



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 08:28 pm BST

PDB ID : 2IVF / pdb_00002ivf
Title : Ethylbenzene dehydrogenase from Aromatoleum aromaticum
Authors : Kloer, D.P.; Hagel, C.; Heider, J.; Schulz, G.E.
Deposited on : 2006-06-13
Resolution : 1.88 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

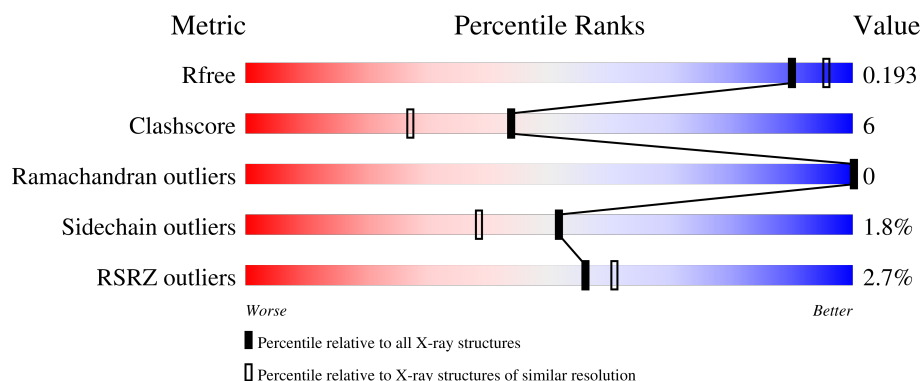
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

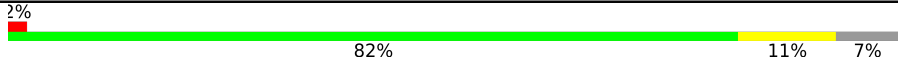
The reported resolution of this entry is 1.88 Å.

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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	976	
2	B	352	
3	C	214	

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
10	MD1	A	1987	X	-	-	-
5	ACT	A	1978	-	-	X	-
6	GOL	A	1981	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 12639 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 ETHYLBENZENE DEHYDROGENASE ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	912	7285	4651	1254	1331	49	0	0	0

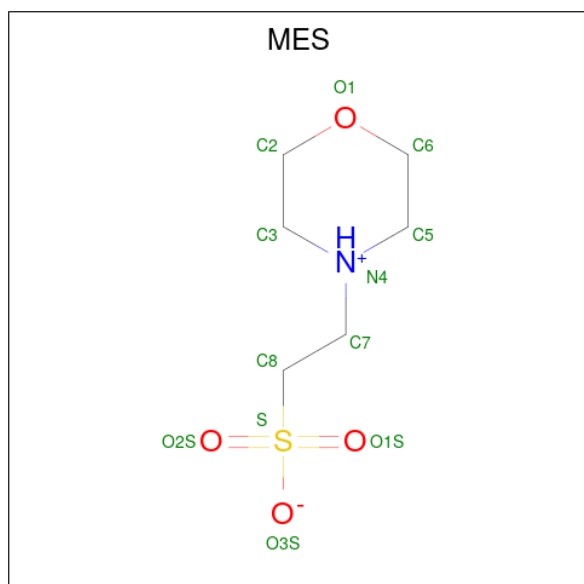
- Molecule 2 is a protein called ETHYLBENZENE DEHYDROGENASE BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	337	2669	1686	479	484	20	0	0	0

- Molecule 3 is a protein called ETHYLBENZENE DEHYDROGENASE GAMMA-SUBUNIT.

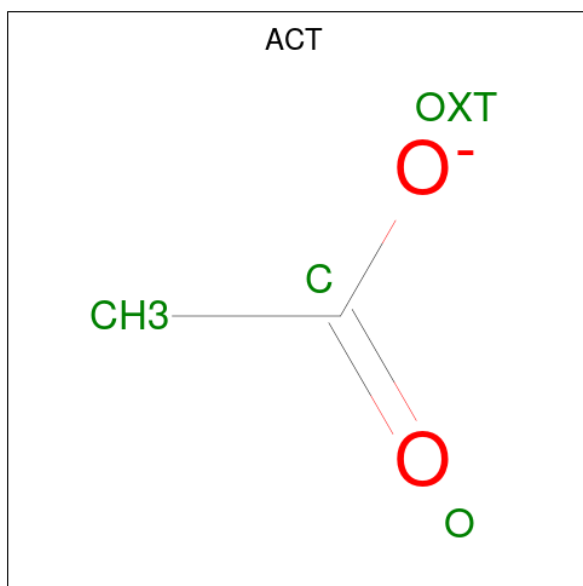
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	214	1617	1026	288	293	10	0	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



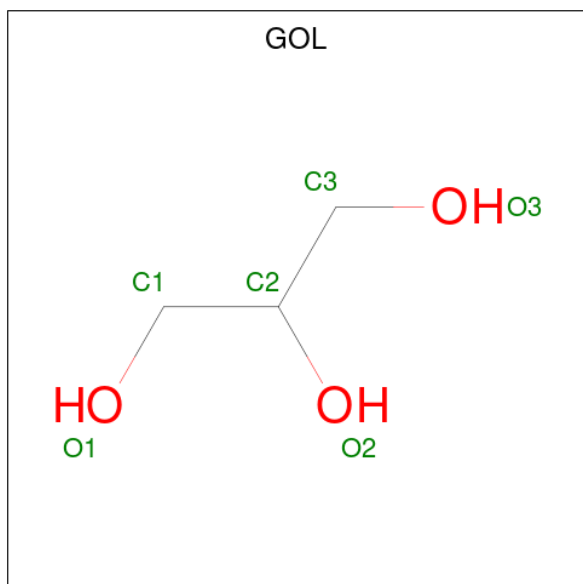
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



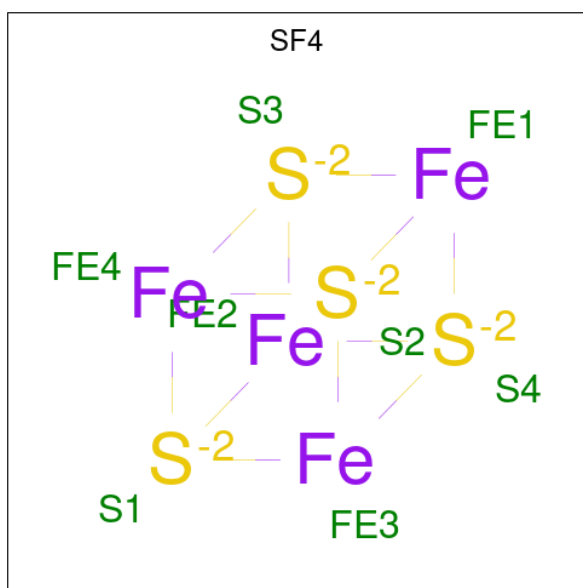
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

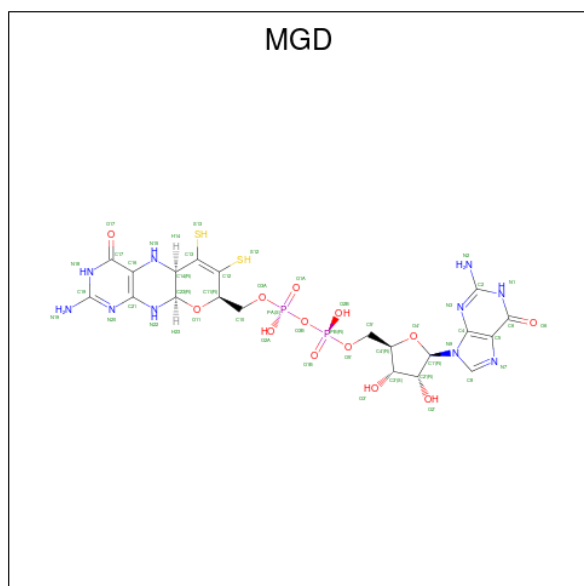


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0

- Molecule 8 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

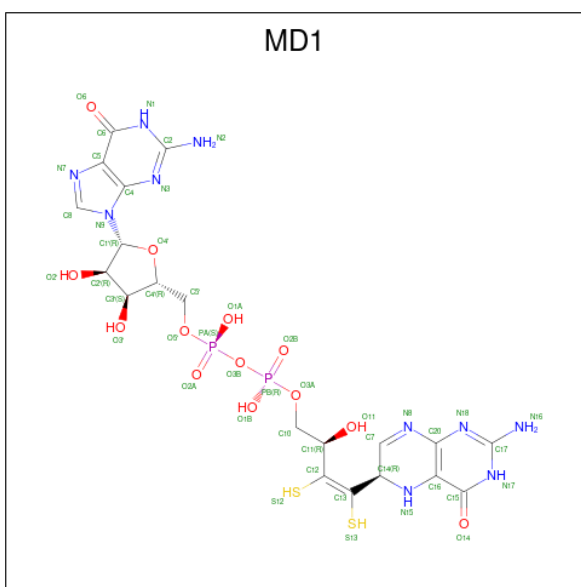
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mo	0	0
			1	1		

- Molecule 9 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



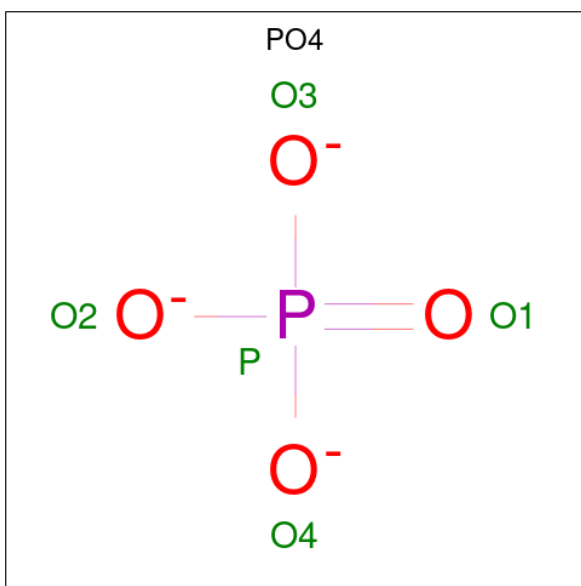
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 10 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (CCD ID: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



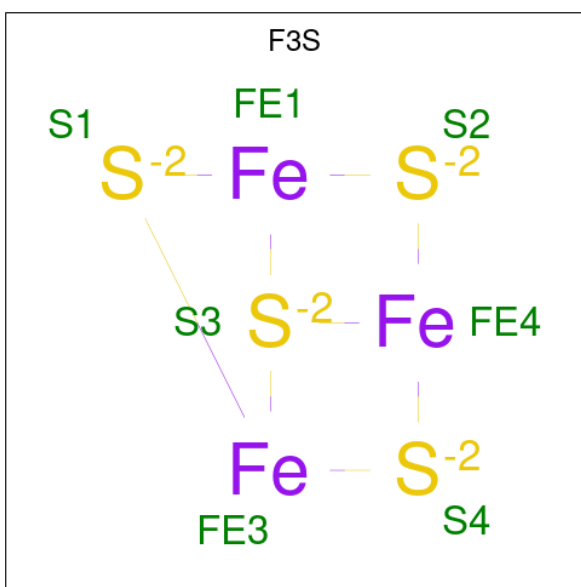
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



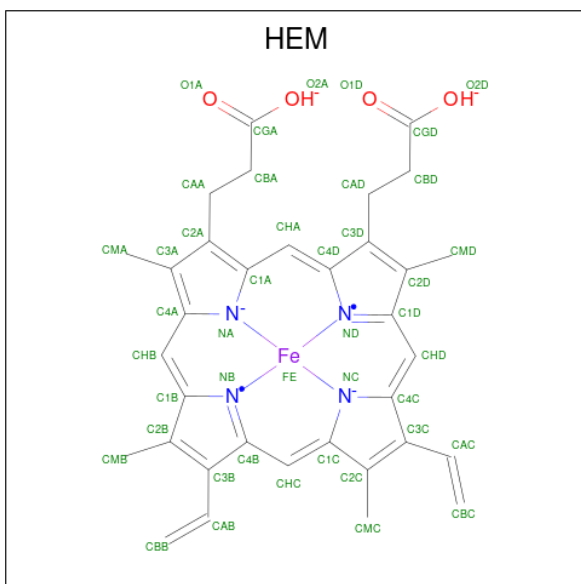
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 12 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			7	3	4		

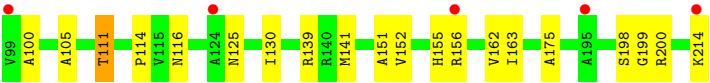
- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	492	Total 492	O 492	0	0
14	B	237	Total 237	O 237	0	0
14	C	89	Total 89	O 89	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.53Å 67.32Å 114.77Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	46.42 – 1.88 46.42 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.42-1.88) 98.1 (46.42-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.148 , 0.183 0.161 , 0.193	Depositor DCC
R_{free} test set	6423 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12639	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, F3S, HEM, MES, PO4, MGD, GOL, SF4, MO, MD1

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	0.91	2/7494 (0.0%)	0.92	1/10140 (0.0%)
2	B	0.96	1/2744 (0.0%)	0.93	0/3715
3	C	0.74	0/1651	0.87	2/2225 (0.1%)
All	All	0.90	3/11889 (0.0%)	0.92	3/16080 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	ALA	CA-CB	9.99	1.61	1.52
2	B	292	ARG	CG-CD	-5.35	1.36	1.52
1	A	792	ILE	C-O	-5.10	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	96	MET	CG-SD-CE	-5.90	87.92	100.90
1	A	67	ILE	N-CA-C	5.15	117.53	111.09
3	C	12	LEU	N-CA-C	-5.14	107.07	113.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	11	GLU	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	7285	0	7052	77	0
2	B	2669	0	2581	31	0
3	C	1617	0	1628	31	0
4	A	12	0	12	0	0
5	A	8	0	6	2	0
6	A	24	0	32	7	0
6	B	12	0	16	3	0
6	C	12	0	16	1	0
7	A	8	0	0	0	0
7	B	24	0	0	0	0
8	A	1	0	0	0	0
9	A	47	0	22	1	0
10	A	47	0	21	4	0
11	B	5	0	0	0	0
12	B	7	0	0	0	0
13	C	43	0	30	3	0
14	A	492	0	0	7	1
14	B	237	0	0	5	1
14	C	89	0	0	2	0
All	All	12639	0	11416	142	1

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 6.

All (142) 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)
3:C:116:ASN:HD22	3:C:175:ALA:H	1.21	0.89
1:A:944:HIS:HA	6:A:1981:GOL:H12	1.64	0.80
3:C:16:LEU:O	3:C:72:ARG:NH1	2.12	0.79
1:A:206:MET:HE1	1:A:604:MET:SD	2.27	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:ARG:HG2	3:C:141:MET:HE2	1.68	0.74
3:C:8:GLY:HA3	3:C:12:LEU:HD12	1.70	0.74
1:A:67:ILE:HB	14:A:2002:HOH:O	1.87	0.72
1:A:944:HIS:HA	6:A:1981:GOL:C1	2.23	0.68
6:A:1981:GOL:H31	6:A:1982:GOL:O1	1.95	0.66
1:A:134:ASN:HD21	2:B:44:LYS:NZ	1.95	0.65
3:C:6:VAL:HG11	3:C:20:ILE:HG12	1.79	0.64
2:B:165:THR:HG22	13:C:1217:HEM:CGD	2.26	0.64
1:A:505:GLU:HA	1:A:508:GLN:HE21	1.63	0.64
1:A:87:TRP:HA	1:A:88:PRO:C	2.22	0.63
1:A:836:MET:HE2	1:A:840:ASP:HA	1.79	0.63
10:A:1987:MD1:H11	10:A:1987:MD1:C7	2.29	0.62
1:A:209:LEU:HD22	1:A:726:LYS:HE3	1.82	0.61
1:A:891:MET:HE1	1:A:904:MET:HE3	1.83	0.60
6:B:1355:GOL:H12	14:B:2237:HOH:O	2.00	0.60
1:A:593:ARG:HA	1:A:594:PRO:C	2.26	0.60
3:C:6:VAL:HG13	3:C:7:PRO:HD2	1.83	0.60
1:A:554:VAL:O	1:A:554:VAL:HG12	2.04	0.58
3:C:39:VAL:O	3:C:42:VAL:HG13	2.04	0.57
1:A:841:HIS:HD2	1:A:972:SER:OG	1.87	0.57
1:A:588:THR:H	1:A:591:HIS:HD2	1.52	0.57
1:A:850:PRO:HB3	14:A:2463:HOH:O	2.05	0.57
2:B:340:ARG:CZ	14:B:2225:HOH:O	2.53	0.56
1:A:357:TYR:HB3	1:A:366:VAL:HG22	1.88	0.56
1:A:334:LEU:CD1	1:A:366:VAL:HG23	2.35	0.56
1:A:206:MET:HG2	1:A:210:MET:HE2	1.86	0.56
3:C:100:ALA:HB2	3:C:114:PRO:HD2	1.88	0.56
1:A:437:LYS:CE	14:A:2197:HOH:O	2.54	0.55
2:B:27:LYS:HB2	2:B:234:VAL:HG22	1.88	0.55
1:A:337:MET:HA	1:A:337:MET:HE2	1.87	0.55
3:C:116:ASN:ND2	3:C:175:ALA:H	1.99	0.55
3:C:36:LEU:O	3:C:39:VAL:HG22	2.07	0.55
1:A:206:MET:HE1	1:A:604:MET:CE	2.37	0.54
1:A:849:HIS:HD1	9:A:1986:MGD:H15	1.56	0.54
1:A:192:HIS:CE1	5:A:1978:ACT:H3	2.44	0.53
1:A:783:ALA:HA	1:A:797:TRP:CE3	2.43	0.53
1:A:203:GLY:HA2	1:A:206:MET:HE2	1.90	0.53
1:A:337:MET:HE3	1:A:399:ARG:HG2	1.91	0.53
2:B:167:ALA:HA	2:B:183:ARG:HE	1.73	0.53
2:B:218:ILE:C	2:B:218:ILE:HD12	2.35	0.52
1:A:116:ASN:HD22	1:A:118:ASP:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LYS:HD3	2:B:111:VAL:HG11	1.92	0.52
3:C:6:VAL:CG2	3:C:63:LEU:HD22	2.40	0.52
1:A:927:LYS:NZ	14:A:2467:HOH:O	2.42	0.52
2:B:165:THR:HG22	13:C:1217:HEM:O1D	2.10	0.52
1:A:385:THR:HG21	1:A:397:GLN:OE1	2.10	0.52
1:A:619:LYS:NZ	1:A:623:ASP:OD2	2.42	0.52
1:A:192:HIS:HE1	5:A:1978:ACT:H3	1.74	0.51
2:B:189:HIS:CE1	3:C:46:LEU:HD13	2.45	0.51
1:A:195:ALA:HA	10:A:1987:MD1:C6	2.41	0.51
1:A:206:MET:HE1	1:A:604:MET:HE1	1.93	0.50
1:A:841:HIS:HE1	1:A:897:ASP:OD1	1.95	0.50
1:A:207:THR:HG21	1:A:214:SER:OG	2.11	0.50
3:C:90:VAL:HG22	6:C:1215:GOL:H11	1.94	0.50
10:A:1987:MD1:H11	10:A:1987:MD1:H7	1.94	0.50
1:A:879:LYS:NZ	14:A:2440:HOH:O	2.44	0.49
13:C:1217:HEM:HHC	13:C:1217:HEM:HBB2	1.94	0.49
1:A:936:LEU:HD13	1:A:966:ASP:HB2	1.94	0.49
3:C:79:LYS:HD3	3:C:155:HIS:HB3	1.94	0.49
1:A:586:TRP:O	6:A:1982:GOL:H2	2.13	0.49
1:A:289:THR:N	1:A:290:PRO:CD	2.76	0.48
3:C:96:MET:HE1	3:C:105:ALA:HA	1.96	0.48
1:A:673:PHE:CZ	1:A:763:LYS:HG2	2.49	0.47
3:C:49:SER:OG	3:C:200:ARG:NH1	2.45	0.47
2:B:229:GLN:O	2:B:231:PRO:HD3	2.14	0.47
3:C:152:VAL:HG22	3:C:163:ILE:HB	1.97	0.47
2:B:62:LYS:HE2	14:B:2032:HOH:O	2.15	0.46
2:B:195:PRO:HB2	2:B:264:TYR:CD2	2.51	0.46
3:C:83:ILE:HA	3:C:88:SER:OG	2.15	0.46
1:A:491:LEU:HD22	1:A:743:MET:HE3	1.98	0.46
1:A:218:ASN:ND2	1:A:481:TRP:HZ2	2.14	0.46
1:A:534:MET:HG3	1:A:777:VAL:CG2	2.46	0.45
2:B:27:LYS:CB	2:B:234:VAL:HG22	2.46	0.45
3:C:40:LYS:NZ	14:C:2017:HOH:O	2.46	0.45
1:A:669:PRO:HG2	6:A:1979:GOL:H32	1.98	0.45
1:A:440:THR:H	1:A:470:ASN:ND2	2.15	0.45
1:A:187:ILE:HD11	1:A:600:PRO:HB3	1.98	0.44
1:A:187:ILE:CD1	1:A:600:PRO:HB3	2.46	0.44
1:A:437:LYS:HE2	14:A:2197:HOH:O	2.17	0.44
1:A:589:ASN:O	1:A:589:ASN:OD1	2.34	0.44
1:A:533:PHE:CZ	1:A:537:VAL:HG11	2.53	0.44
6:A:1981:GOL:C3	6:A:1982:GOL:O1	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:NZ	1:A:950:GLU:OE1	2.50	0.44
2:B:59:TYR:HA	2:B:60:PRO:C	2.43	0.44
3:C:139:ARG:HG2	3:C:141:MET:CE	2.43	0.44
1:A:224:THR:O	1:A:449:ALA:HB2	2.18	0.44
1:A:439:ARG:HA	1:A:470:ASN:HD21	1.83	0.44
1:A:872:PRO:HA	1:A:921:TRP:CE2	2.53	0.44
2:B:190:CYS:HB2	2:B:199:ILE:HD12	1.99	0.44
1:A:240:SER:HA	1:A:666:SER:O	2.18	0.44
2:B:180:ASP:OD1	2:B:180:ASP:C	2.61	0.43
1:A:224:THR:HG22	1:A:449:ALA:HB1	1.99	0.43
2:B:253:LYS:HZ3	2:B:327:GLU:CD	2.26	0.43
3:C:6:VAL:CG1	3:C:7:PRO:HD2	2.48	0.43
1:A:87:TRP:CA	1:A:88:PRO:C	2.89	0.43
2:B:151:CYS:HB3	2:B:211:CYS:HB3	2.01	0.43
2:B:228:ARG:HE	6:B:1353:GOL:H31	1.83	0.43
1:A:218:ASN:ND2	1:A:481:TRP:CZ2	2.87	0.42
2:B:159:CYS:HB2	2:B:199:ILE:HD11	2.00	0.42
1:A:206:MET:HE2	1:A:206:MET:HB3	1.73	0.42
1:A:836:MET:CE	1:A:840:ASP:HA	2.47	0.42
3:C:28:THR:HG23	3:C:59:ASP:OD1	2.19	0.42
3:C:71:LEU:O	3:C:163:ILE:HA	2.19	0.42
1:A:229:PHE:HB2	1:A:235:MET:HE2	2.01	0.42
3:C:198:SER:OG	3:C:199:GLY:N	2.44	0.42
2:B:131:ASP:HA	2:B:134:GLN:OE1	2.20	0.42
3:C:19:PRO:O	3:C:22:ALA:HB3	2.19	0.42
1:A:949:TYR:O	1:A:950:GLU:C	2.62	0.42
1:A:534:MET:HG3	1:A:777:VAL:HG22	2.02	0.42
2:B:154:CYS:HB3	2:B:266:THR:O	2.19	0.42
3:C:151:ALA:HA	3:C:163:ILE:O	2.20	0.42
3:C:28:THR:CG2	3:C:57:ARG:HG3	2.50	0.41
2:B:165:THR:HG21	2:B:185:LYS:HD2	2.02	0.41
2:B:340:ARG:NH2	14:B:2225:HOH:O	2.53	0.41
2:B:256:VAL:HG21	2:B:328:LEU:HD11	2.02	0.41
3:C:111:THR:HG23	14:C:2046:HOH:O	2.20	0.41
1:A:324:PHE:CD1	1:A:469:GLY:HA2	2.56	0.41
1:A:76:LYS:HE3	1:A:98:VAL:HG21	2.03	0.41
1:A:312:GLN:NE2	1:A:414:PRO:HD3	2.36	0.41
1:A:967:ARG:HH12	10:A:1987:MD1:H17	1.68	0.41
1:A:405:LEU:HD21	1:A:463:LEU:HD21	2.03	0.41
1:A:790:LYS:NZ	14:A:2375:HOH:O	2.54	0.41
1:A:797:TRP:O	1:A:801:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG23	1:A:292:ALA:HB2	2.03	0.41
2:B:16:LYS:NZ	2:B:17:ARG:O	2.54	0.41
2:B:168:ILE:HG12	2:B:179:VAL:HG22	2.01	0.41
3:C:13:LEU:O	3:C:163:ILE:HD13	2.21	0.41
1:A:944:HIS:O	6:A:1981:GOL:H32	2.21	0.40
2:B:188:ARG:HD3	2:B:201:PHE:CG	2.55	0.40
3:C:97:PHE:HB2	3:C:175:ALA:HB2	2.02	0.40
3:C:100:ALA:CB	3:C:114:PRO:HD2	2.51	0.40
1:A:116:ASN:ND2	1:A:118:ASP:H	2.20	0.40
1:A:252:MET:HE3	1:A:268:LEU:HD13	2.02	0.40
2:B:171:ARG:HD2	14:B:2118:HOH:O	2.21	0.40
1:A:220:ASP:OD2	1:A:614:LYS:NZ	2.53	0.40
2:B:228:ARG:HE	6:B:1353:GOL:C2	2.34	0.40
1:A:696:LYS:NZ	1:A:700:GLU:OE2	2.27	0.40
1:A:910:ASN:HA	2:B:142:PRO:HG3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:2120:HOH:O	14:B:2149:HOH:O[2_645]	2.09	0.11

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	910/976 (93%)	887 (98%)	23 (2%)	0	100	100
2	B	335/352 (95%)	323 (96%)	12 (4%)	0	100	100
3	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	1457/1542 (94%)	1414 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	766/816 (94%)	755 (99%)	11 (1%)	59	48
2	B	285/298 (96%)	283 (99%)	2 (1%)	76	69
3	C	163/164 (99%)	154 (94%)	9 (6%)	19	5
All	All	1214/1278 (95%)	1192 (98%)	22 (2%)	51	38

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	106	GLU
1	A	234	LYS
1	A	325	VAL
1	A	366	VAL
1	A	387	SER
1	A	582	LYS
1	A	608	GLN
1	A	670	PHE
1	A	924	HIS
1	A	932	TYR
2	B	213	LEU
2	B	218	ILE
3	C	10	LYS
3	C	42	VAL
3	C	88	SER
3	C	111	THR
3	C	125	ASN
3	C	130	ILE
3	C	156	ARG
3	C	162	VAL
3	C	214	LYS

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

Mol	Chain	Res	Type
1	A	116	ASN
1	A	134	ASN
1	A	218	ASN
1	A	312	GLN
1	A	470	ASN
1	A	507	HIS
1	A	508	GLN
1	A	589	ASN
1	A	591	HIS
1	A	601	GLN
1	A	714	ASN
1	A	747	ASN
1	A	841	HIS
2	B	55	ASN
2	B	112	HIS
2	B	269	ASN
3	C	116	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\# Z > 2$
6	GOL	B	1355	-	5,5,5	0.46	0	5,5,5	0.43	0
7	SF4	B	1359	2	0,12,12	-	-	-	-	-
9	MGD	A	1986	8	45,52,52	1.47	6 (13%)	54,81,81	1.77	12 (22%)
6	GOL	A	1982	-	5,5,5	0.28	0	5,5,5	0.60	0
6	GOL	A	1979	-	5,5,5	0.47	0	5,5,5	0.74	0
10	MD1	A	1987	8	43,51,51	2.18	4 (9%)	53,78,78	1.56	10 (18%)
7	SF4	A	1984	1	0,12,12	-	-	-	-	-
7	SF4	B	1358	2	0,12,12	-	-	-	-	-
5	ACT	A	1983	-	3,3,3	0.74	0	3,3,3	1.03	0
6	GOL	B	1353	-	5,5,5	0.78	0	5,5,5	2.20	3 (60%)
7	SF4	B	1357	2	0,12,12	-	-	-	-	-
6	GOL	A	1980	-	5,5,5	0.38	0	5,5,5	0.63	0
5	ACT	A	1978	8	3,3,3	0.47	0	3,3,3	2.15	2 (66%)
11	PO4	B	1354	-	4,4,4	0.73	0	6,6,6	0.57	0
12	F3S	B	1356	2	0,9,9	-	-	-	-	-
6	GOL	A	1981	-	5,5,5	0.40	0	5,5,5	1.59	1 (20%)
6	GOL	C	1216	-	5,5,5	0.33	0	5,5,5	0.23	0
6	GOL	C	1215	-	5,5,5	0.31	0	5,5,5	0.66	0
4	MES	A	1977	-	12,12,12	1.53	1 (8%)	14,16,16	2.90	5 (35%)
13	HEM	C	1217	3	50,50,50	1.74	7 (14%)	66,82,82	1.34	5 (7%)

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
12	F3S	B	1356	2	-	-	0/3/3/3
6	GOL	A	1981	-	-	3/4/4/4	-
6	GOL	B	1355	-	-	2/4/4/4	-
10	MD1	A	1987	8	1/1/10/12	4/22/59/59	0/5/5/5
6	GOL	B	1353	-	-	2/4/4/4	-
9	MGD	A	1986	8	-	0/22/66/66	0/6/6/6
7	SF4	B	1359	2	-	-	0/6/5/5
6	GOL	C	1216	-	-	0/4/4/4	-
6	GOL	A	1980	-	-	0/4/4/4	-
7	SF4	B	1357	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	1215	-	-	0/4/4/4	-
13	HEM	C	1217	3	-	2/14/54/54	-
6	GOL	A	1982	-	-	1/4/4/4	-
7	SF4	A	1984	1	-	-	0/6/5/5
4	MES	A	1977	-	-	4/6/14/14	0/1/1/1
7	SF4	B	1358	2	-	-	0/6/5/5
6	GOL	A	1979	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1987	MD1	C7-N8	12.32	1.44	1.28
13	C	1217	HEM	C3D-C2D	7.79	1.53	1.36
9	A	1986	MGD	O11-C11	-4.84	1.37	1.43
4	A	1977	MES	C8-S	-4.67	1.70	1.77
13	C	1217	HEM	FE-ND	4.01	2.07	1.94
9	A	1986	MGD	C21-N22	3.74	1.39	1.35
13	C	1217	HEM	FE-NB	3.34	2.05	1.94
10	A	1987	MD1	C5-N7	-2.98	1.33	1.39
9	A	1986	MGD	C23-C14	2.84	1.55	1.53
13	C	1217	HEM	CAC-C3C	2.65	1.54	1.47
9	A	1986	MGD	C14-N15	2.64	1.49	1.46
10	A	1987	MD1	C14-C13	-2.59	1.48	1.51
9	A	1986	MGD	C4-N9	-2.55	1.31	1.38
13	C	1217	HEM	CMD-C2D	2.42	1.55	1.50
13	C	1217	HEM	CAB-C3B	2.32	1.53	1.47
13	C	1217	HEM	CMC-C2C	2.13	1.55	1.50
9	A	1986	MGD	PA-O2A	-2.08	1.45	1.55
10	A	1987	MD1	O11-C11	2.04	1.47	1.42

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1977	MES	C5-N4-C3	6.25	122.89	108.83
4	A	1977	MES	O2S-S-C8	6.10	114.26	106.92
9	A	1986	MGD	C19-N20-C21	4.70	121.91	113.43
9	A	1986	MGD	C2-N3-C4	4.48	120.29	112.30
10	A	1987	MD1	C2-N3-C4	4.39	120.12	112.30
13	C	1217	HEM	C4D-ND-C1D	4.35	109.57	105.07
4	A	1977	MES	C7-N4-C5	4.06	121.61	111.23
9	A	1986	MGD	N1-C2-N3	-3.56	116.69	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1987	MD1	C5-C4-N3	-3.34	123.04	128.46
9	A	1986	MGD	N18-C19-N20	-3.24	117.27	123.32
9	A	1986	MGD	C5'-C4'-C3'	-3.19	103.22	115.18
13	C	1217	HEM	C1B-NB-C4B	3.15	108.33	105.07
9	A	1986	MGD	C6-C5-N7	3.07	135.96	130.25
13	C	1217	HEM	CHD-C4C-NC	3.02	127.70	124.44
10	A	1987	MD1	C17-N18-C20	3.01	118.37	114.20
9	A	1986	MGD	C4'-O4'-C1'	-2.92	103.03	109.47
13	C	1217	HEM	C1D-C2D-C3D	-2.91	103.90	106.96
13	C	1217	HEM	CAA-CBA-CGA	-2.90	107.37	113.60
10	A	1987	MD1	N1-C2-N3	-2.80	118.10	123.32
4	A	1977	MES	C2-C3-N4	2.78	114.33	110.10
6	B	1353	GOL	O1-C1-C2	2.75	123.38	110.20
5	A	1978	ACT	OXT-C-CH3	2.64	126.09	115.18
10	A	1987	MD1	O4'-C1'-N9	2.64	114.39	108.36
6	A	1981	GOL	O1-C1-C2	2.63	122.80	110.20
6	B	1353	GOL	O2-C2-C3	-2.60	97.65	109.12
5	A	1978	ACT	OXT-C-O	-2.60	112.46	122.05
9	A	1986	MGD	C5-C4-N3	-2.59	124.26	128.46
9	A	1986	MGD	O17-C17-C16	-2.54	121.42	127.24
9	A	1986	MGD	N19-C19-N20	2.50	124.60	119.73
10	A	1987	MD1	O14-C15-C16	-2.48	121.55	127.24
10	A	1987	MD1	C6-C5-N7	2.47	134.85	130.25
6	B	1353	GOL	C3-C2-C1	2.45	121.23	111.70
4	A	1977	MES	O1S-S-C8	-2.40	104.02	106.92
9	A	1986	MGD	C17-C16-N15	2.35	123.07	116.76
10	A	1987	MD1	C4'-O4'-C1'	-2.33	104.34	109.47
10	A	1987	MD1	N2-C2-N1	2.12	121.24	116.71
10	A	1987	MD1	O1B-PB-O2B	2.10	122.63	112.24
9	A	1986	MGD	O11-C23-N22	-2.09	106.42	108.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	1987	MD1	C14

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1981	GOL	C1-C2-C3-O3
6	B	1353	GOL	O1-C1-C2-O2
6	B	1353	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1977	MES	C7-C8-S-O3S
6	A	1979	GOL	O1-C1-C2-C3
6	A	1982	GOL	C1-C2-C3-O3
6	B	1355	GOL	C1-C2-C3-O3
6	A	1981	GOL	O2-C2-C3-O3
4	A	1977	MES	C8-C7-N4-C3
6	A	1979	GOL	O1-C1-C2-O2
10	A	1987	MD1	PB-O3B-PA-O5'
4	A	1977	MES	C7-C8-S-O1S
4	A	1977	MES	C7-C8-S-O2S
13	C	1217	HEM	C3D-CAD-CBD-CGD
6	B	1355	GOL	O2-C2-C3-O3
6	A	1981	GOL	O1-C1-C2-C3
10	A	1987	MD1	C10-O3A-PB-O1B
10	A	1987	MD1	C10-O3A-PB-O2B
10	A	1987	MD1	O4'-C4'-C5'-O5'
13	C	1217	HEM	CAD-CBD-CGD-O2D

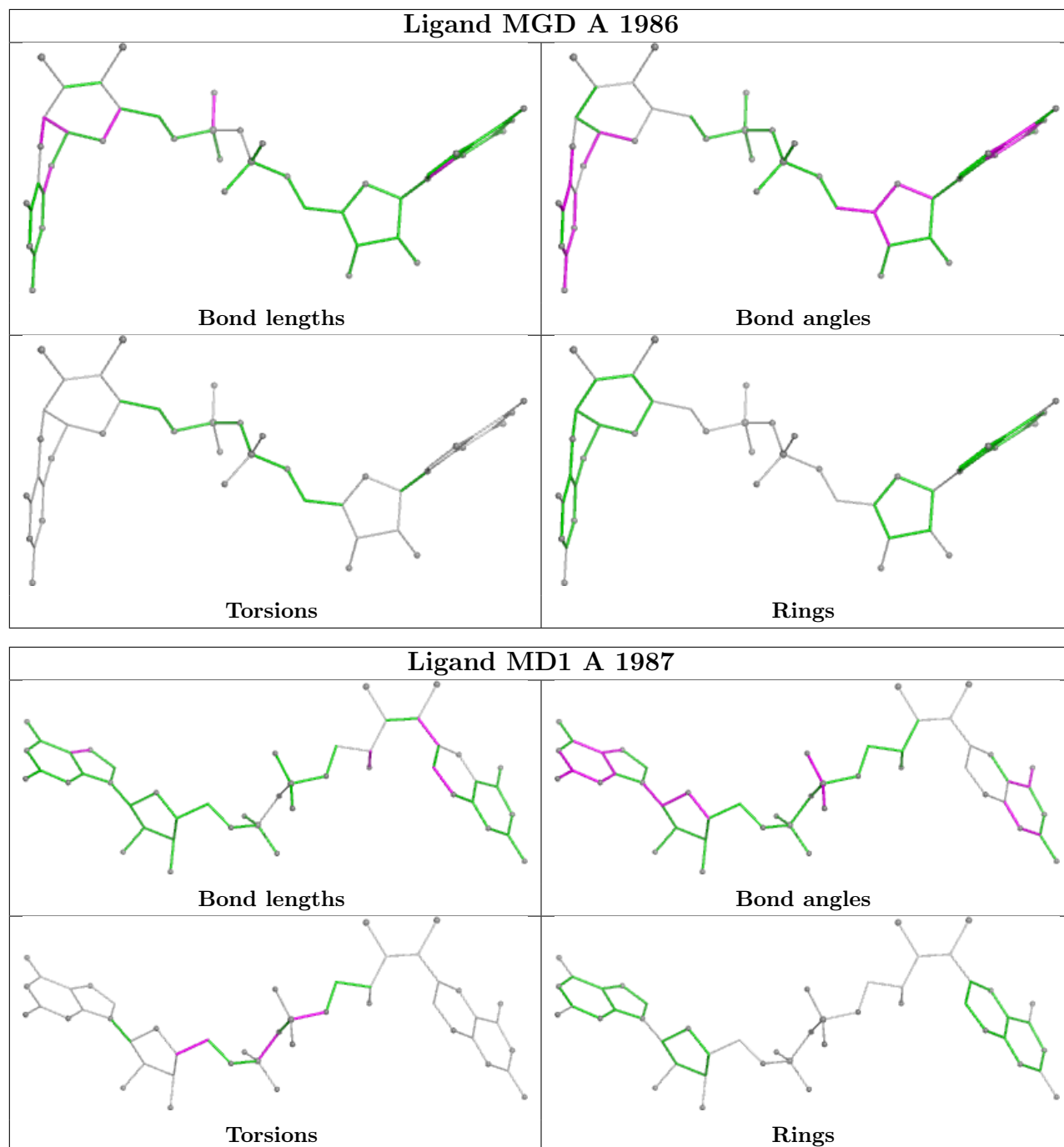
There are no ring outliers.

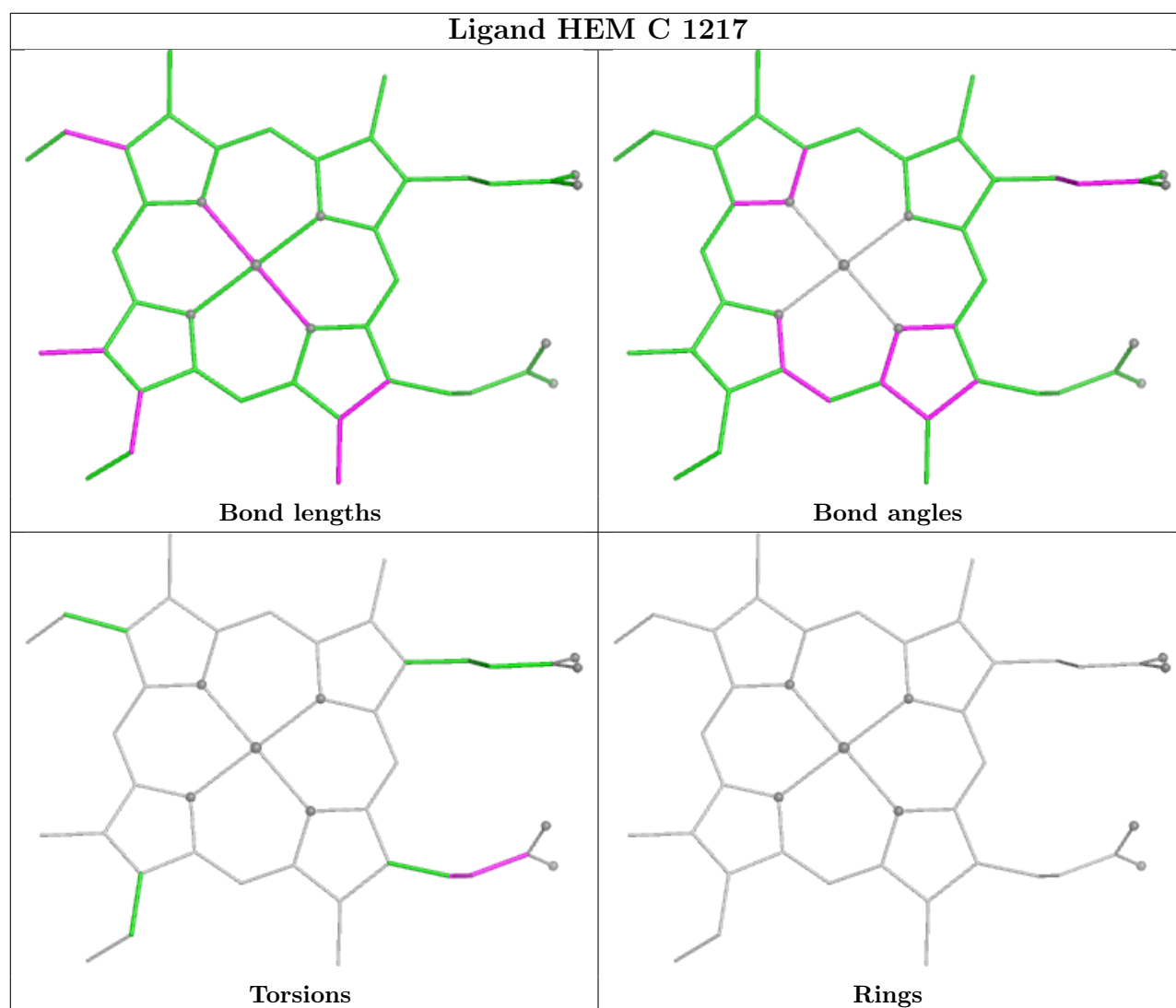
10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1355	GOL	1	0
9	A	1986	MGD	1	0
6	A	1982	GOL	3	0
6	A	1979	GOL	1	0
10	A	1987	MD1	4	0
6	B	1353	GOL	2	0
5	A	1978	ACT	2	0
6	A	1981	GOL	5	0
6	C	1215	GOL	1	0
13	C	1217	HEM	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.





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	912/976 (93%)	0.44	18 (1%) 65 71	19, 24, 33, 50	0
2	B	337/352 (95%)	0.22	6 (1%) 67 73	18, 24, 31, 46	0
3	C	214/214 (100%)	0.88	16 (7%) 20 23	17, 25, 34, 42	0
All	All	1463/1542 (94%)	0.45	40 (2%) 56 61	17, 24, 33, 50	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ILE	4.0
1	A	138	TYR	3.9
1	A	589	ASN	3.8
2	B	76	LEU	3.6
3	C	86	LEU	3.4
3	C	124	ALA	3.3
1	A	506	LEU	3.3
3	C	84	VAL	3.2
1	A	513	PHE	3.2
1	A	520	ALA	3.1
1	A	882	ALA	3.0
2	B	77	ARG	2.9
3	C	83	ILE	2.9
3	C	8	GLY	2.9
3	C	9	GLY	2.9
3	C	99	VAL	2.7
3	C	214	LYS	2.7
1	A	516	ARG	2.7
1	A	509	MET	2.6
3	C	25	GLU	2.6
3	C	12	LEU	2.6
1	A	101	GLY	2.6
1	A	392	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	518	LEU	2.5
1	A	68	TYR	2.3
2	B	78	GLY	2.3
3	C	156	ARG	2.3
2	B	79	GLU	2.3
2	B	172	GLU	2.3
1	A	483	TYR	2.2
1	A	507	HIS	2.2
2	B	183	ARG	2.2
3	C	82	LYS	2.1
1	A	362	LYS	2.1
1	A	505	GLU	2.1
1	A	363	ALA	2.1
3	C	24	ALA	2.1
3	C	195	ALA	2.1
3	C	68	MET	2.0
3	C	10	LYS	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
6	GOL	A	1980	6/6	0.83	0.17	33,36,36,37	0
6	GOL	B	1355	6/6	0.84	0.16	45,46,47,47	0
11	PO4	B	1354	5/5	0.84	0.14	44,47,47,48	0
6	GOL	A	1981	6/6	0.88	0.13	32,36,38,39	0
6	GOL	A	1982	6/6	0.88	0.14	40,41,43,44	0
5	ACT	A	1983	4/4	0.89	0.15	34,37,38,38	0

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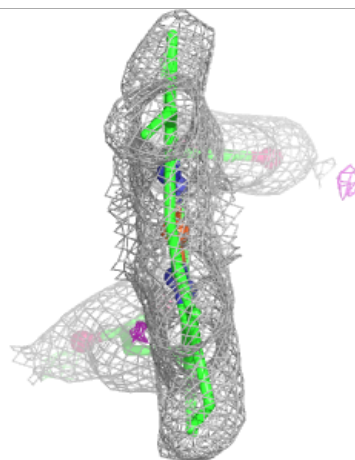
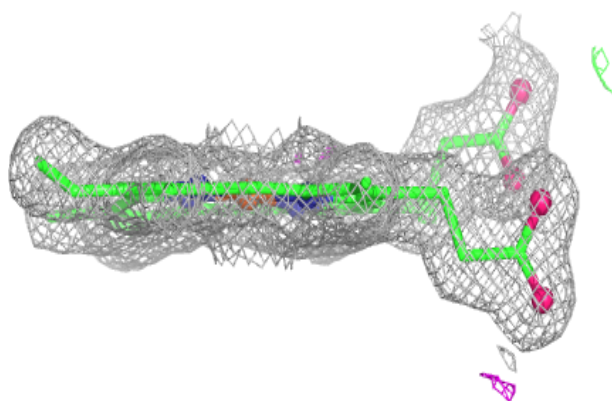
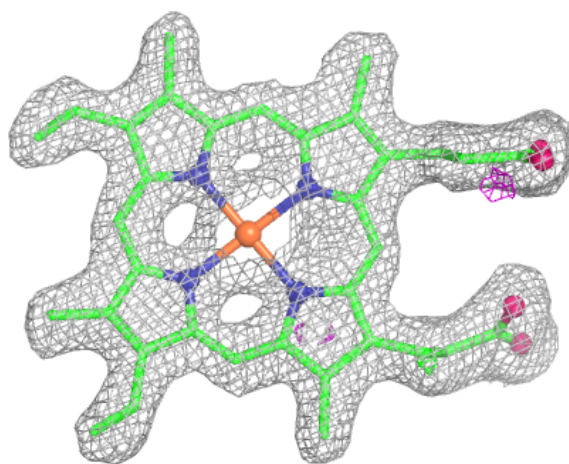
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	B	1353	6/6	0.89	0.18	24,31,33,37	0
6	GOL	C	1216	6/6	0.91	0.14	33,34,35,36	0
5	ACT	A	1978	4/4	0.91	0.18	23,25,26,28	0
6	GOL	C	1215	6/6	0.93	0.13	23,27,30,30	0
4	MES	A	1977	12/12	0.95	0.12	24,27,28,32	0
6	GOL	A	1979	6/6	0.96	0.12	16,20,23,24	0
13	HEM	C	1217	43/43	0.97	0.09	21,24,27,28	0
9	MGD	A	1986	47/47	0.98	0.07	10,14,16,17	0
10	MD1	A	1987	47/47	0.98	0.08	14,16,18,18	0
7	SF4	A	1984	8/8	0.99	0.06	23,25,26,26	0
7	SF4	B	1357	8/8	0.99	0.05	21,22,23,24	0
7	SF4	B	1358	8/8	0.99	0.04	24,24,25,25	0
12	F3S	B	1356	7/7	0.99	0.04	20,21,22,22	0
7	SF4	B	1359	8/8	0.99	0.04	23,24,24,26	0
8	MO	A	1985	1/1	1.00	0.11	19,19,19,19	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.

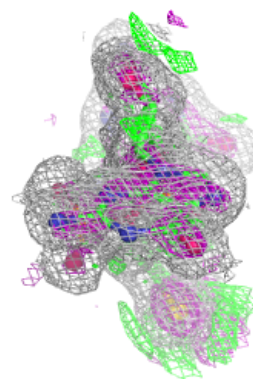
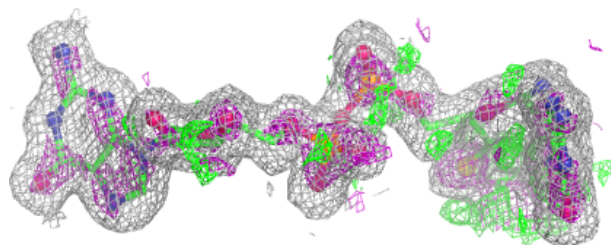
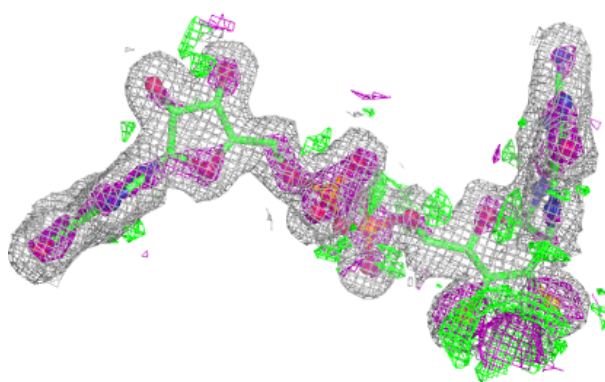
Electron density around HEM C 1217:

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

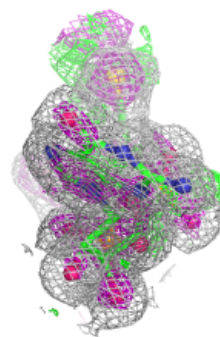
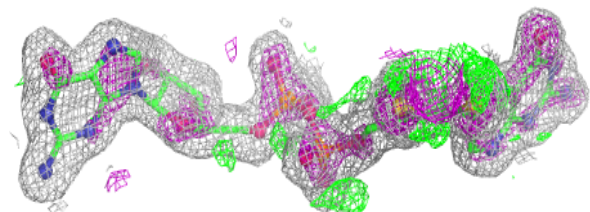
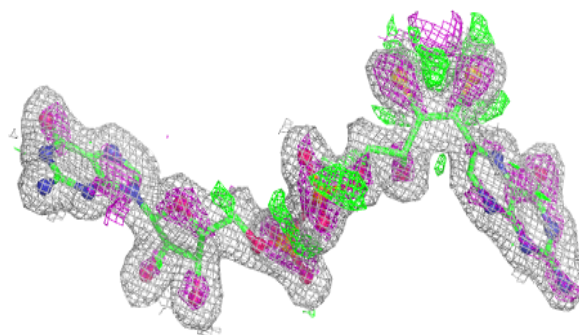


Electron density around MGD A 1986:

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

**Electron density around MD1 A 1987:**

$2mF_o-DF_c$ (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.