



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:00 PM BST

PDB ID : 4KLA  
Title : E343D variant of human ferrochelatase  
Authors : Lanzilotta, W.N.; Medlock, A.E.  
Deposited on : 2013-05-07  
Resolution : 2.60 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

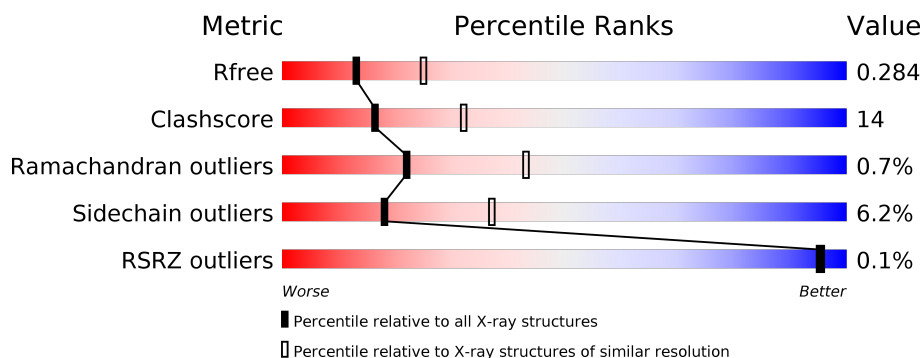
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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
5	PP9	B	502	-	-	X	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6184 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.

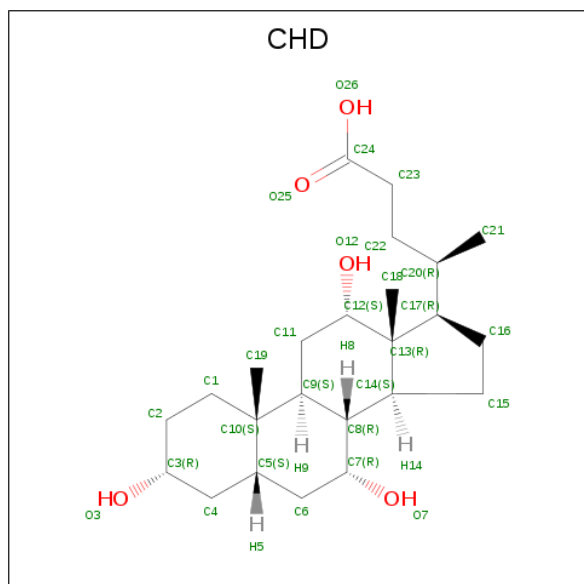
- Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2890	1840	503	529	18			
1	B	359	Total	C	N	O	S	0	1	0
			2896	1845	504	529	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	ASP	GLU	ENGINEERED MUTATION	UNP P22830
B	343	ASP	GLU	ENGINEERED MUTATION	UNP P22830

- Molecule 2 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



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

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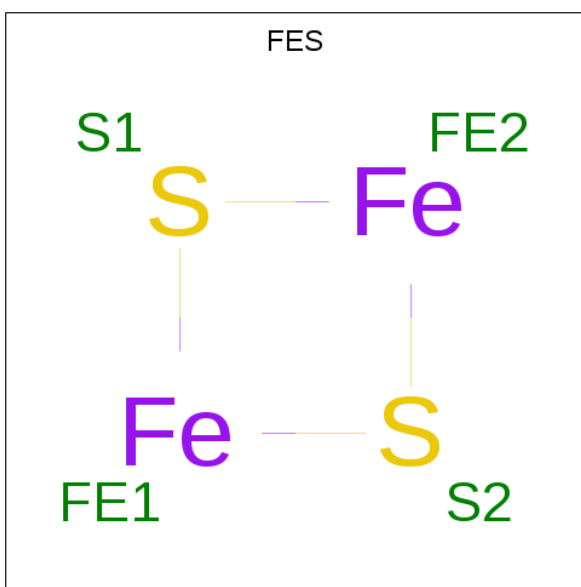
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			29	24	5		
2	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



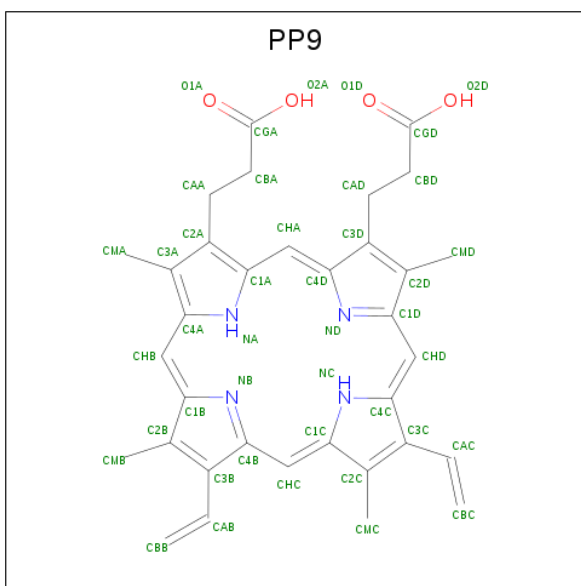
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



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

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



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

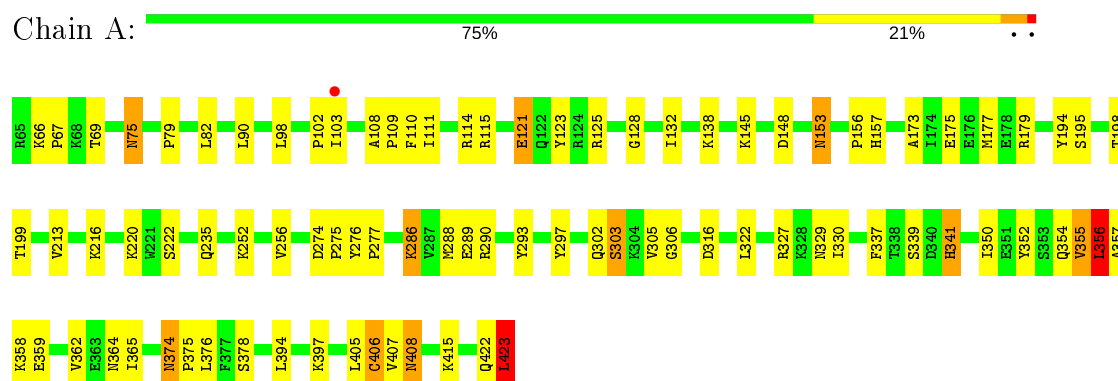
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total 142	O 142	0	0
6	B	113	Total 113	O 113	0	0

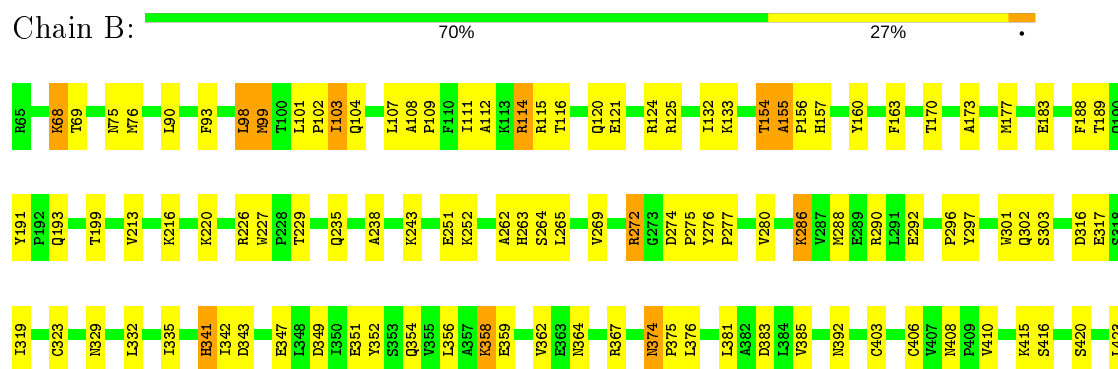
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	87.99 Å 93.43 Å 111.74 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.68 – 2.60 47.95 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.68-2.60) 99.0 (47.95-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.212 , 0.285 0.214 , 0.284	Depositor DCC
$R_{free}$ test set	1473 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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 56.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6504e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PP9, CHD, 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	0.67	1/2960 (0.0%)	0.76	1/4010 (0.0%)
1	B	0.71	4/2969 (0.1%)	0.75	4/4021 (0.1%)
All	All	0.69	5/5929 (0.1%)	0.76	5/8031 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	LEU	C-O	-8.82	1.06	1.23
1	B	98	LEU	CG-CD2	-7.91	1.22	1.51
1	B	99	MET	C-O	-5.42	1.13	1.23
1	B	99	MET	CG-SD	-5.39	1.67	1.81
1	A	286	LYS	CE-NZ	5.26	1.62	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	LEU	CB-CG-CD2	-9.94	94.10	111.00
1	A	423	LEU	CA-CB-CG	9.25	136.58	115.30
1	B	98	LEU	CA-CB-CG	7.64	132.88	115.30
1	B	356	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	99	MET	CA-CB-CG	5.25	122.22	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	406	CYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2890	0	2895	58	0
1	B	2896	0	2910	89	0
2	A	58	0	78	11	0
2	B	29	0	39	6	0
3	A	6	0	8	2	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	B	42	0	32	22	0
6	A	142	0	0	5	0
6	B	113	0	0	1	0
All	All	6184	0	5962	170	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 14.

All (170) 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:220:LYS:HE3	1:A:423:LEU:HD11	1.17	1.14
5:B:502:PP9:HMB1	5:B:502:PP9:HBB1	1.17	1.11
5:B:502:PP9:CBD	5:B:502:PP9:HHA	1.86	1.05
1:B:155:ALA:HB1	1:B:156:PRO:CD	1.85	1.05
5:B:502:PP9:HMB1	5:B:502:PP9:CBB	1.83	1.04
5:B:502:PP9:HHA	5:B:502:PP9:HBD2	1.35	1.03
5:B:502:PP9:CMB	5:B:502:PP9:HBB1	1.82	1.02
1:B:155:ALA:HB1	1:B:156:PRO:HD2	1.39	1.01
5:B:502:PP9:HMA3	5:B:502:PP9:HBA1	1.45	0.96
5:B:502:PP9:CBA	5:B:502:PP9:CMA	2.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:GOL:H2	1:B:277:PRO:HB3	1.53	0.88
2:B:501:CHD:H192	5:B:502:PP9:HMB3	1.56	0.87
2:A:501:CHD:H212	2:A:501:CHD:H12	1.58	0.86
1:A:115:ARG:HD2	2:A:501:CHD:H231	1.58	0.85
1:B:115:ARG:HH21	2:B:501:CHD:H231	1.43	0.83
5:B:502:PP9:CMA	5:B:502:PP9:HBA1	2.03	0.83
5:B:502:PP9:CBA	5:B:502:PP9:HMA3	2.13	0.79
1:B:155:ALA:CB	1:B:156:PRO:CD	2.62	0.75
1:A:115:ARG:NH1	2:A:501:CHD:H222	2.02	0.74
2:B:501:CHD:H192	5:B:502:PP9:CMB	2.17	0.74
1:A:374:ASN:ND2	1:A:376:LEU:H	1.84	0.74
5:B:502:PP9:CMA	5:B:502:PP9:HBA2	2.18	0.73
2:B:501:CHD:C19	5:B:502:PP9:HMB3	2.19	0.73
1:A:374:ASN:HD22	1:A:375:PRO:N	1.85	0.72
5:B:502:PP9:CBD	5:B:502:PP9:CHA	2.63	0.71
5:B:502:PP9:HBD1	5:B:502:PP9:HHA	1.73	0.70
1:B:329:ASN:HD22	1:B:364:ASN:HB2	1.56	0.70
3:A:503:GOL:H2	1:B:277:PRO:CB	2.22	0.69
1:B:75:ASN:OD1	1:B:132:ILE:HD11	1.92	0.69
1:A:220:LYS:HD3	1:A:423:LEU:HD21	1.76	0.67
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.77	0.66
1:A:153:ASN:H	1:A:153:ASN:ND2	1.95	0.65
1:B:68:LYS:HB2	1:B:155:ALA:HB3	1.80	0.63
1:A:305:VAL:HG21	2:A:502:CHD:H161	1.81	0.63
5:B:502:PP9:HMA2	5:B:502:PP9:HBA2	1.81	0.63
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.82	0.62
1:A:374:ASN:HD22	1:A:374:ASN:C	2.03	0.61
1:A:355:VAL:O	1:A:358:LYS:N	2.32	0.61
1:B:68:LYS:CB	1:B:155:ALA:HB3	2.30	0.61
1:A:330:ILE:HB	1:A:365:ILE:HD12	1.83	0.61
1:A:306:GLY:HA2	6:A:675:HOH:O	2.00	0.60
1:A:110:PHE:CZ	1:A:114:ARG:HD2	2.37	0.59
1:A:355:VAL:O	1:A:356:LEU:C	2.41	0.59
1:B:115:ARG:NH2	2:B:501:CHD:H231	2.17	0.58
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.15	0.58
1:A:357:ALA:HB1	1:A:362:VAL:HG11	1.84	0.58
1:A:350:ILE:O	1:A:354:GLN:HB2	2.03	0.58
1:B:229:THR:HB	1:B:286[A]:LYS:HE3	1.84	0.58
1:B:269:VAL:HG21	5:B:502:PP9:HBB2	1.85	0.58
1:B:155:ALA:CB	1:B:156:PRO:HD2	2.24	0.57
1:A:375:PRO:O	1:A:378:SER:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLU:O	1:B:125:ARG:HG2	2.05	0.56
1:B:374:ASN:ND2	1:B:376:LEU:H	2.04	0.56
1:B:155:ALA:HB1	1:B:156:PRO:HD3	1.80	0.56
1:A:148:ASP:OD2	1:A:157:HIS:ND1	2.31	0.56
1:B:99:MET:HG2	1:B:101:LEU:HG	1.87	0.56
1:B:173:ALA:O	1:B:177:MET:HG3	2.06	0.56
1:A:194:TYR:HA	6:A:615:HOH:O	2.06	0.56
1:B:133:LYS:HG3	1:B:163:PHE:HE1	1.71	0.55
1:B:229:THR:HB	1:B:286[A]:LYS:HD3	1.88	0.55
1:B:229:THR:O	1:B:286[A]:LYS:HE3	2.07	0.55
1:B:132:ILE:HG23	1:B:133:LYS:N	2.22	0.54
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.43	0.54
1:B:93:PHE:HB2	1:B:108:ALA:HB1	1.89	0.54
1:A:198:THR:OG1	1:A:199:THR:N	2.41	0.54
1:B:408:ASN:OD1	1:B:410:VAL:HG12	2.08	0.53
1:B:374:ASN:HD22	1:B:376:LEU:H	1.56	0.53
1:B:115:ARG:NH1	6:B:602:HOH:O	2.37	0.53
1:B:235:GLN:HG3	1:B:290:ARG:CZ	2.39	0.53
1:B:319:ILE:HD11	1:B:332:LEU:HD21	1.90	0.53
1:A:405:LEU:HD11	1:B:317:GLU:HB3	1.90	0.52
1:A:121:GLU:O	1:A:125:ARG:HG2	2.10	0.52
2:A:501:CHD:H12	2:A:501:CHD:C21	2.36	0.52
1:A:102:PRO:O	1:A:103:ILE:HG13	2.09	0.51
1:B:189:THR:HB	1:B:199:THR:HG23	1.93	0.51
5:B:502:PP9:HBD2	5:B:502:PP9:CHA	2.22	0.51
1:B:235:GLN:HG3	1:B:290:ARG:NH2	2.26	0.51
1:A:82:LEU:HD21	1:A:128:GLY:HA2	1.93	0.51
1:B:154:THR:OG1	1:B:157:HIS:NE2	2.41	0.50
1:A:98:LEU:HD13	6:A:658:HOH:O	2.12	0.50
1:B:349:ASP:OD2	1:B:367:ARG:NH2	2.45	0.50
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.47	0.49
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.47	0.49
1:A:341:HIS:CD2	1:A:341:HIS:N	2.81	0.49
1:A:422:GLN:HG2	6:A:721:HOH:O	2.11	0.49
1:B:354:GLN:O	1:B:358:LYS:HB2	2.12	0.49
1:B:102:PRO:C	1:B:103:ILE:HG13	2.34	0.49
1:B:238:ALA:CB	1:B:290:ARG:HD3	2.43	0.49
1:B:193:GLN:HG2	1:B:280:VAL:HA	1.95	0.48
1:B:343:ASP:O	1:B:347:GLU:HB3	2.13	0.48
5:B:502:PP9:HBD1	5:B:502:PP9:CHA	2.38	0.48
1:B:116:THR:O	1:B:120:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PRO:O	1:B:103:ILE:C	2.51	0.48
1:B:323:CYS:SG	1:B:362:VAL:HG23	2.53	0.48
1:A:407:VAL:O	1:A:408:ASN:CB	2.62	0.48
1:A:79:PRO:HD2	1:A:123:TYR:CZ	2.48	0.47
1:B:101:LEU:O	1:B:104:GLN:HG3	2.14	0.47
1:B:374:ASN:HD22	1:B:374:ASN:C	2.16	0.47
1:B:381:LEU:O	1:B:385:VAL:HG23	2.14	0.47
1:B:265:LEU:HD11	1:B:276:TYR:CD2	2.49	0.47
1:B:302:GLN:HG3	1:B:303:SER:OG	2.14	0.47
1:B:238:ALA:HB3	1:B:290:ARG:HD3	1.97	0.47
1:B:329:ASN:ND2	1:B:364:ASN:HB2	2.27	0.47
1:B:416:SER:O	1:B:420:SER:OG	2.24	0.47
1:B:347:GLU:HA	1:B:351:GLU:HG2	1.97	0.47
1:B:262:ALA:O	1:B:301:TRP:HA	2.15	0.47
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.14	0.47
1:A:406:CYS:SG	1:A:407:VAL:O	2.72	0.47
1:A:111:ILE:O	1:A:115:ARG:HG2	2.14	0.46
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.30	0.46
1:B:342:ILE:HG21	5:B:502:PP9:HAD2	1.97	0.46
1:B:341:HIS:N	1:B:341:HIS:CD2	2.82	0.46
1:A:69:THR:HB	1:A:157:HIS:CD2	2.50	0.46
1:B:102:PRO:O	1:B:107:LEU:HD12	2.15	0.46
1:B:90:LEU:HD13	1:B:109:PRO:HA	1.97	0.46
2:A:502:CHD:H41	2:A:502:CHD:O7	2.15	0.46
1:B:374:ASN:HD22	1:B:375:PRO:N	2.13	0.46
1:A:374:ASN:ND2	1:A:374:ASN:C	2.68	0.46
1:B:342:ILE:CG2	5:B:502:PP9:HAD2	2.46	0.46
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.81	0.45
1:B:374:ASN:HD22	1:B:376:LEU:N	2.14	0.45
2:A:501:CHD:H12A	2:A:501:CHD:H112	1.65	0.45
1:B:288:MET:HG3	1:B:297:TYR:CD2	2.52	0.45
1:B:115:ARG:HH21	2:B:501:CHD:C23	2.23	0.45
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.98	0.45
2:A:501:CHD:C21	2:A:501:CHD:C12	2.94	0.45
1:B:272:ARG:O	1:B:272:ARG:HG2	2.16	0.45
1:B:403:CYS:HB2	1:B:406:CYS:HB2	1.99	0.45
1:B:229:THR:HB	1:B:286[A]:LYS:CD	2.47	0.45
1:B:263:HIS:HB3	5:B:502:PP9:HBC1	1.99	0.44
1:A:173:ALA:O	1:A:177:MET:HG3	2.16	0.44
1:A:90:LEU:HD13	1:A:109:PRO:HA	1.99	0.44
1:B:154:THR:HG1	1:B:157:HIS:CE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:O	1:B:335:ILE:HG13	2.17	0.44
1:B:68:LYS:HD3	1:B:183:GLU:OE1	2.18	0.44
1:A:322:LEU:HB3	1:A:327:ARG:HB2	1.99	0.43
1:B:76:MET:HG2	1:B:191:TYR:OH	2.19	0.43
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.87	0.43
1:B:101:LEU:HB2	1:B:104:GLN:HG3	2.00	0.43
1:B:251:GLU:HG2	1:B:252:LYS:HG2	2.01	0.43
1:B:112:ALA:C	1:B:114:ARG:N	2.71	0.43
1:A:195:SER:HB2	1:A:276:TYR:HB2	2.00	0.42
1:B:133:LYS:HG3	1:B:163:PHE:CE1	2.53	0.42
1:B:288:MET:HG3	1:B:297:TYR:CE2	2.54	0.42
1:A:75:ASN:OD1	1:A:337:PHE:CZ	2.72	0.42
1:A:115:ARG:HD2	2:A:501:CHD:C23	2.41	0.42
1:B:69:THR:HB	1:B:157:HIS:CD2	2.54	0.42
1:B:69:THR:HB	1:B:157:HIS:HD2	1.85	0.42
1:A:222:SER:HB2	1:A:394:LEU:HA	2.01	0.42
1:A:175:GLU:HG2	1:A:179:ARG:HH22	1.85	0.41
1:B:160:TYR:CD2	1:B:177:MET:HG2	2.55	0.41
1:A:302:GLN:O	1:A:303:SER:HB2	2.20	0.41
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.74	0.41
1:B:68:LYS:HB3	1:B:154:THR:O	2.21	0.41
1:A:252:LYS:O	1:A:256:VAL:HG23	2.19	0.41
1:B:132:ILE:HG23	1:B:133:LYS:H	1.85	0.41
1:B:69:THR:OG1	1:B:154:THR:HB	2.21	0.41
1:A:67:PRO:HA	1:A:156:PRO:HG2	2.02	0.41
1:A:288:MET:HG3	1:A:297:TYR:CE2	2.56	0.41
1:A:330:ILE:O	1:A:365:ILE:HA	2.21	0.41
1:A:75:ASN:ND2	6:A:729:HOH:O	2.53	0.41
1:B:264:SER:HB2	1:B:301:TRP:HB3	2.03	0.41
1:B:226:ARG:C	1:B:227:TRP:CD1	2.94	0.41
1:B:154:THR:OG1	1:B:157:HIS:CE1	2.74	0.41
1:B:265:LEU:HD11	1:B:276:TYR:HB3	2.04	0.40
1:A:397:LYS:HD2	1:B:296:PRO:HD3	2.03	0.40
1:A:422:GLN:O	1:A:423:LEU:HD22	2.21	0.40
2:A:501:CHD:C18	2:A:502:CHD:H162	2.51	0.40
2:A:502:CHD:H12	2:A:502:CHD:H212	2.03	0.40
1:B:111:ILE:O	1:B:111:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/359 (99%)	332 (93%)	21 (6%)	4 (1%)	14	30
1	B	358/359 (100%)	328 (92%)	29 (8%)	1 (0%)	41	64
All	All	715/718 (100%)	660 (92%)	50 (7%)	5 (1%)	22	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	VAL
1	A	303	SER
1	B	155	ALA
1	A	356	LEU
1	A	408	ASN

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/324 (100%)	307 (95%)	17 (5%)	23	46
1	B	325/324 (100%)	301 (93%)	24 (7%)	13	28
All	All	649/648 (100%)	608 (94%)	41 (6%)	18	36

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	121	GLU
1	A	132	ILE
1	A	138	LYS
1	A	145	LYS
1	A	153	ASN
1	A	213	VAL
1	A	216	LYS
1	A	286	LYS
1	A	339	SER
1	A	341	HIS
1	A	356	LEU
1	A	359	GLU
1	A	374	ASN
1	A	415	LYS
1	A	423	LEU
1	B	68	LYS
1	B	98	LEU
1	B	103	ILE
1	B	114	ARG
1	B	124	ARG
1	B	154	THR
1	B	170	THR
1	B	188	PHE
1	B	213	VAL
1	B	216	LYS
1	B	220	LYS
1	B	243	LYS
1	B	272	ARG
1	B	286[A]	LYS
1	B	286[B]	LYS
1	B	292	GLU
1	B	341	HIS
1	B	358	LYS
1	B	359	GLU
1	B	374	ASN
1	B	383	ASP
1	B	392	ASN
1	B	415	LYS
1	B	423	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	153	ASN
1	A	247	HIS
1	A	314	GLN
1	A	329	ASN
1	A	364	ASN
1	A	374	ASN
1	A	421	GLN
1	B	105	ASN
1	B	314	GLN
1	B	329	ASN
1	B	374	ASN
1	B	421	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	503	-	5,5,5	0.55	0	5,5,5	0.74	0
2	CHD	B	501	-	29,32,32	0.57	0	48,51,51	2.53	19 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FES	A	504	1	0,4,4	0.00	-	-		
4	FES	B	503	1	0,4,4	0.00	-	-		
5	PP9	B	502	-	34,46,46	4.54	9 (26%)	33,68,68	2.77	18 (54%)
2	CHD	A	501	-	29,32,32	0.82	1 (3%)	48,51,51	2.58	20 (41%)
2	CHD	A	502	-	29,32,32	0.68	0	48,51,51	1.60	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	503	-	-	2/4/4/4	-
2	CHD	B	501	-	-	0/7/74/74	0/4/4/4
4	FES	A	504	1	-	-	0/1/1/1
4	FES	B	503	1	-	-	0/1/1/1
5	PP9	B	502	-	-	4/20/62/62	0/4/5/5
2	CHD	A	501	-	-	1/7/74/74	0/4/4/4
2	CHD	A	502	-	-	1/7/74/74	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PP9	CHD-C1D	17.24	1.49	1.35
5	B	502	PP9	CHC-C4B	16.87	1.49	1.35
5	B	502	PP9	C3C-C2C	5.27	1.47	1.40
5	B	502	PP9	C3D-C2D	5.10	1.47	1.36
5	B	502	PP9	C3B-C2B	3.66	1.44	1.37
5	B	502	PP9	C3B-C4B	3.08	1.49	1.43
5	B	502	PP9	C1A-C2A	2.58	1.48	1.42
5	B	502	PP9	C2A-C3A	2.42	1.44	1.37
5	B	502	PP9	CAA-C2A	-2.15	1.48	1.52
2	A	501	CHD	C13-C14	-2.12	1.51	1.55

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	PP9	CBA-CAA-C2A	-6.80	99.95	112.48
2	A	501	CHD	C9-C8-C7	-6.11	104.57	111.88
2	B	501	CHD	C17-C13-C14	-5.64	94.41	100.09
5	B	502	PP9	CMB-C2B-C1B	5.54	133.60	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	CHD	C9-C10-C5	5.43	116.20	108.58
2	A	501	CHD	C4-C5-C10	5.35	118.34	112.66
2	B	501	CHD	C4-C5-C10	5.16	118.14	112.66
2	B	501	CHD	C18-C13-C14	5.06	119.13	111.21
2	B	501	CHD	C13-C17-C20	5.04	125.52	119.50
2	B	501	CHD	C17-C13-C12	4.86	122.10	117.67
2	B	501	CHD	C9-C8-C7	-4.84	106.09	111.88
2	B	501	CHD	C13-C14-C8	4.66	120.68	114.74
2	A	501	CHD	C13-C17-C20	-4.60	114.01	119.50
2	A	501	CHD	C23-C22-C20	-4.58	108.56	114.72
2	B	501	CHD	C9-C10-C5	4.49	114.88	108.58
5	B	502	PP9	CAD-CBD-CGD	-4.09	105.80	112.67
5	B	502	PP9	CHD-C1D-ND	-4.06	123.19	128.83
2	A	501	CHD	C17-C13-C12	-4.06	113.96	117.67
2	A	501	CHD	C4-C3-C2	-3.84	105.97	110.55
2	A	501	CHD	C10-C9-C8	3.80	115.90	111.82
2	B	501	CHD	C23-C22-C20	3.64	119.62	114.72
2	A	501	CHD	C16-C17-C20	3.63	117.77	112.15
5	B	502	PP9	C1D-C2D-C3D	-3.63	102.34	106.51
2	A	501	CHD	C1-C10-C9	-3.52	105.83	111.35
5	B	502	PP9	CAA-CBA-CGA	-3.43	106.92	112.67
5	B	502	PP9	CHC-C4B-NB	-3.43	124.07	128.83
2	A	501	CHD	C15-C14-C8	3.42	123.11	118.33
5	B	502	PP9	C2D-C1D-ND	3.40	114.92	109.79
2	A	502	CHD	C18-C13-C12	3.39	112.52	109.07
2	A	502	CHD	C13-C17-C20	3.35	123.50	119.50
2	A	501	CHD	O3-C3-C4	3.35	116.51	109.85
5	B	502	PP9	CMD-C2D-C1D	3.21	130.01	125.06
5	B	502	PP9	C2B-C1B-NB	3.09	117.12	110.53
2	A	501	CHD	C1-C10-C5	3.08	112.32	107.77
2	A	501	CHD	C22-C20-C17	3.08	116.64	110.28
5	B	502	PP9	CBB-CAB-C3B	-3.04	112.48	127.62
2	B	501	CHD	C15-C14-C13	3.03	106.52	103.55
5	B	502	PP9	CAB-C3B-C2B	-2.97	118.83	128.60
2	A	502	CHD	C13-C14-C8	2.96	118.51	114.74
2	A	501	CHD	C21-C20-C22	-2.95	105.74	110.36
5	B	502	PP9	CMC-C2C-C3C	2.93	130.16	124.68
2	A	501	CHD	C11-C9-C10	-2.93	110.71	113.73
2	B	501	CHD	C19-C10-C9	-2.88	107.21	111.18
2	B	501	CHD	C11-C9-C10	2.84	116.65	113.73
2	B	501	CHD	C6-C7-C8	2.81	114.48	111.48
5	B	502	PP9	C3D-C4D-ND	2.77	114.58	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	CHD	C5-C4-C3	2.73	116.77	112.76
2	A	502	CHD	C9-C11-C12	-2.68	110.77	114.30
2	B	501	CHD	C18-C13-C12	-2.67	106.34	109.07
2	A	502	CHD	C9-C10-C5	2.67	112.33	108.58
2	A	501	CHD	C15-C14-C13	-2.60	101.00	103.55
2	A	501	CHD	C19-C10-C5	-2.55	106.04	110.36
2	A	502	CHD	C14-C8-C7	2.55	115.19	111.81
5	B	502	PP9	CMA-C3A-C2A	2.48	129.62	124.94
2	A	501	CHD	C5-C6-C7	2.48	117.19	114.46
5	B	502	PP9	CAB-C3B-C4B	2.42	134.38	124.38
2	A	502	CHD	C17-C13-C14	-2.36	97.71	100.09
2	B	501	CHD	C10-C9-C8	-2.34	109.31	111.82
2	B	501	CHD	C16-C15-C14	-2.27	100.62	105.13
2	A	501	CHD	C14-C13-C12	2.27	109.52	107.40
5	B	502	PP9	C4D-C3D-C2D	-2.20	104.35	106.78
5	B	502	PP9	CHA-C4D-C3D	-2.20	120.03	124.49
2	B	501	CHD	C18-C13-C17	-2.11	107.91	111.21
2	B	501	CHD	C6-C5-C4	-2.11	108.77	111.19
2	B	501	CHD	C22-C23-C24	2.01	117.92	113.59
2	A	502	CHD	C19-C10-C1	-2.01	105.02	108.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	C1-C2-C3-O3
5	B	502	PP9	C1A-C2A-CAA-CBA
5	B	502	PP9	C3A-C2A-CAA-CBA
5	B	502	PP9	C2D-C3D-CAD-CBD
5	B	502	PP9	C4D-C3D-CAD-CBD
3	A	503	GOL	O2-C2-C3-O3
2	A	501	CHD	C20-C22-C23-C24
2	A	502	CHD	C21-C20-C22-C23

There are no ring outliers.

5 monomers are involved in 38 short contacts:

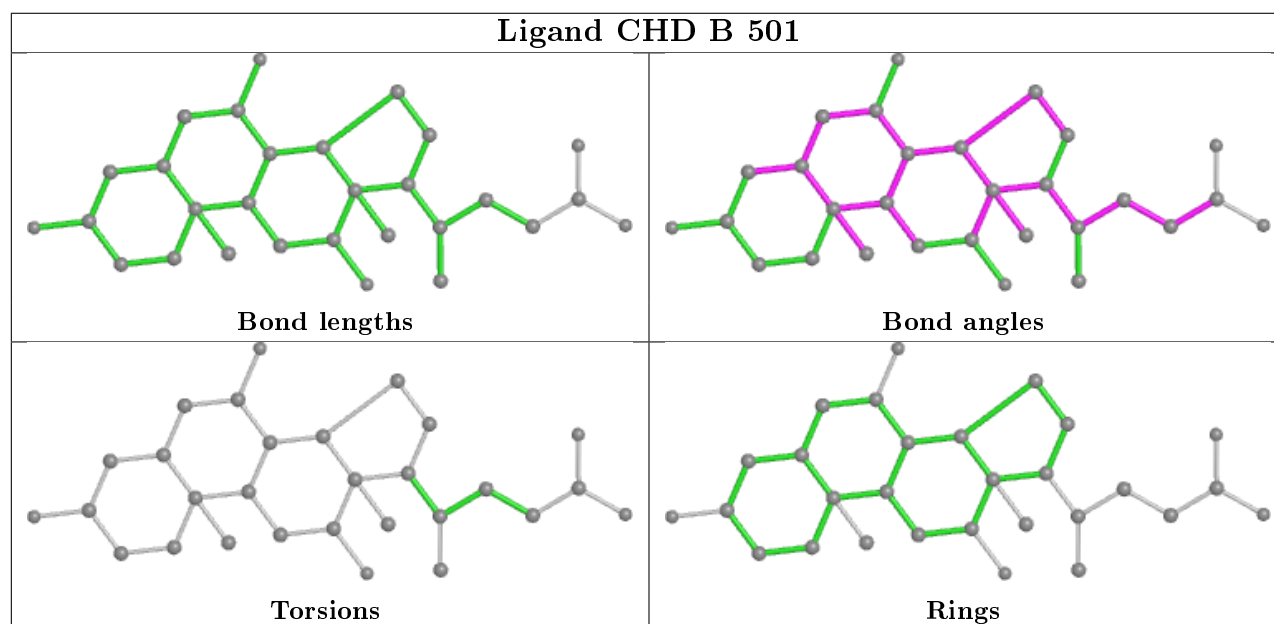
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	GOL	2	0
2	B	501	CHD	6	0
5	B	502	PP9	22	0

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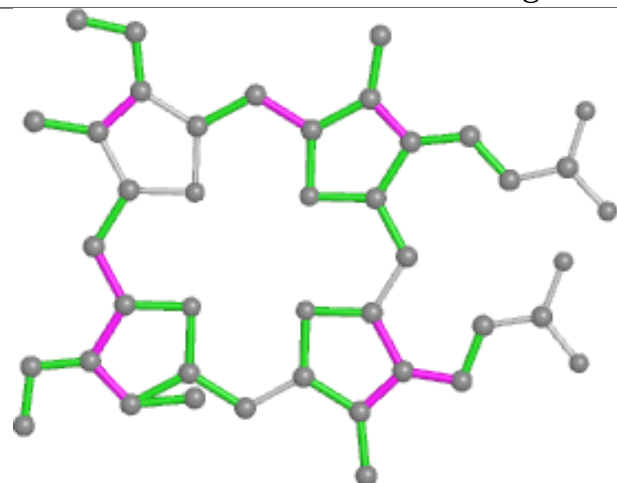
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CHD	8	0
2	A	502	CHD	4	0

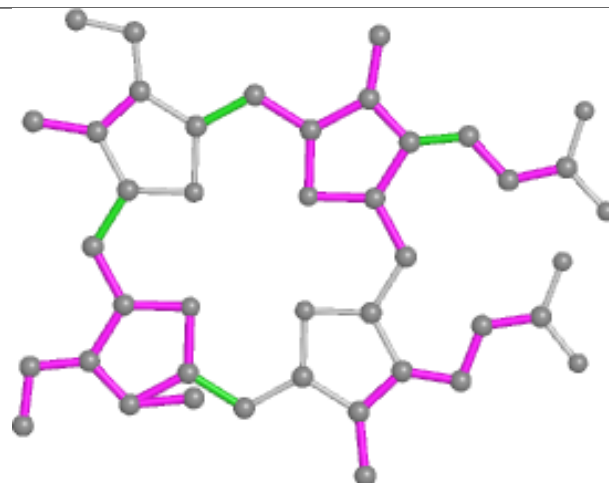
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



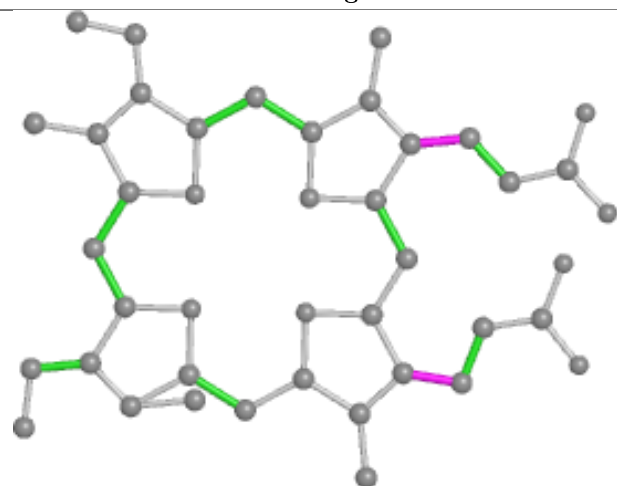
## Ligand PP9 B 502



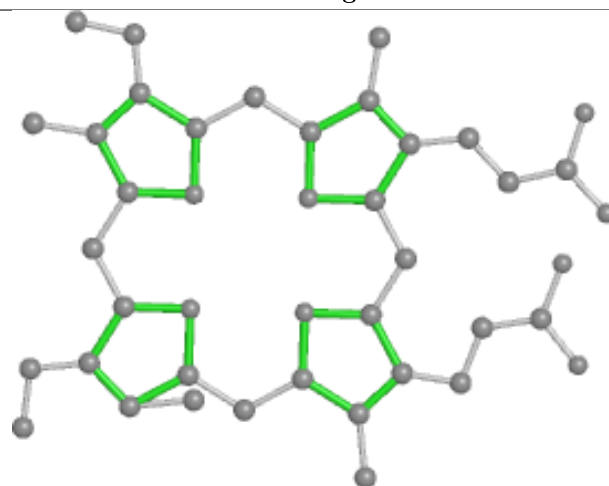
Bond lengths



Bond angles

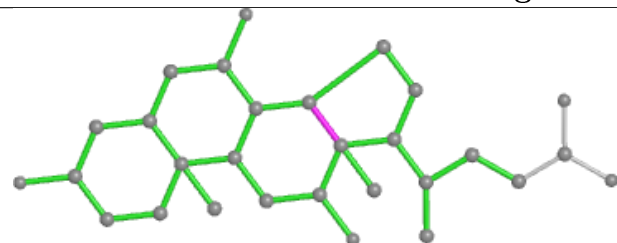


Torsions

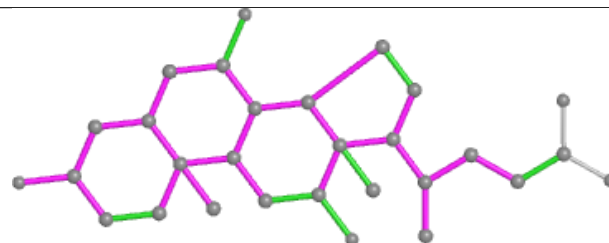


Rings

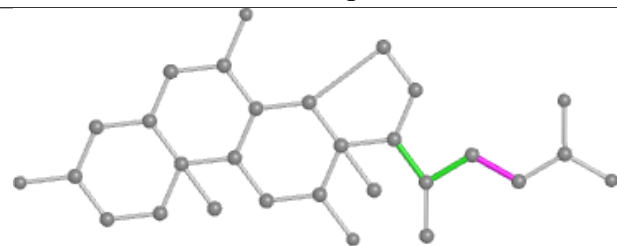
## Ligand CHD A 501



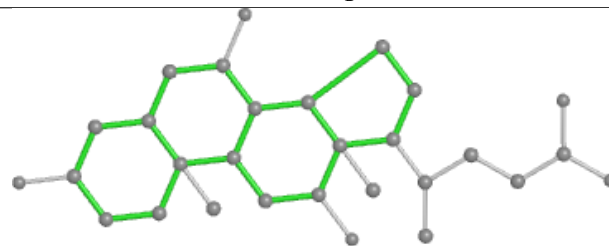
Bond lengths



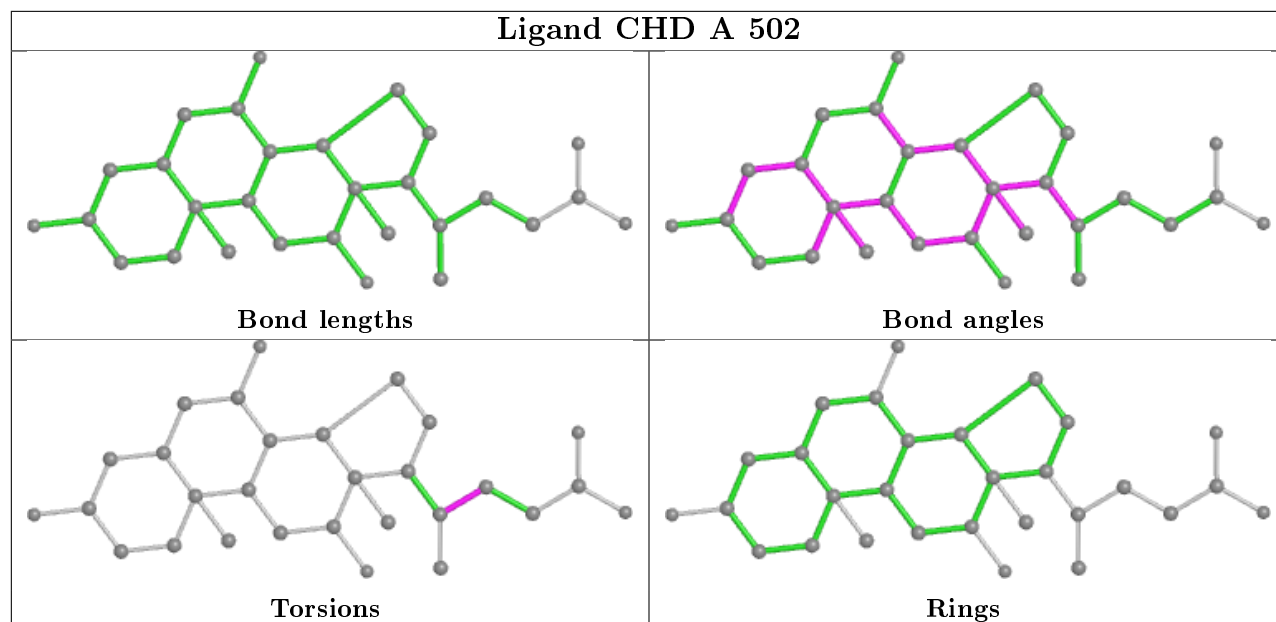
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/359 (100%)	-0.55	1 (0%) 94 93	2, 13, 32, 39	0
1	B	359/359 (100%)	-0.52	0 100 100	2, 12, 37, 44	0
All	All	718/718 (100%)	-0.53	1 (0%) 95 95	2, 13, 34, 44	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	3.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	PP9	B	502	42/42	0.73	0.44	4,9,10,11	42
2	CHD	B	501	29/29	0.74	0.27	47,50,60,61	0
2	CHD	A	501	29/29	0.76	0.32	40,44,68,70	0
2	CHD	A	502	29/29	0.88	0.21	21,24,27,27	0

*Continued on next page...*

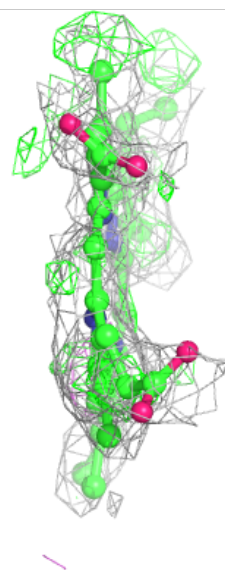
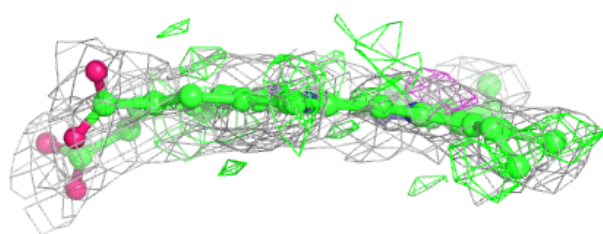
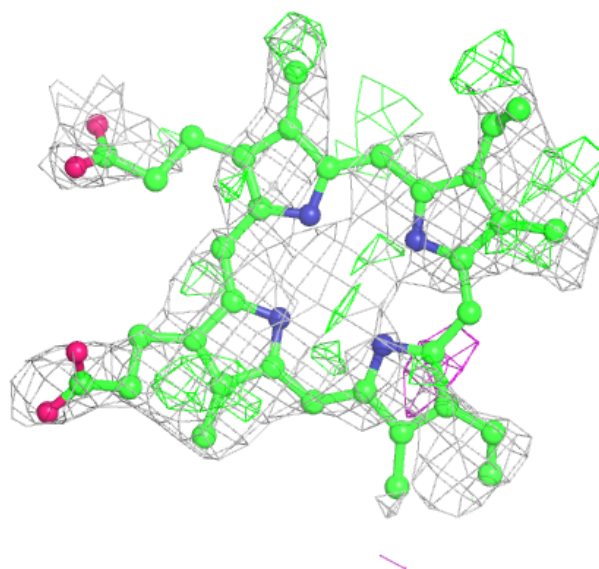
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	503	6/6	0.94	0.51	2,2,2,2	6
4	FES	B	503	4/4	0.98	0.06	8,9,13,13	0
4	FES	A	504	4/4	0.99	0.04	7,8,10,12	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.

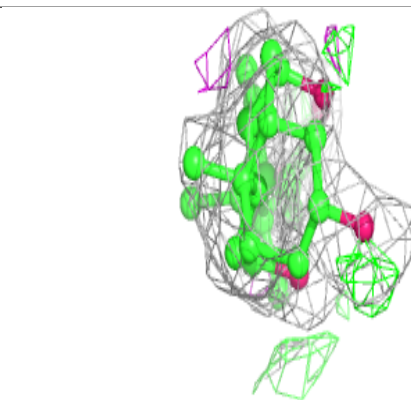
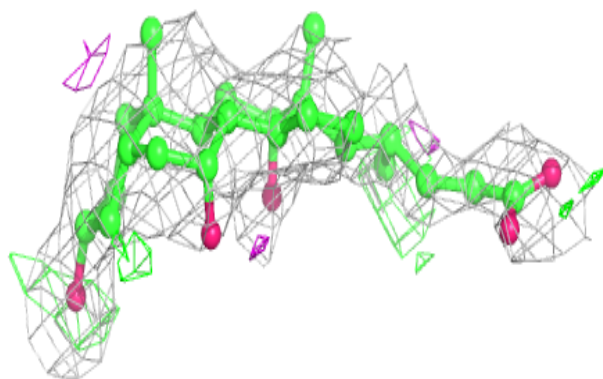
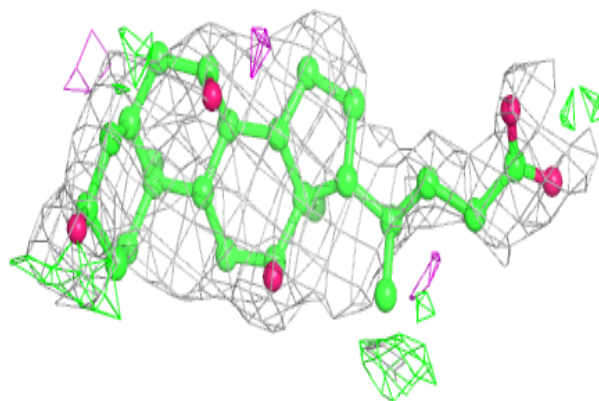
**Electron density around PP9 B 502:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

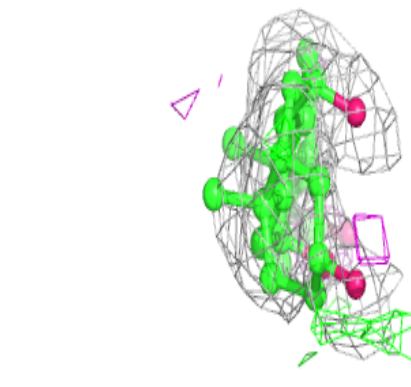
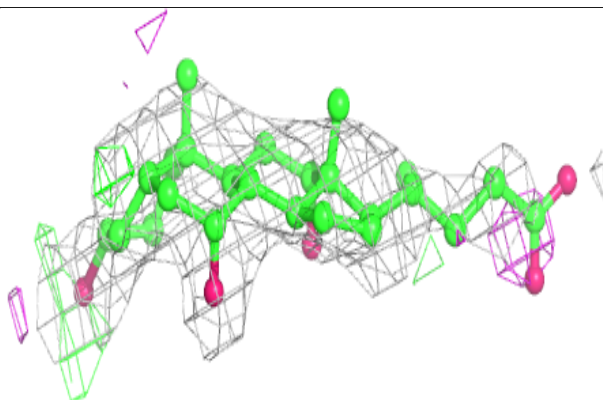
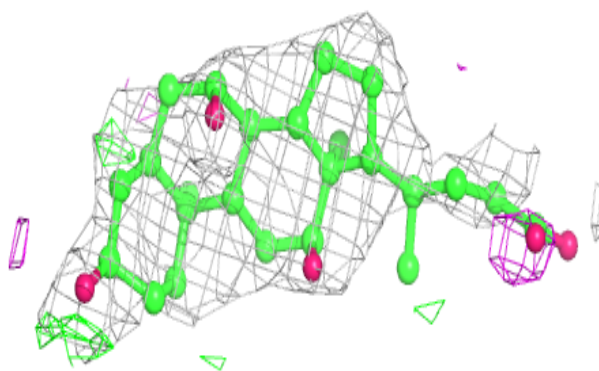


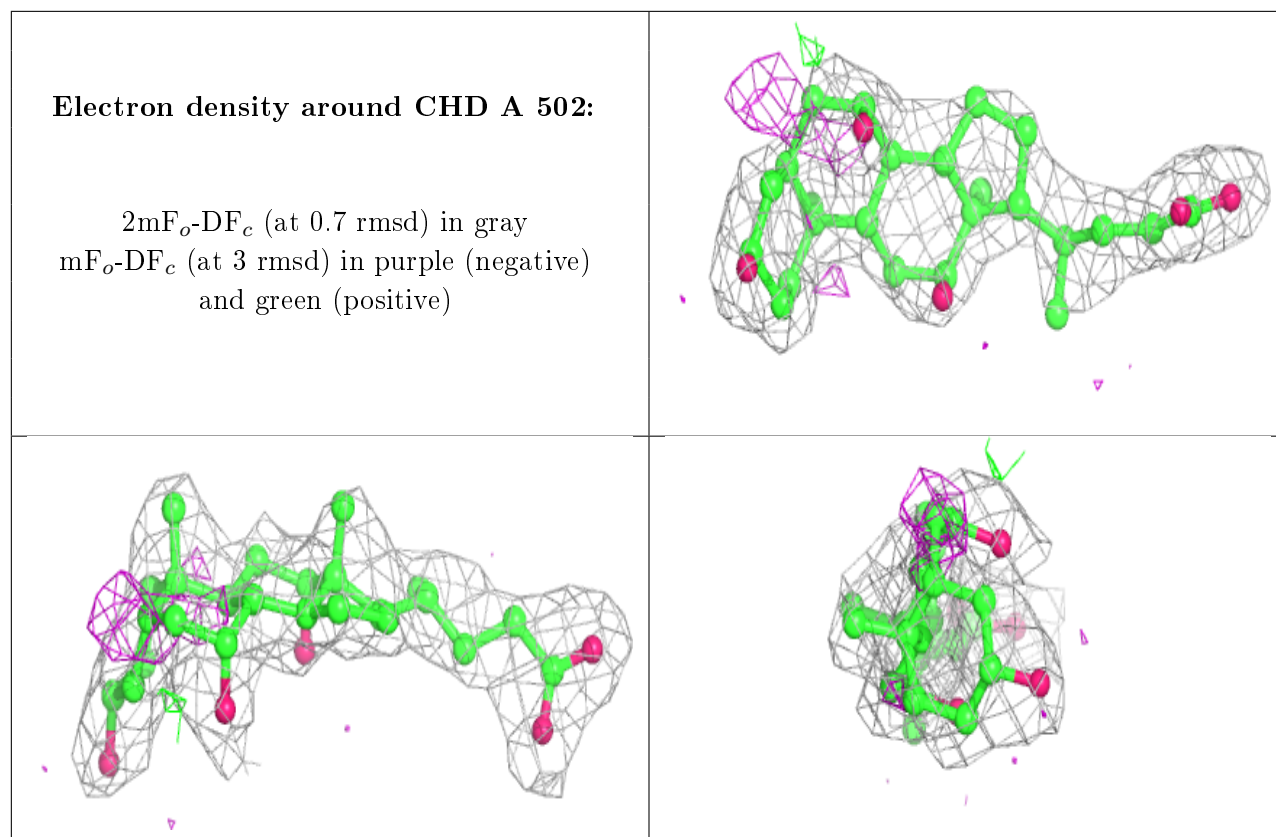
**Electron density around CHD B 501:**

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

**Electron density around CHD A 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.