:C	2.36	0.45
1:A:270:VAL:HG12	1:B:812:GLY:HA2	1.98	0.45
1:B:635:TRP:HA	1:B:635:TRP:CE3	2.51	0.45
1:B:570:GLY:HA3	1:B:682:LEU:HD13	1.98	0.45
1:B:858:LYS:CE	1:B:858:LYS:HA	2.45	0.45
1:B:897:LYS:HZ2	1:B:897:LYS:HB2	1.79	0.45
1:A:134:ILE:O	1:A:138[B]:LYS:HG2	2.17	0.45
1:A:369[B]:GLU:HG2	9:A:1113:HOH:O	2.15	0.45
1:B:654:THR:OG1	1:B:657:HIS:NE2	2.48	0.45
1:B:708:ARG:CZ	1:B:910:VAL:HG21	2.46	0.45
1:B:828:LYS:HD3	1:B:861:GLY:O	2.16	0.45
1:B:876:LEU:HD12	1:B:879:LYS:HD3	1.98	0.45
1:A:303:SER:C	1:A:304:LYS:HG3	2.37	0.45
1:B:804:LYS:HZ2	1:B:814:GLN:HA	1.81	0.44
1:A:107:LEU:O	1:A:111:ILE:HG13	2.17	0.44
1:A:115:ARG:NH1	1:A:115:ARG:HG2	2.32	0.44
1:B:715:ARG:H	1:B:715:ARG:HG2	1.62	0.44
1:B:810:TRP:CZ3	7:B:1106:ACY:H3	2.53	0.44
1:A:101:LEU:H	1:A:104:GLN:NE2	2.16	0.44
1:B:851[A]:GLU:N	1:B:851[A]:GLU:CD	2.71	0.43
1:B:761:SER:OG	1:B:802:GLN:HB3	2.18	0.43
1:B:877:PHE:O	1:B:880:ALA:HB3	2.18	0.43
1:A:286:LYS:HZ1	1:B:786:LYS:HE2	1.84	0.43
1:B:569:THR:OG1	1:B:654:THR:HB	2.18	0.43
1:A:322:LEU:HG	1:B:904:PRO:HB3	1.99	0.43
1:A:106:LYS:HA	1:A:106:LYS:NZ	2.33	0.43
1:A:266:PRO:HG2	1:A:269:VAL:HG23	2.00	0.43
1:A:107:LEU:HD23	1:A:107:LEU:C	2.38	0.43
1:A:91:ARG:HD2	1:A:165:TYR:O	2.19	0.43
1:B:693:GLN:HG2	1:B:780:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:VAL:HA	1:B:834:PRO:HD3	1.93	0.43
1:A:320:LYS:HA	1:A:356:LEU:HD11	2.01	0.43
1:B:602:PRO:O	1:B:603:ILE:C	2.57	0.43
1:B:658:LYS:HD3	1:B:660:TYR:OH	2.19	0.43
1:A:272:ARG:HA	1:A:405:LEU:HB2	2.01	0.43
1:B:678:GLU:OE2	1:B:718:THR:HG23	2.19	0.43
1:A:103:ILE:CD1	1:A:107:LEU:HD13	2.49	0.42
1:A:141:GLU:O	1:A:145:LYS:HG2	2.18	0.42
1:A:323:CYS:HB3	1:A:360:CYS:HB3	2.02	0.42
1:A:117:PRO:HD2	9:A:1120:HOH:O	2.18	0.42
1:A:320:LYS:HE2	1:A:324:GLU:OE2	2.20	0.42
1:B:858:LYS:HE2	1:B:858:LYS:CA	2.48	0.42
1:B:654:THR:HG21	1:B:889:ILE:HG21	2.01	0.42
1:A:259:LEU:HD23	1:A:298:ARG:HB2	2.00	0.42
1:A:208:ARG:CZ	1:A:410:VAL:HG21	2.49	0.42
1:A:103:ILE:H	1:A:103:ILE:CD1	2.28	0.42
1:A:104:GLN:HE21	1:A:104:GLN:HB2	1.55	0.42
1:A:270:VAL:O	1:B:813:PRO:HD3	2.20	0.42
1:B:825:ARG:HH11	1:B:825:ARG:HG3	1.84	0.42
1:A:80:GLU:H	1:A:80:GLU:HG2	1.44	0.41
1:B:712:GLN:C	1:B:714:GLY:H	2.24	0.41
1:A:210:TYR:HE2	1:A:217:PRO:HA	1.85	0.41
1:B:614:ARG:HH11	1:B:614:ARG:HG2	1.85	0.41
1:B:712:GLN:HA	1:B:712:GLN:OE1	2.20	0.41
1:A:121:GLU:CD	1:A:124:ARG:HH21	2.24	0.41
1:A:385:VAL:O	1:A:388:HIS:HB3	2.20	0.41
1:A:106:LYS:C	1:A:109:PRO:HD2	2.41	0.41
1:A:139:GLN:HG3	9:A:1177:HOH:O	2.21	0.41
1:B:808[A]:MET:CB	1:B:809:PRO:HD2	2.51	0.41
1:A:118:LYS:O	1:A:122:GLN:HG2	2.21	0.41
6:A:601:GOL:H31	1:B:777:PRO:HB2	2.03	0.41
1:B:823:CYS:HB3	1:B:860:CYS:CB	2.51	0.41
1:A:91:ARG:NH2	1:A:169:LEU:HD11	2.36	0.41
1:B:808[A]:MET:CE	4:B:1103:CHD:H21	2.51	0.41
1:A:215:ARG:HA	1:A:215:ARG:HD3	1.82	0.40
1:A:171:GLU:N	1:A:171:GLU:OE1	2.24	0.40
1:B:808[A]:MET:SD	4:B:1103:CHD:H112	2.61	0.40
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.87	0.40
9:A:1128:HOH:O	1:B:785:GLN:HG2	2.22	0.40
1:A:159:TYR:C	1:A:159:TYR:CD1	2.95	0.40
1:A:193:GLN:HG2	1:A:280:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:H	1:A:251:GLU:CD	2.24	0.40
1:A:315:THR:O	1:A:319:ILE:HG13	2.21	0.40
1:A:407:VAL:O	1:A:407:VAL:HG23	2.21	0.40
1:B:716:LYS:HB2	1:B:717:PRO:HD2	2.02	0.40
9:A:1128:HOH:O	1:B:785:GLN:CG	2.68	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	361/359 (101%)	332 (92%)	24 (7%)	5 (1%)	11	11
1	B	360/359 (100%)	336 (93%)	18 (5%)	6 (2%)	9	8
All	All	721/718 (100%)	668 (93%)	42 (6%)	11 (2%)	10	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PRO
1	A	312	GLY
1	A	372	ASN
1	B	812	GLY
1	B	872	ASN
1	A	304	LYS
1	B	804	LYS
1	A	303	SER
1	B	803	SER
1	B	807	PRO
1	B	714	GLY

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	328/324 (101%)	316 (96%)	12 (4%)	34	48
1	B	327/324 (101%)	315 (96%)	12 (4%)	34	48
All	All	655/648 (101%)	631 (96%)	24 (4%)	37	48

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	103	ILE
1	A	104	GLN
1	A	106	LYS
1	A	107	LEU
1	A	115	ARG
1	A	255	GLU
1	A	308[A]	MET
1	A	308[B]	MET
1	A	356	LEU
1	A	374	ASN
1	A	392	ASN
1	B	606	LYS
1	B	688	PHE
1	B	715	ARG
1	B	750	LEU
1	B	786	LYS
1	B	790	ARG
1	B	807	PRO
1	B	808[A]	MET
1	B	808[B]	MET
1	B	827	ARG
1	B	858	LYS
1	B	897	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	153	ASN
1	A	211	ASN
1	A	285	GLN
1	A	302	GLN
1	A	314	GLN
1	A	354	GLN
1	A	374	ASN
1	B	653	ASN
1	B	711	ASN
1	B	735	GLN
1	B	778	GLN
1	B	814	GLN
1	B	874	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\#\|Z\|>2$
8	OXY	B	1001	-	1,1,1	1.27	0	-		
5	PP9	A	901	-	34,46,46	5.39	16 (47%)	33,68,68	2.54	14 (42%)
7	ACY	A	801	-	1,3,3	1.91	0	0,3,3	0.00	-
5	PP9	B	1105	-	34,46,46	5.28	20 (58%)	33,68,68	2.92	15 (45%)
4	CHD	B	1103	-	29,32,32	2.03	12 (41%)	48,51,51	1.87	17 (35%)
6	GOL	A	601	-	5,5,5	0.10	0	5,5,5	0.13	0
4	CHD	A	701	-	29,32,32	1.97	10 (34%)	48,51,51	1.85	15 (31%)
7	ACY	A	803	-	1,3,3	1.91	0	0,3,3	0.00	-
4	CHD	B	1104	-	29,32,32	2.05	13 (44%)	48,51,51	1.79	17 (35%)
3	FES	A	501	-	0,4,4	0.00	-	-		
4	CHD	A	702	-	29,32,32	2.02	13 (44%)	48,51,51	1.78	16 (33%)
7	ACY	B	1106	-	1,3,3	1.87	0	0,3,3	0.00	-
3	FES	B	502	-	0,4,4	0.00	-	-		

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	1103	-	-	1/7/74/74	0/4/4/4
5	PP9	A	901	-	-	2/20/62/62	0/4/5/5
5	PP9	B	1105	-	-	3/20/62/62	0/4/5/5
6	GOL	A	601	-	-	2/4/4/4	-
4	CHD	A	701	-	-	1/7/74/74	0/4/4/4
4	CHD	B	1104	-	-	3/7/74/74	0/4/4/4
3	FES	A	501	-	-	-	0/1/1/1
4	CHD	A	702	-	-	2/7/74/74	0/4/4/4
3	FES	B	502	-	-	-	0/1/1/1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	PP9	CHD-C1D	19.83	1.51	1.35
5	B	1105	PP9	CHD-C1D	17.03	1.49	1.35
5	A	901	PP9	C1D-ND	-14.60	1.07	1.38
5	B	1105	PP9	C1D-ND	-12.10	1.12	1.38
5	B	1105	PP9	C3B-C2B	9.85	1.57	1.37
5	B	1105	PP9	CHC-C4B	9.37	1.42	1.35
5	A	901	PP9	C3B-C2B	8.75	1.55	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1105	PP9	C4A-C3A	8.41	1.61	1.42
5	A	901	PP9	C1D-C2D	7.61	1.62	1.45
5	A	901	PP9	CHC-C4B	7.45	1.41	1.35
5	B	1105	PP9	C4A-NA	-6.80	1.16	1.38
5	A	901	PP9	C4A-C3A	6.38	1.57	1.42
5	B	1105	PP9	C2A-C3A	5.49	1.53	1.37
5	B	1105	PP9	C3C-CAC	-5.40	1.36	1.47
5	A	901	PP9	C2A-C3A	5.14	1.52	1.37
5	A	901	PP9	C3C-CAC	-5.07	1.37	1.47
5	B	1105	PP9	C1D-C2D	4.98	1.56	1.45
5	B	1105	PP9	C3D-C2D	4.31	1.45	1.36
5	A	901	PP9	C4A-NA	-4.10	1.25	1.38
5	B	1105	PP9	C3C-C2C	4.05	1.46	1.40
5	B	1105	PP9	C4B-NB	-3.98	1.30	1.38
5	A	901	PP9	CBD-CAD	3.91	1.72	1.52
4	B	1104	CHD	C11-C9	3.81	1.60	1.53
4	A	701	CHD	C11-C9	3.80	1.60	1.53
4	A	702	CHD	C11-C9	3.79	1.60	1.53
4	A	701	CHD	C10-C9	3.71	1.62	1.56
4	B	1103	CHD	C11-C9	3.70	1.59	1.53
4	B	1104	CHD	C16-C17	3.68	1.62	1.54
4	B	1103	CHD	C16-C17	3.53	1.61	1.54
5	B	1105	PP9	C3B-C4B	3.45	1.50	1.43
4	A	702	CHD	C16-C17	3.40	1.61	1.54
4	A	701	CHD	C16-C17	3.36	1.61	1.54
4	B	1103	CHD	C10-C9	3.33	1.62	1.56
5	B	1105	PP9	C4C-CHD	-3.29	1.28	1.41
4	A	702	CHD	C6-C5	3.19	1.59	1.53
5	A	901	PP9	C3C-C2C	3.15	1.44	1.40
4	A	701	CHD	C6-C5	3.10	1.58	1.53
4	B	1104	CHD	O12-C12	3.00	1.48	1.43
4	B	1104	CHD	C6-C5	2.98	1.58	1.53
5	A	901	PP9	C3B-C4B	2.98	1.49	1.43
4	A	702	CHD	C10-C9	2.86	1.61	1.56
4	A	702	CHD	O12-C12	2.84	1.48	1.43
4	B	1103	CHD	C6-C5	2.83	1.58	1.53
4	B	1103	CHD	O12-C12	2.80	1.48	1.43
5	A	901	PP9	C1A-C2A	2.80	1.48	1.42
4	B	1104	CHD	C13-C12	2.77	1.58	1.54
4	A	701	CHD	O12-C12	2.73	1.48	1.43
4	B	1103	CHD	C8-C14	2.71	1.59	1.53
4	B	1104	CHD	C18-C13	2.71	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	CHD	C10-C9	2.70	1.61	1.56
4	B	1103	CHD	C18-C13	2.65	1.58	1.54
5	B	1105	PP9	C1A-C2A	2.64	1.48	1.42
4	A	702	CHD	C8-C7	2.63	1.58	1.53
5	B	1105	PP9	C1B-NB	-2.62	1.30	1.36
5	B	1105	PP9	C1A-NA	2.62	1.47	1.38
5	A	901	PP9	C4D-C3D	-2.60	1.41	1.45
4	B	1104	CHD	C8-C7	2.57	1.57	1.53
4	A	702	CHD	C18-C13	2.56	1.58	1.54
5	B	1105	PP9	C1C-CHC	-2.55	1.31	1.41
4	A	701	CHD	C18-C13	2.55	1.58	1.54
4	A	702	CHD	C8-C14	2.53	1.58	1.53
4	A	701	CHD	C8-C14	2.47	1.58	1.53
4	B	1104	CHD	C8-C14	2.46	1.58	1.53
4	A	701	CHD	O7-C7	2.43	1.48	1.43
4	B	1103	CHD	C20-C17	2.37	1.58	1.54
5	A	901	PP9	C4C-CHD	-2.36	1.31	1.41
4	B	1104	CHD	C19-C10	2.36	1.58	1.54
4	A	702	CHD	C13-C12	2.34	1.58	1.54
4	A	702	CHD	C19-C10	2.34	1.58	1.54
4	B	1103	CHD	C19-C10	2.33	1.58	1.54
4	A	702	CHD	C20-C17	2.31	1.58	1.54
4	B	1104	CHD	C20-C17	2.31	1.58	1.54
4	B	1103	CHD	O7-C7	2.22	1.48	1.43
5	B	1105	PP9	CMD-C2D	2.20	1.55	1.50
4	B	1103	CHD	C8-C7	2.19	1.57	1.53
4	B	1103	CHD	C4-C3	2.19	1.55	1.51
4	A	702	CHD	O7-C7	2.19	1.48	1.43
4	A	701	CHD	C8-C7	2.16	1.57	1.53
4	B	1104	CHD	C4-C3	2.13	1.55	1.51
4	B	1104	CHD	O7-C7	2.11	1.47	1.43
5	B	1105	PP9	C4D-C3D	-2.06	1.42	1.45
4	A	701	CHD	C13-C12	2.04	1.57	1.54
5	A	901	PP9	C1C-CHC	-2.03	1.33	1.41
4	A	702	CHD	C4-C3	2.03	1.55	1.51

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1105	PP9	CAD-CBD-CGD	6.40	123.42	112.67
5	B	1105	PP9	CHC-C4B-NB	-5.79	120.80	128.83
5	A	901	PP9	CHC-C4B-NB	-5.63	121.01	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	901	PP9	C1D-C2D-C3D	-5.43	100.27	106.51
5	B	1105	PP9	C1D-ND-C4D	5.00	115.94	106.51
5	B	1105	PP9	C1D-C2D-C3D	-4.98	100.79	106.51
5	A	901	PP9	CAD-CBD-CGD	4.88	120.86	112.67
5	A	901	PP9	C1D-ND-C4D	4.60	115.18	106.51
5	B	1105	PP9	C4C-CHD-C1D	4.40	134.06	128.81
5	B	1105	PP9	CHD-C1D-ND	-4.38	122.75	128.83
4	A	701	CHD	C19-C10-C1	-4.04	101.75	108.26
5	B	1105	PP9	CMC-C2C-C3C	3.97	132.10	124.68
4	B	1103	CHD	C19-C10-C1	-3.96	101.88	108.26
4	B	1104	CHD	C18-C13-C12	-3.89	105.10	109.07
5	A	901	PP9	C1C-CHC-C4B	3.84	133.40	128.81
4	A	701	CHD	O12-C12-C13	-3.81	104.59	111.03
5	B	1105	PP9	CMB-C2B-C1B	3.75	130.84	125.06
5	B	1105	PP9	CMA-C3A-C2A	3.71	131.93	124.94
4	B	1104	CHD	C19-C10-C1	-3.69	102.31	108.26
4	B	1103	CHD	O12-C12-C13	-3.62	104.90	111.03
5	B	1105	PP9	C2B-C1B-NB	3.61	118.23	110.53
5	A	901	PP9	CMA-C3A-C2A	3.58	131.69	124.94
4	B	1103	CHD	C18-C13-C12	-3.55	105.45	109.07
4	A	702	CHD	C18-C13-C12	-3.55	105.45	109.07
4	A	702	CHD	C19-C10-C1	-3.52	102.59	108.26
5	A	901	PP9	C4C-CHD-C1D	3.43	132.91	128.81
4	B	1103	CHD	C6-C5-C4	3.37	115.07	111.19
4	B	1104	CHD	C17-C13-C14	3.36	103.48	100.09
5	B	1105	PP9	CAD-C3D-C4D	3.30	130.85	125.01
5	A	901	PP9	C2B-C1B-NB	3.30	117.57	110.53
4	A	701	CHD	C18-C13-C12	-3.29	105.71	109.07
4	A	702	CHD	C17-C13-C14	3.29	103.41	100.09
4	B	1103	CHD	C17-C13-C12	3.26	120.64	117.67
4	B	1104	CHD	C17-C13-C12	3.24	120.63	117.67
4	B	1103	CHD	C17-C13-C14	3.22	103.33	100.09
4	A	701	CHD	C17-C13-C14	3.20	103.32	100.09
5	B	1105	PP9	CMD-C2D-C1D	3.16	129.94	125.06
4	A	702	CHD	O12-C12-C13	-3.15	105.71	111.03
4	A	701	CHD	C17-C13-C12	3.08	120.48	117.67
5	A	901	PP9	CMC-C2C-C3C	3.06	130.40	124.68
4	A	702	CHD	C17-C13-C12	3.05	120.45	117.67
4	B	1104	CHD	O12-C12-C13	-3.00	105.96	111.03
4	B	1103	CHD	C6-C5-C10	-2.98	109.49	112.66
4	B	1103	CHD	C9-C8-C7	-2.97	108.33	111.88
5	A	901	PP9	CMB-C2B-C1B	2.83	129.42	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	CHD	C11-C12-C13	2.82	114.14	111.24
4	A	701	CHD	C6-C5-C10	-2.79	109.69	112.66
4	B	1104	CHD	C6-C5-C10	-2.63	109.86	112.66
4	A	702	CHD	C11-C12-C13	2.63	113.94	111.24
4	A	702	CHD	C6-C5-C10	-2.63	109.87	112.66
5	B	1105	PP9	C1C-CHC-C4B	2.62	131.94	128.81
4	A	701	CHD	C9-C8-C7	-2.61	108.75	111.88
4	A	701	CHD	C6-C5-C4	2.61	114.19	111.19
5	A	901	PP9	CHB-C1B-NB	-2.59	119.52	124.93
4	B	1103	CHD	C16-C17-C13	-2.59	101.02	103.55
4	A	702	CHD	C16-C17-C13	-2.58	101.03	103.55
4	B	1103	CHD	C11-C12-C13	2.55	113.86	111.24
4	B	1103	CHD	C1-C10-C5	2.55	111.53	107.77
4	A	701	CHD	C1-C10-C5	2.48	111.44	107.77
4	B	1104	CHD	C11-C9-C10	-2.48	111.17	113.73
5	A	901	PP9	CMD-C2D-C3D	2.45	132.77	126.12
4	A	702	CHD	C9-C11-C12	-2.44	111.08	114.30
4	B	1104	CHD	C11-C12-C13	2.44	113.75	111.24
4	A	702	CHD	C9-C8-C7	-2.42	108.97	111.88
4	B	1104	CHD	C1-C10-C5	2.41	111.33	107.77
4	A	702	CHD	C6-C5-C4	2.40	113.95	111.19
5	A	901	PP9	CHD-C1D-ND	-2.36	125.55	128.83
4	A	701	CHD	C9-C11-C12	-2.36	111.18	114.30
5	A	901	PP9	CAD-C3D-C4D	2.36	129.18	125.01
4	B	1104	CHD	C22-C23-C24	-2.33	108.59	113.59
4	B	1104	CHD	C9-C11-C12	-2.32	111.24	114.30
4	B	1104	CHD	C9-C8-C7	-2.32	109.10	111.88
4	A	702	CHD	C1-C10-C5	2.31	111.19	107.77
4	B	1104	CHD	C6-C5-C4	2.31	113.85	111.19
4	A	702	CHD	C11-C9-C10	-2.30	111.35	113.73
4	B	1104	CHD	C16-C17-C13	-2.28	101.32	103.55
4	B	1103	CHD	C11-C9-C10	-2.28	111.38	113.73
4	A	702	CHD	C22-C23-C24	-2.27	108.71	113.59
5	B	1105	PP9	C4D-C3D-C2D	-2.26	104.28	106.78
4	A	701	CHD	C19-C10-C9	2.22	114.24	111.18
4	B	1103	CHD	C22-C23-C24	-2.21	108.85	113.59
4	A	702	CHD	C19-C10-C9	2.20	114.21	111.18
4	B	1103	CHD	C9-C11-C12	-2.20	111.40	114.30
4	A	701	CHD	C16-C17-C20	-2.18	108.78	112.15
4	B	1104	CHD	C21-C20-C22	-2.09	107.08	110.36
4	A	701	CHD	C19-C10-C5	-2.08	106.83	110.36
4	B	1104	CHD	C19-C10-C9	2.06	114.02	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	CHD	C5-C4-C3	-2.04	109.77	112.76
4	B	1103	CHD	C21-C20-C22	-2.03	107.18	110.36
5	B	1105	PP9	CAB-C3B-C4B	2.03	132.78	124.38
4	A	702	CHD	C21-C20-C22	-2.03	107.18	110.36
4	B	1103	CHD	C19-C10-C9	2.01	113.95	111.18
4	B	1104	CHD	C16-C17-C20	-2.00	109.04	112.15
4	B	1103	CHD	C19-C10-C5	-2.00	106.97	110.36

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	CHD	C20-C22-C23-C24
4	A	702	CHD	C17-C20-C22-C23
4	A	702	CHD	C21-C20-C22-C23
4	B	1104	CHD	C17-C20-C22-C23
5	B	1105	PP9	C3D-CAD-CBD-CGD
4	B	1104	CHD	C21-C20-C22-C23
5	A	901	PP9	C2B-C3B-CAB-CBB
5	B	1105	PP9	C2B-C3B-CAB-CBB
6	A	601	GOL	O1-C1-C2-O2
4	B	1104	CHD	C20-C22-C23-C24
4	B	1103	CHD	C20-C22-C23-C24
5	A	901	PP9	C4B-C3B-CAB-CBB
5	B	1105	PP9	C4B-C3B-CAB-CBB
6	A	601	GOL	O1-C1-C2-C3

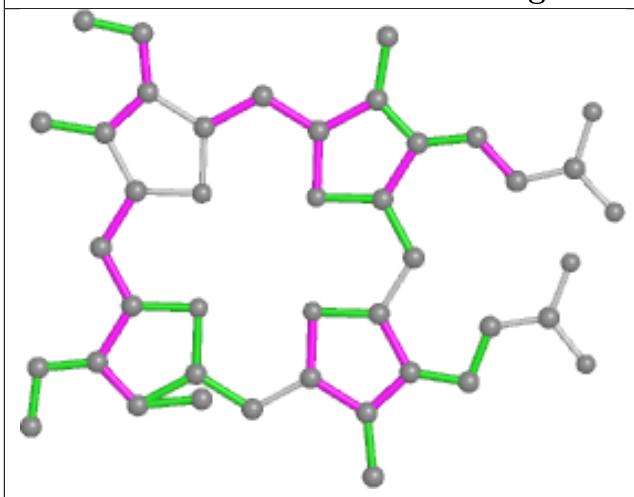
There are no ring outliers.

9 monomers are involved in 26 short contacts:

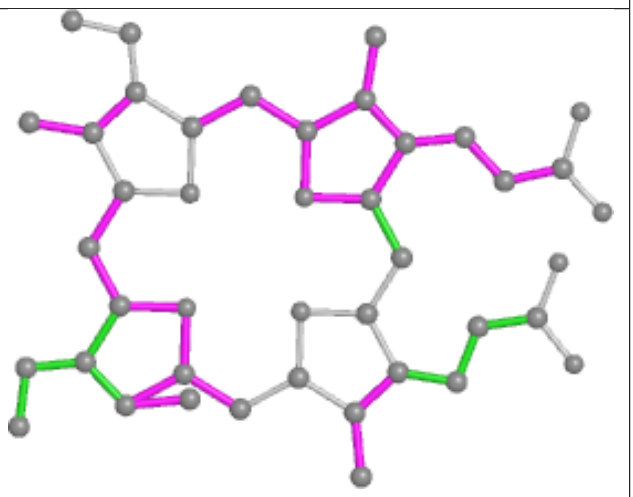
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	PP9	1	0
7	A	801	ACY	1	0
5	B	1105	PP9	4	0
4	B	1103	CHD	3	0
6	A	601	GOL	2	0
4	A	701	CHD	5	0
7	A	803	ACY	4	0
4	A	702	CHD	3	0
7	B	1106	ACY	4	0

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 then 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.

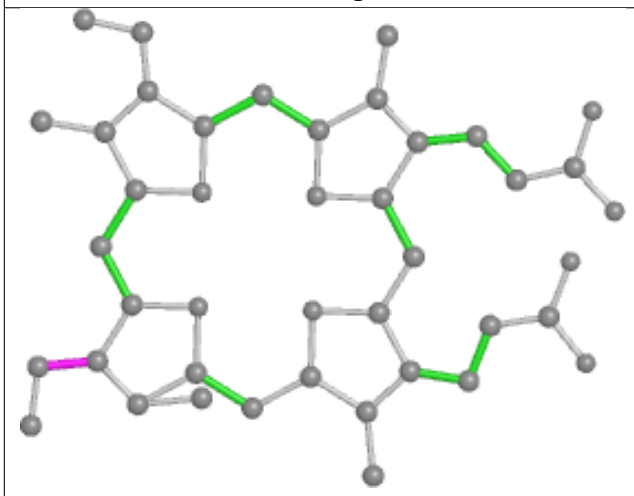
Ligand PP9 A 901



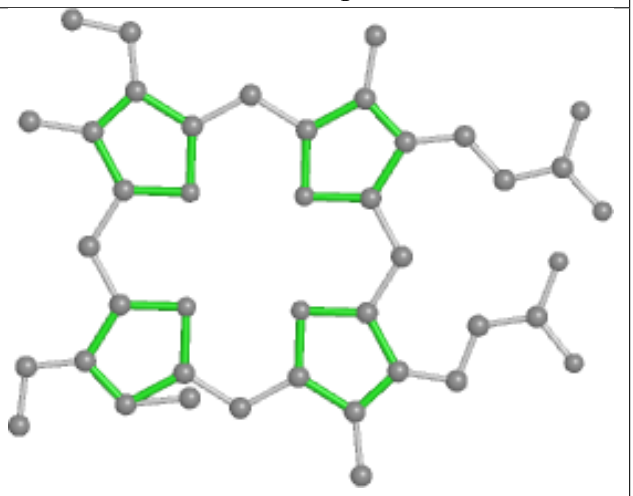
Bond lengths



Bond angles

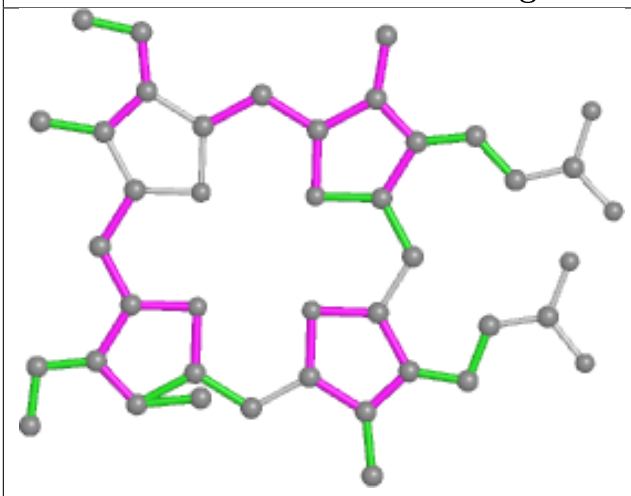


Torsions

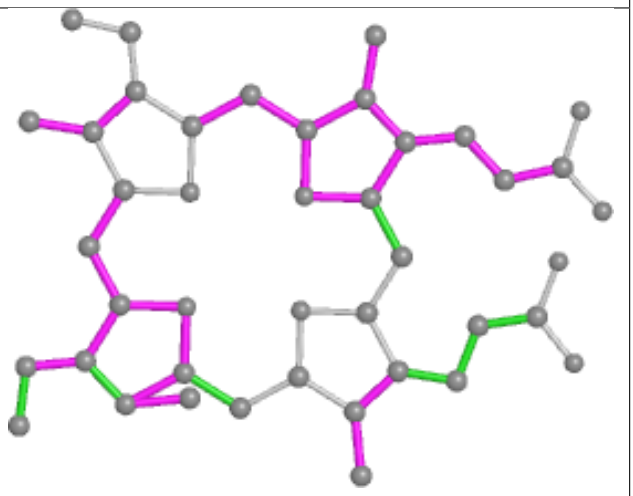


Rings

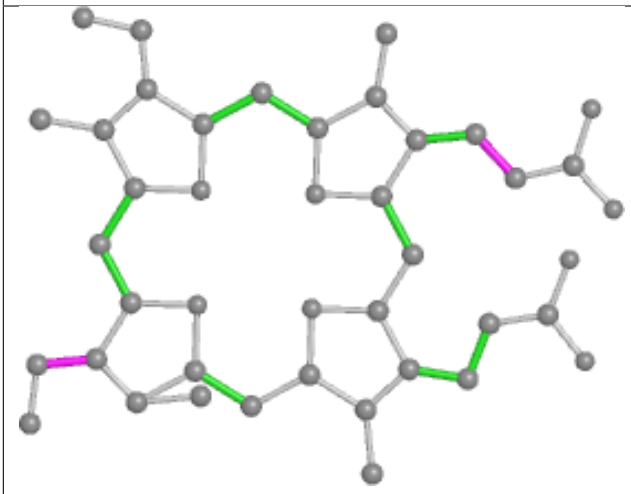
Ligand PP9 B 1105



Bond lengths



Bond angles



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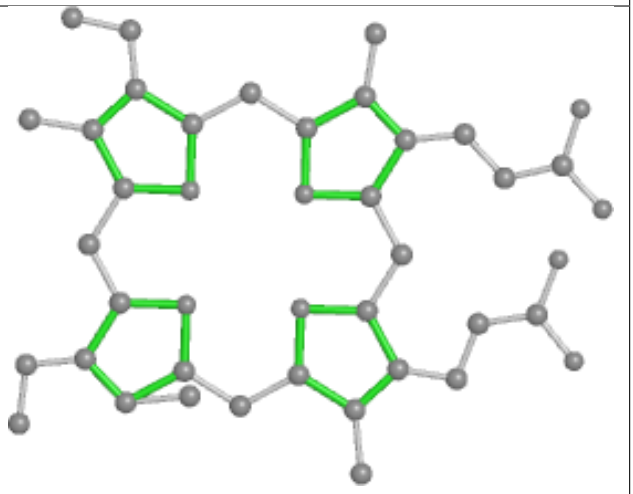
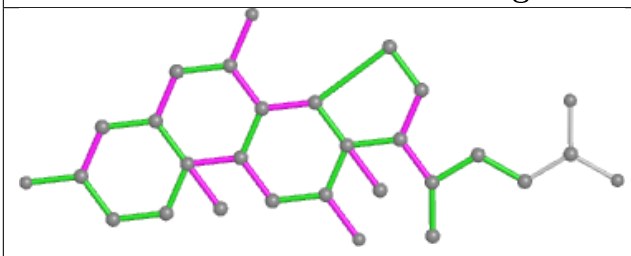
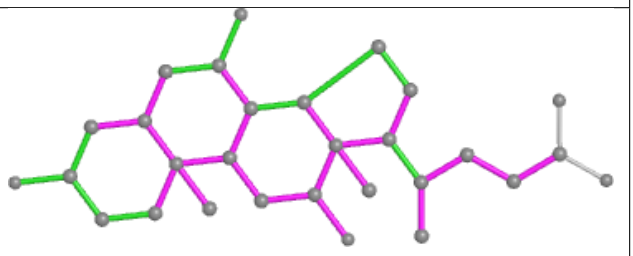


Rings

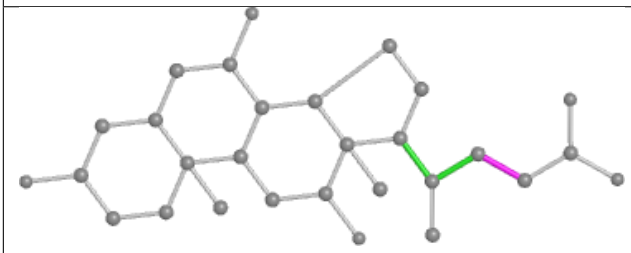
Ligand CHD B 1103



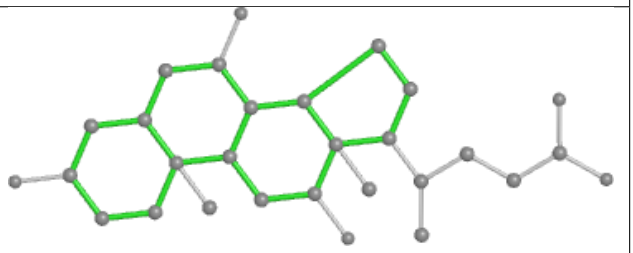
Bond lengths



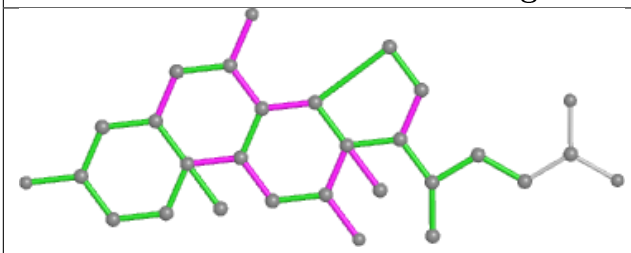
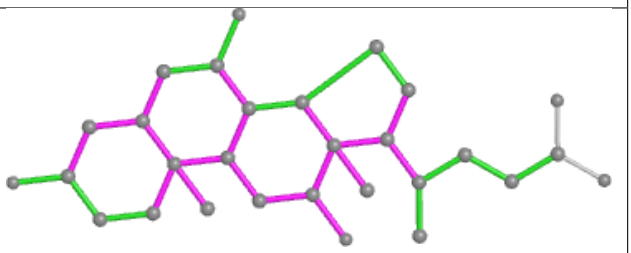
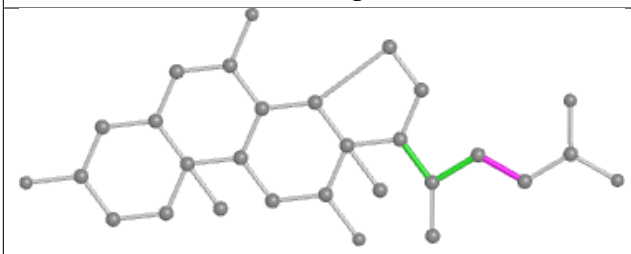
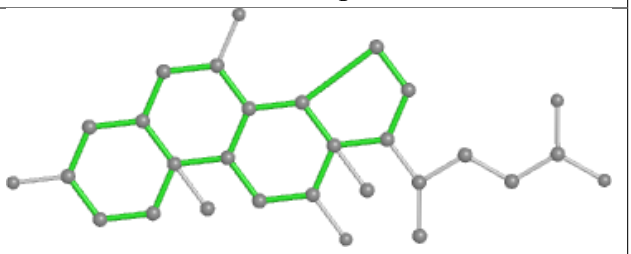
Bond angles

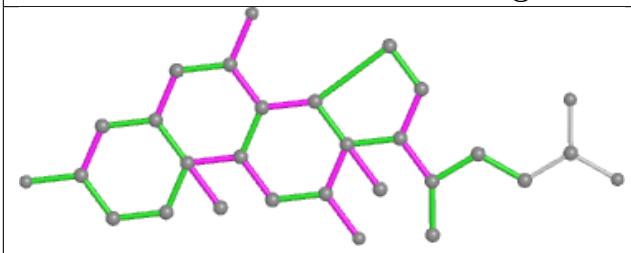
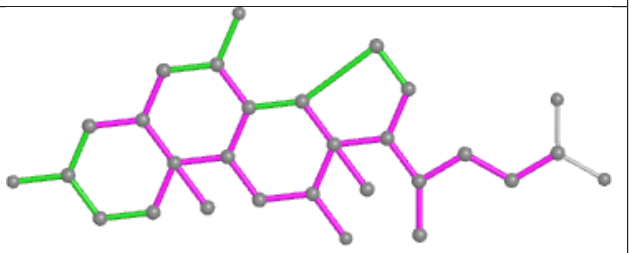
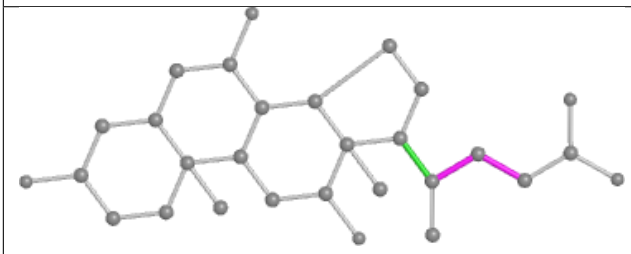
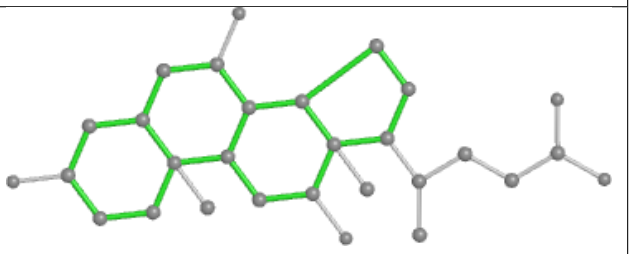


Torsions

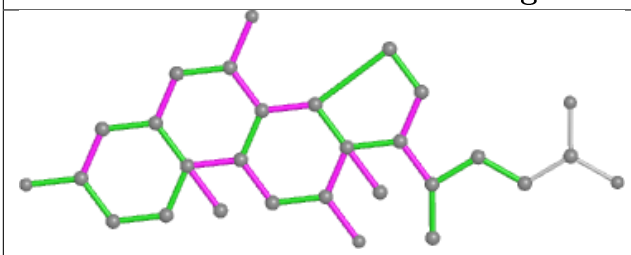


Rings

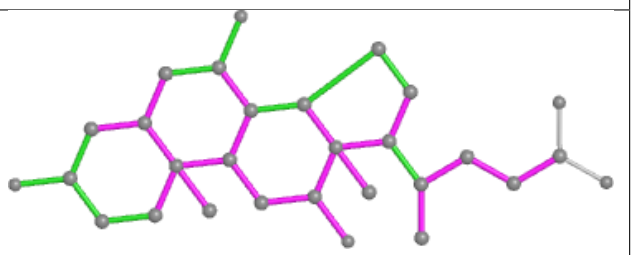
Ligand CHD A 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD B 1104	
 Bond lengths	 Bond angles
 Torsions	 Rings

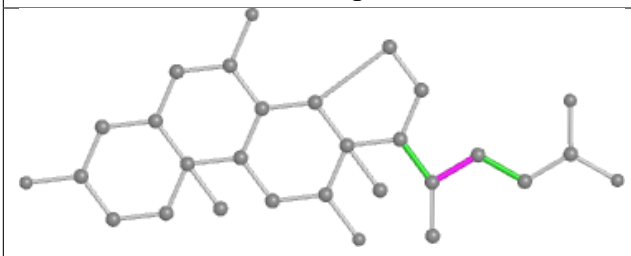
Ligand CHD A 702



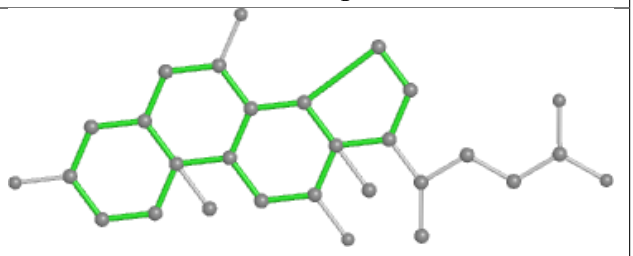
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.48	20 (5%)	24	30	27, 56, 82, 92	0
1	B	359/359 (100%)	0.38	13 (3%)	42	49	24, 51, 75, 86	0
All	All	718/718 (100%)	0.43	33 (4%)	32	39	24, 54, 79, 92	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	6.6
1	B	923	LEU	5.8
1	B	565	ARG	5.5
1	B	850	ILE	4.5
1	A	107	LEU	4.4
1	A	110	PHE	4.0
1	A	350	ILE	3.9
1	A	65	ARG	3.7
1	B	803	SER	3.7
1	A	102	PRO	3.4
1	A	356	LEU	3.4
1	A	409	PRO	2.9
1	B	715	ARG	2.8
1	A	106	LYS	2.7
1	B	858	LYS	2.7
1	A	66	LYS	2.7
1	B	713	VAL	2.6
1	B	854	GLN	2.6
1	B	607	LEU	2.5
1	B	566	LYS	2.5
1	B	806	GLY	2.5
1	A	212	GLN	2.5
1	A	213	VAL	2.4
1	A	407	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	277	PRO	2.2
1	A	150	LEU	2.2
1	B	606	LYS	2.1
1	B	610	PHE	2.1
1	A	280	VAL	2.0
1	A	346	TYR	2.0
1	A	111	ILE	2.0
1	A	183	GLU	2.0
1	A	312	GLY	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 carbohydrates 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, 95^{th} 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	CHD	B	1103	29/29	0.71	0.28	80,80,84,84	0
8	OXY	B	1001	2/2	0.73	0.26	62,62,62,63	0
4	CHD	A	701	29/29	0.78	0.28	96,97,97,98	0
4	CHD	B	1104	29/29	0.80	0.35	98,98,100,100	0
4	CHD	A	702	29/29	0.81	0.31	96,96,97,97	0
7	ACY	A	803	4/4	0.81	0.29	64,64,64,65	4
7	ACY	B	1106	4/4	0.82	0.28	42,42,43,44	4
2	PB	A	1101[B]	1/1	0.83	0.15	49,49,49,49	1
2	PB	A	1101[A]	1/1	0.83	0.15	51,51,51,51	1
5	PP9	A	901	42/42	0.88	0.19	43,49,51,53	0
6	GOL	A	601	6/6	0.89	0.29	48,49,50,50	0
7	ACY	A	801	4/4	0.89	0.25	55,55,55,55	4
3	FES	A	501	4/4	0.90	0.08	55,56,56,56	0
2	PB	B	1102[A]	1/1	0.91	0.14	43,43,43,43	1

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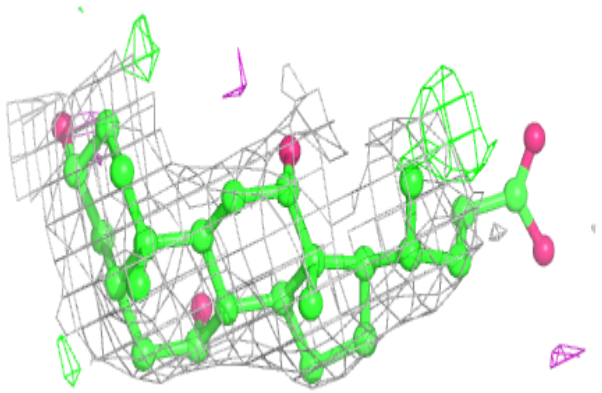
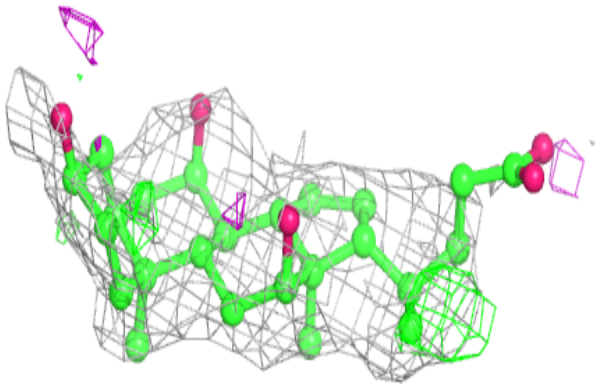
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PB	B	1102[B]	1/1	0.91	0.14	43,43,43,43	1
5	PP9	B	1105	42/42	0.92	0.18	38,42,46,47	0
3	FES	B	502	4/4	0.95	0.06	53,54,54,55	0

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 B 1103:

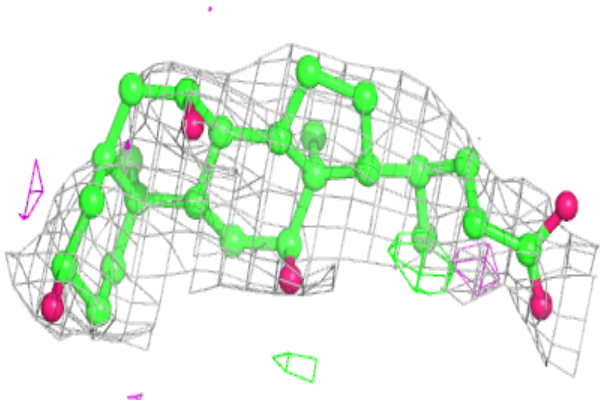
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

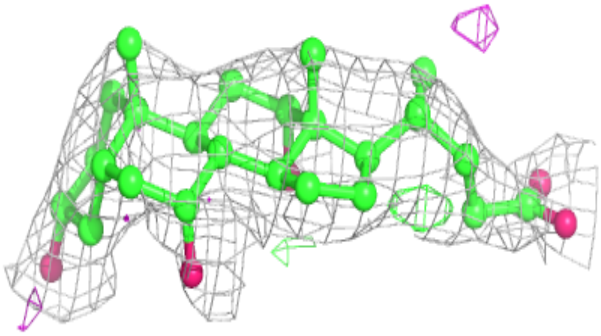


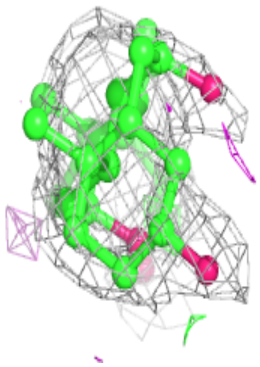


Electron density around CHD A 701:

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

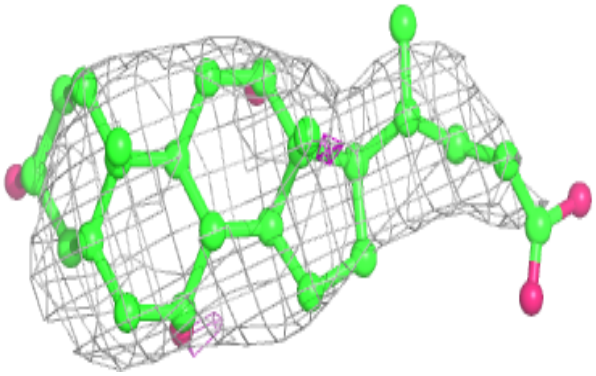


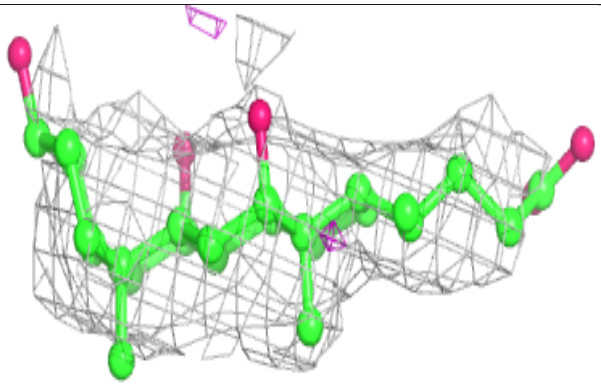


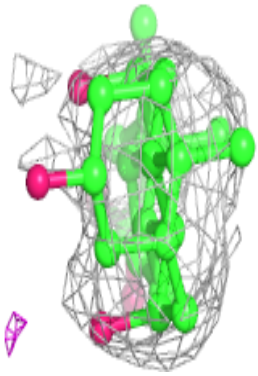


Electron density around CHD B 1104:

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

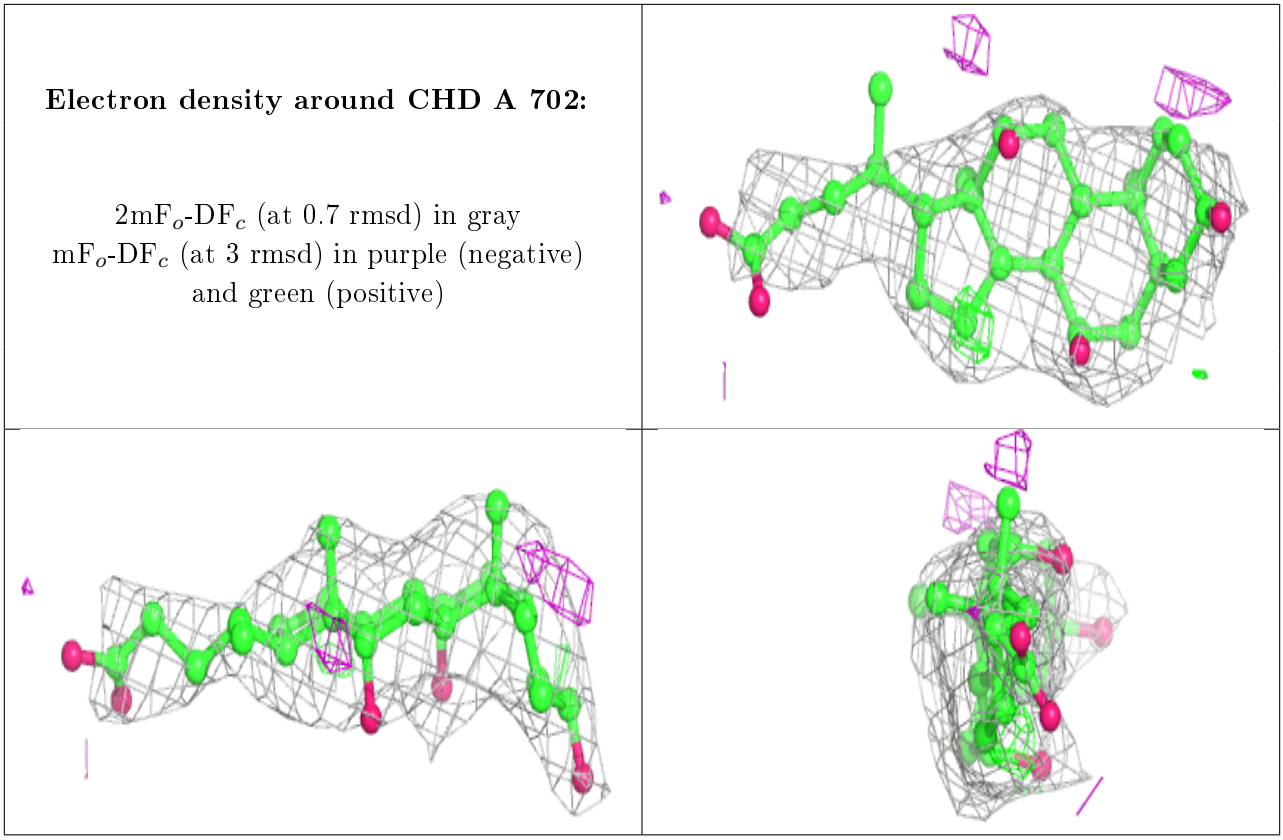






Electron density around CHD A 702:

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



Electron density around PP9 A 901:

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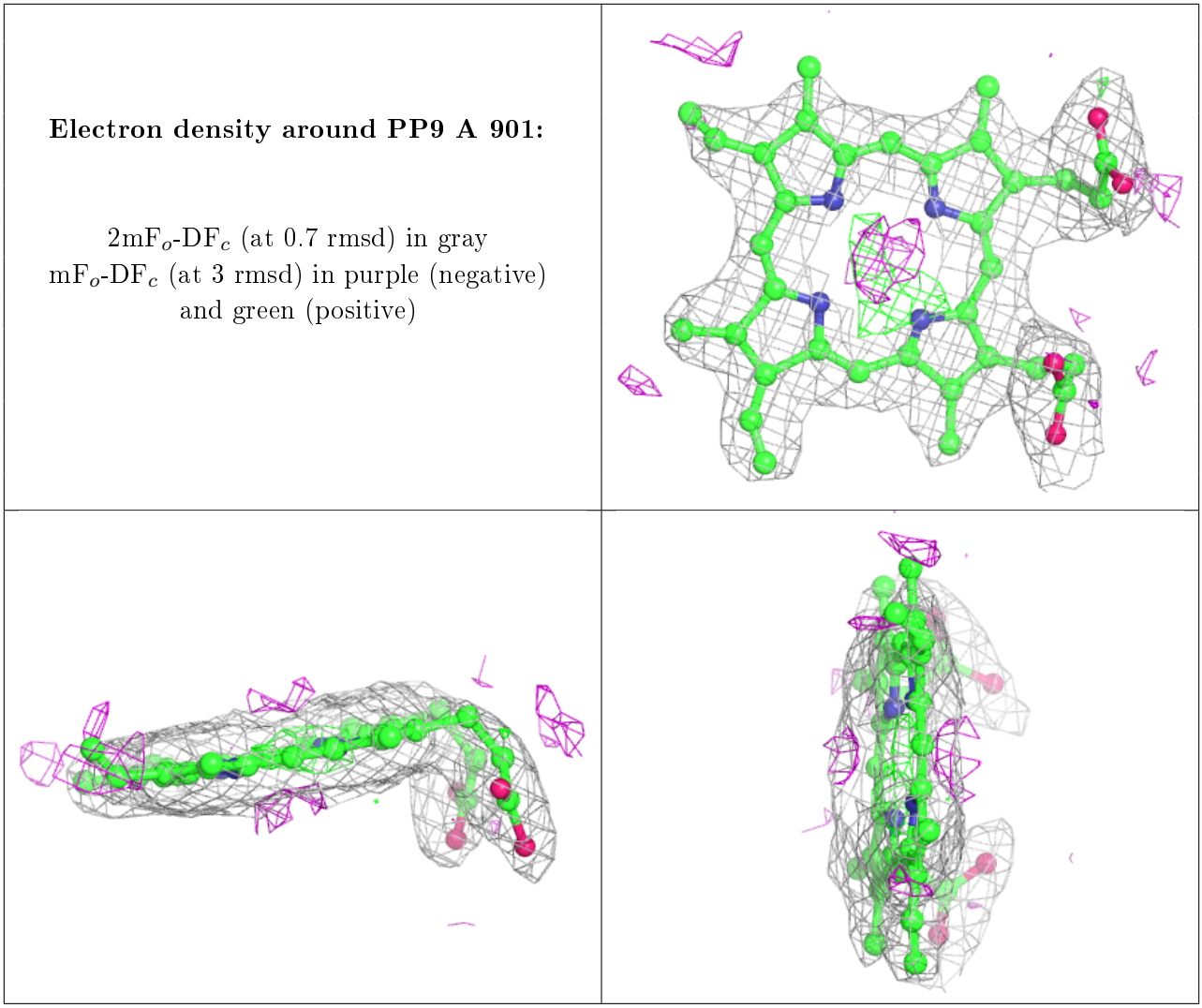
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PP9 B 1105:

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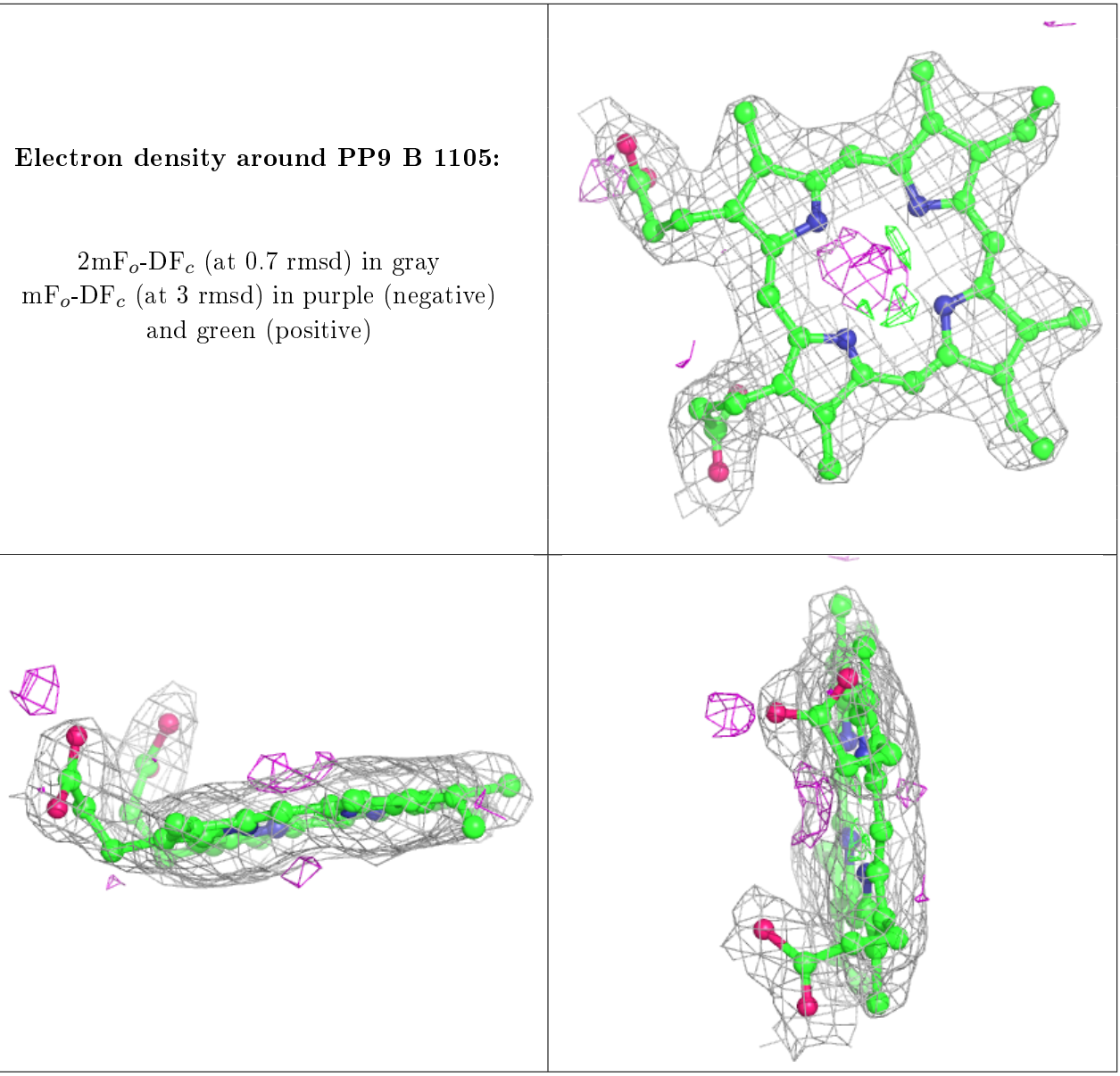
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.