Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 01:00 PM EST

PDB ID	:	1KQG
Title	:	FORMATE DEHYDROGENASE N FROM E. COLI
Authors	:	Jormakka, M.; Tornroth, S.; Byrne, B.; Iwata, S.
Deposited on	:	2002-01-05
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

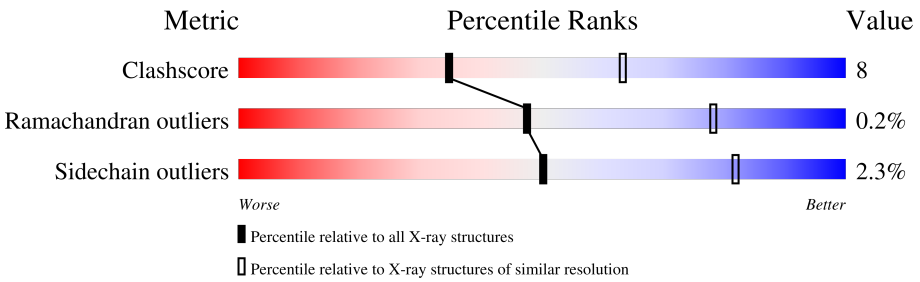
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1015	73% 21% • •
2	B	294	78% 17% • •
3	C	217	61% 32% 6% •

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14003 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 FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	982	7719	4872	1352	1457	37	1	0	0	0

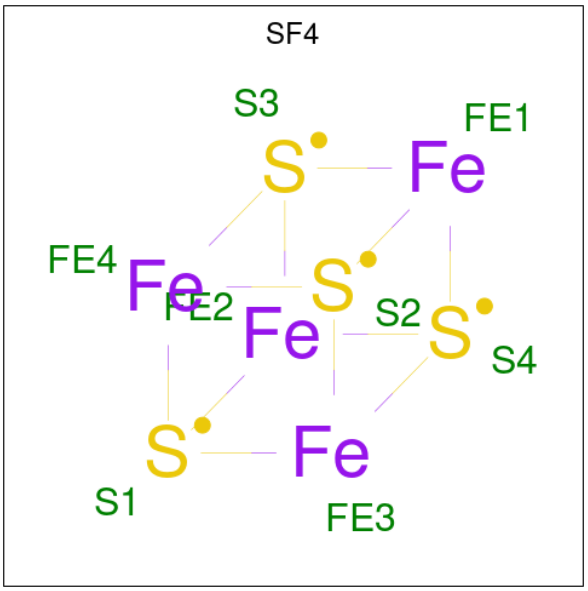
- Molecule 2 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	289	2207	1383	381	421	22	0	0	0

- Molecule 3 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT.

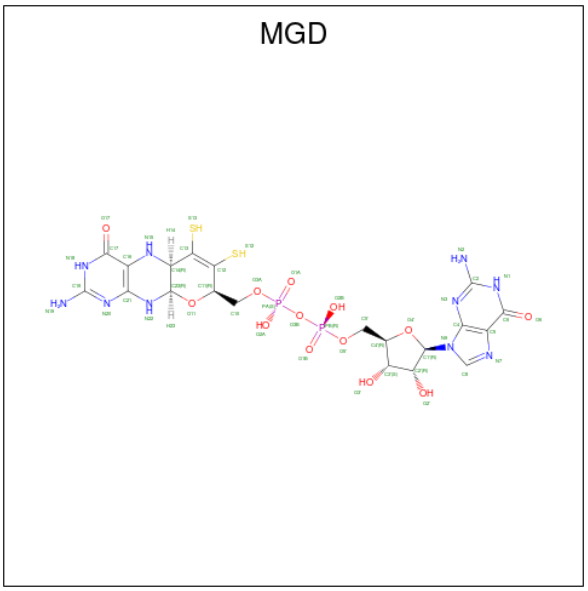
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	216	1783	1192	301	276	14	0	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 5 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 (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).

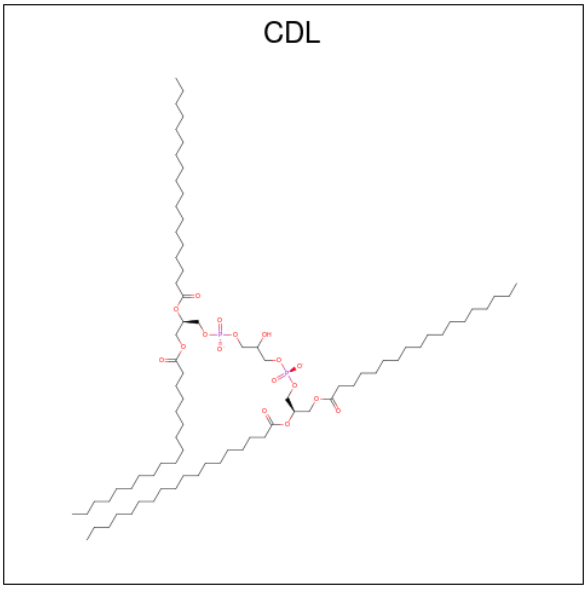


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
5	A	1	47	20	10	13	2	2	0	0

- Molecule 6 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

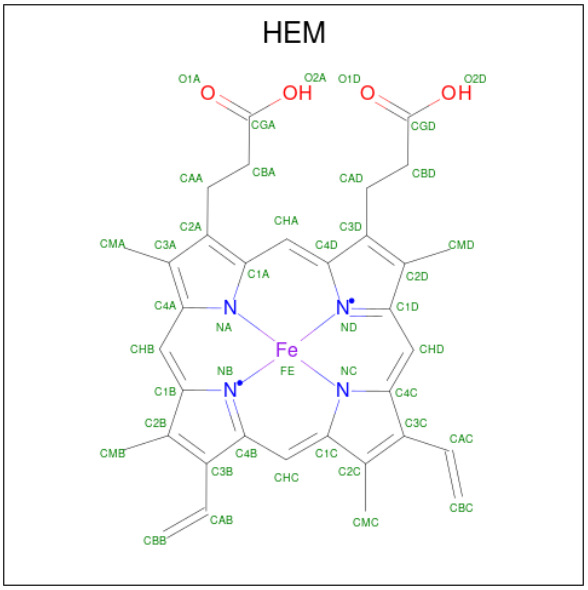
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
6	A	1	1	1	0	0

- Molecule 7 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



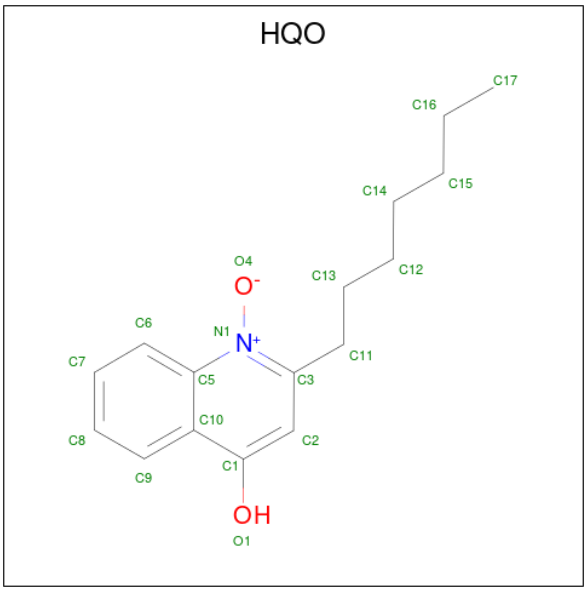
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
7	B	1	70	51	17	2	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 9 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: $C_{16}H_{21}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	C	1	19	16	1	2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	1493	1493	1493	0	0
			Total	O		
10	B	410	410	410	0	0
			Total	O		
10	C	81	81	81	0	0

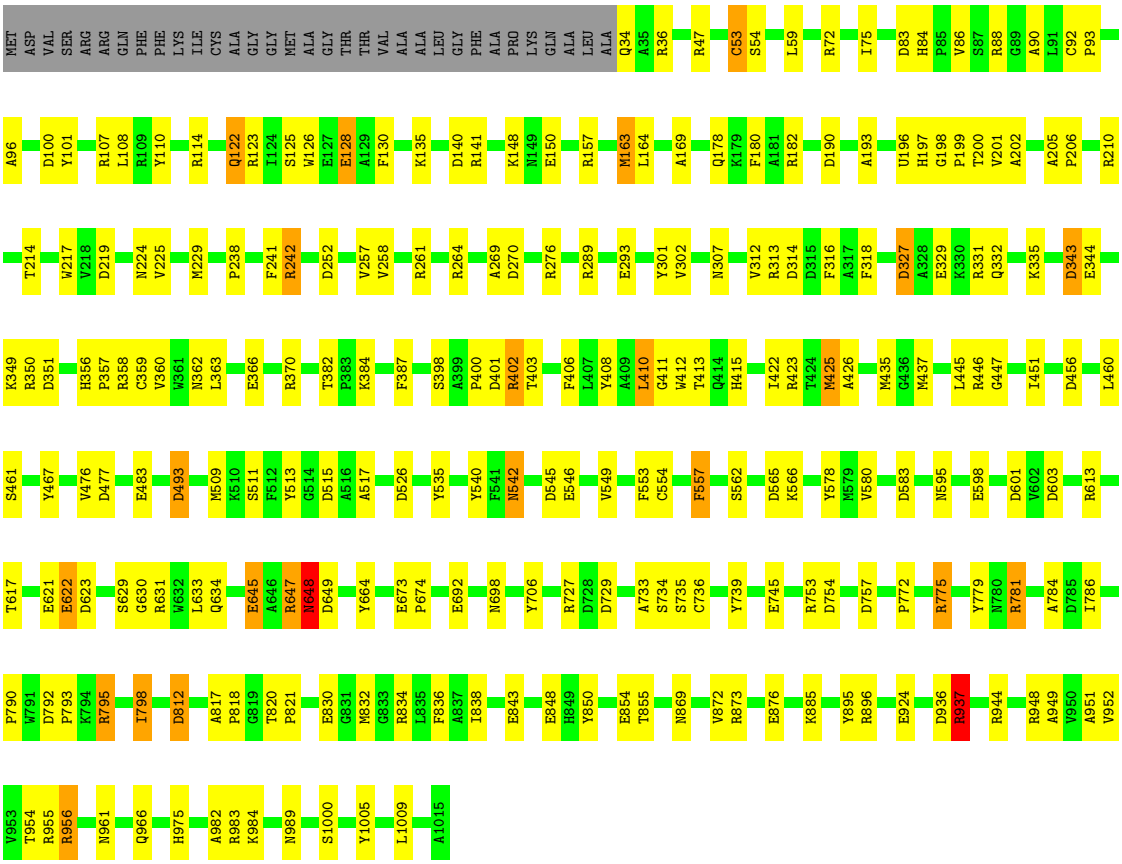
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

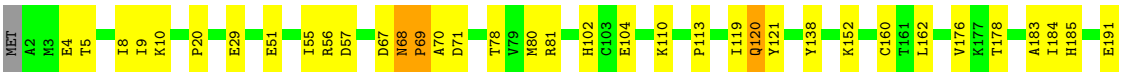
• Molecule 1: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT

Chain A: 73% 21%



• Molecule 2: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT

Chain B: 78% 17%



• Molecule 3: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT

Chain C:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	203.00Å 203.00Å 203.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.8 (40.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14003	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, HEM, 6MO, SF4, SEC, HQO, MGD

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	0.75	1/7910 (0.0%)	1.88	205/10749 (1.9%)
2	B	0.76	0/2255	1.66	39/3056 (1.3%)
3	C	0.67	0/1840	1.65	28/2483 (1.1%)
All	All	0.74	1/12005 (0.0%)	1.81	272/16288 (1.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	GLU	CD-OE1	5.14	1.31	1.25

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	ARG	NE-CZ-NH2	-36.10	102.25	120.30
1	A	937	ARG	NE-CZ-NH2	-21.45	109.57	120.30
1	A	873	ARG	NE-CZ-NH1	18.68	129.64	120.30
1	A	157	ARG	NE-CZ-NH2	16.52	128.56	120.30
3	C	74	ARG	NE-CZ-NH2	-16.10	112.25	120.30
1	A	313	ARG	NE-CZ-NH1	-16.08	112.26	120.30
1	A	88	ARG	NE-CZ-NH1	15.52	128.06	120.30
1	A	834	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	A	182	ARG	NE-CZ-NH1	-14.80	112.90	120.30
1	A	493	ASP	CB-CG-OD2	-14.37	105.37	118.30
1	A	72	ARG	NE-CZ-NH2	14.28	127.44	120.30
3	C	15	ARG	NE-CZ-NH2	-14.20	113.20	120.30
1	A	937	ARG	NH1-CZ-NH2	13.62	134.39	119.40
1	A	956	ARG	NE-CZ-NH1	-13.32	113.64	120.30
1	A	948	ARG	NE-CZ-NH2	-12.42	114.09	120.30
2	B	81	ARG	NE-CZ-NH1	-12.01	114.30	120.30
1	A	757	ASP	CB-CG-OD1	-11.87	107.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	795	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	A	47	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	A	36	ARG	NE-CZ-NH1	-10.79	114.90	120.30
3	C	149	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	A	141	ARG	NE-CZ-NH1	10.74	125.67	120.30
3	C	190	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	219	ASP	CB-CG-OD2	-10.57	108.79	118.30
1	A	446	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	A	613	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	A	955	ARG	NE-CZ-NH2	-10.38	115.11	120.30
3	C	9	ARG	NE-CZ-NH2	10.35	125.48	120.30
1	A	983	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	A	107	ARG	NE-CZ-NH2	10.31	125.45	120.30
1	A	812	ASP	CB-CG-OD1	-10.21	109.11	118.30
1	A	327	ASP	CB-CG-OD1	-10.03	109.28	118.30
3	C	74	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	A	834	ARG	NH1-CZ-NH2	-9.98	108.43	119.40
1	A	242	ARG	NE-CZ-NH1	-9.97	115.31	120.30
3	C	54	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	A	1005	TYR	CB-CG-CD2	9.78	126.87	121.00
1	A	123	ARG	NE-CZ-NH2	-9.74	115.43	120.30
2	B	81	ARG	NH1-CZ-NH2	9.73	130.10	119.40
1	A	114	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	745	GLU	OE1-CD-OE2	-9.70	111.66	123.30
1	A	848	GLU	OE1-CD-OE2	-9.45	111.96	123.30
2	B	81	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	A	88	ARG	NH1-CZ-NH2	9.35	129.69	119.40
1	A	289	ARG	NE-CZ-NH2	9.31	124.95	120.30
1	A	83	ASP	CB-CG-OD1	9.18	126.56	118.30
1	A	406	PHE	CB-CG-CD1	-9.14	114.41	120.80
1	A	157	ARG	NH1-CZ-NH2	-9.04	109.45	119.40
1	A	781	ARG	NE-CZ-NH2	9.00	124.80	120.30
1	A	350	ARG	NE-CZ-NH1	8.90	124.75	120.30
2	B	199	ARG	NE-CZ-NH1	-8.89	115.85	120.30
3	C	149	ARG	NH1-CZ-NH2	8.88	129.17	119.40
1	A	261	ARG	NE-CZ-NH1	8.83	124.71	120.30
3	C	149	ARG	NE-CZ-NH1	-8.81	115.89	120.30
1	A	122	GLN	OE1-CD-NE2	-8.80	101.66	121.90
1	A	753	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	A	937	ARG	NE-CZ-NH1	-8.55	116.02	120.30
2	B	197	GLU	OE1-CD-OE2	-8.51	113.09	123.30
3	C	191	ARG	NE-CZ-NH1	8.49	124.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	202	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	983	ARG	NH1-CZ-NH2	8.42	128.66	119.40
1	A	83	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	A	406	PHE	CB-CG-CD2	8.27	126.59	120.80
2	B	286	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	983	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	A	944	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	A	270	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	141	ARG	NH1-CZ-NH2	-7.92	110.69	119.40
1	A	107	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	A	727	ARG	NE-CZ-NH1	-7.89	116.36	120.30
3	C	105	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	754	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	140	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	467	TYR	CB-CG-CD2	-7.78	116.33	121.00
1	A	565	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	873	ARG	NH1-CZ-NH2	-7.68	110.95	119.40
1	A	313	ARG	NH1-CZ-NH2	7.65	127.82	119.40
1	A	601	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	645	GLU	OE1-CD-OE2	-7.58	114.20	123.30
1	A	276	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	A	613	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	727	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	937	ARG	CG-CD-NE	-7.54	95.97	111.80
2	B	197	GLU	CG-CD-OE2	7.50	133.30	118.30
1	A	123	ARG	NH1-CZ-NH2	7.44	127.59	119.40
1	A	293	GLU	OE1-CD-OE2	7.42	132.21	123.30
1	A	1005	TYR	CA-CB-CG	7.36	127.38	113.40
2	B	195	LEU	CB-CG-CD1	-7.34	98.52	111.00
1	A	540	TYR	CB-CG-CD2	7.30	125.38	121.00
2	B	288	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	622	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	A	664	TYR	CB-CG-CD1	-7.16	116.71	121.00
1	A	598	GLU	OE1-CD-OE2	-7.08	114.81	123.30
2	B	290	GLU	CA-C-O	-7.06	105.27	120.10
1	A	261	ARG	NH1-CZ-NH2	-7.05	111.64	119.40
1	A	648	ASN	OD1-CG-ND2	7.03	138.06	121.90
1	A	318	PHE	CB-CG-CD1	-7.02	115.89	120.80
1	A	948	ARG	NH1-CZ-NH2	6.99	127.09	119.40
1	A	727	ARG	NH1-CZ-NH2	6.97	127.07	119.40
1	A	647	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	100	ASP	CB-CG-OD1	6.93	124.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	219	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	706	TYR	CB-CG-CD2	-6.78	116.93	121.00
1	A	895	TYR	CB-CG-CD2	-6.76	116.95	121.00
1	A	398	SER	N-CA-CB	6.75	120.63	110.50
1	A	956	ARG	NH1-CZ-NH2	6.74	126.82	119.40
1	A	261	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	A	123	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	A	141	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	A	834	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	225	VAL	CG1-CB-CG2	-6.66	100.25	110.90
2	B	232	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	944	ARG	CD-NE-CZ	6.61	132.85	123.60
2	B	191	GLU	OE1-CD-OE2	-6.56	115.43	123.30
2	B	276	TYR	CB-CG-CD1	-6.56	117.07	121.00
1	A	210	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	595	ASN	CB-CG-OD1	-6.51	108.58	121.60
1	A	540	TYR	CB-CG-CD1	-6.48	117.11	121.00
3	C	109	TYR	CB-CG-CD2	-6.44	117.13	121.00
1	A	477	ASP	CB-CG-OD1	6.44	124.09	118.30
2	B	121	TYR	CB-CG-CD2	6.43	124.86	121.00
1	A	792	ASP	CB-CG-OD1	-6.42	112.52	118.30
2	B	232	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	178	GLN	CG-CD-OE1	-6.41	108.79	121.60
1	A	402	ARG	NE-CZ-NH1	-6.41	117.10	120.30
3	C	202	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	739	TYR	CB-CG-CD1	6.38	124.83	121.00
2	B	289	GLU	CA-CB-CG	6.38	127.43	113.40
1	A	779	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	A	944	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	A	387	PHE	CB-CG-CD2	-6.36	116.35	120.80
2	B	71	ASP	CB-CG-OD2	-6.35	112.58	118.30
2	B	57	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	895	TYR	CB-CG-CD1	6.32	124.79	121.00
1	A	210	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	343	ASP	CB-CG-OD1	6.31	123.98	118.30
2	B	199	ARG	CG-CD-NE	-6.28	98.62	111.80
2	B	121	TYR	CB-CG-CD1	-6.25	117.25	121.00
3	C	54	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	314	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	72	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
1	A	387	PHE	CB-CG-CD1	6.18	125.12	120.80
1	A	225	VAL	O-C-N	6.16	132.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	335	LYS	N-CA-CB	-6.16	99.52	110.60
2	B	232	ASP	OD1-CG-OD2	-6.16	111.60	123.30
1	A	729	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	698	ASN	OD1-CG-ND2	-6.14	107.77	121.90
1	A	733	ALA	N-CA-CB	-6.13	101.51	110.10
1	A	182	ARG	NH1-CZ-NH2	6.10	126.11	119.40
1	A	515	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	A	110	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	A	350	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	B	56	ARG	CD-NE-CZ	6.06	132.08	123.60
1	A	190	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	47	ARG	NH1-CZ-NH2	6.02	126.03	119.40
1	A	408	TYR	CB-CG-CD1	6.01	124.61	121.00
2	B	9	ILE	O-C-N	-6.01	113.09	122.70
1	A	219	ASP	O-C-N	-6.00	113.11	122.70
1	A	122	GLN	CG-CD-OE1	5.99	133.58	121.60
3	C	217	ILE	CA-C-O	-5.97	107.55	120.10
2	B	245	LYS	CD-CE-NZ	5.97	125.44	111.70
1	A	425	MET	CA-CB-CG	5.94	123.39	113.30
1	A	483	GLU	OE1-CD-OE2	-5.94	116.18	123.30
1	A	88	ARG	CD-NE-CZ	5.93	131.91	123.60
3	C	12	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	A	545	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	692	GLU	OE1-CD-OE2	-5.92	116.19	123.30
2	B	81	ARG	CD-NE-CZ	5.91	131.87	123.60
1	A	493	ASP	OD1-CG-OD2	5.89	134.49	123.30
1	A	382	THR	CA-CB-CG2	-5.86	104.20	112.40
1	A	621	GLU	OE1-CD-OE2	-5.83	116.31	123.30
3	C	190	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	1000	SER	N-CA-CB	-5.82	101.77	110.50
1	A	649	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	456	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	A	467	TYR	CB-CG-CD1	5.79	124.47	121.00
2	B	208	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	A	542	ASN	O-C-N	-5.78	113.45	122.70
1	A	850	TYR	CB-CG-CD2	5.77	124.46	121.00
1	A	526	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	366	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	A	517	ALA	N-CA-CB	5.74	118.14	110.10
2	B	229	HIS	CA-CB-CG	5.72	123.33	113.60
1	A	107	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	128	GLU	OE1-CD-OE2	5.71	130.15	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	753	ARG	NH1-CZ-NH2	5.70	125.66	119.40
1	A	148	LYS	CB-CG-CD	5.68	126.37	111.60
1	A	535	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	A	252	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	100	ASP	CB-CG-OD2	-5.67	113.20	118.30
3	C	60	PHE	CB-CG-CD1	5.67	124.77	120.80
1	A	745	GLU	CG-CD-OE2	5.66	129.61	118.30
3	C	206	LYS	CD-CE-NZ	5.65	124.70	111.70
1	A	401	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	982	ALA	N-CA-CB	5.62	117.97	110.10
1	A	565	ASP	OD1-CG-OD2	-5.62	112.62	123.30
1	A	114	ARG	NH1-CZ-NH2	5.61	125.57	119.40
1	A	698	ASN	CB-CG-OD1	5.61	132.81	121.60
1	A	332	GLN	CB-CG-CD	5.61	126.17	111.60
1	A	169	ALA	N-CA-CB	5.60	117.94	110.10
2	B	205	ALA	CB-CA-C	5.59	118.48	110.10
1	A	423	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	163	MET	CG-SD-CE	-5.55	91.32	100.20
1	A	141	ARG	CD-NE-CZ	-5.55	115.83	123.60
1	A	241	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	A	350	ARG	CD-NE-CZ	-5.51	115.89	123.60
1	A	779	TYR	CB-CG-CD1	5.51	124.30	121.00
1	A	784	ALA	CB-CA-C	-5.51	101.84	110.10
1	A	952	VAL	CA-CB-CG2	-5.49	102.66	110.90
1	A	775	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	975	HIS	N-CA-CB	-5.48	100.73	110.60
1	A	264	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	314	ASP	OD1-CG-OD2	5.46	133.67	123.30
1	A	955	ARG	NH1-CZ-NH2	5.45	125.40	119.40
1	A	664	TYR	CB-CG-CD2	5.44	124.27	121.00
1	A	90	ALA	N-CA-CB	5.43	117.70	110.10
1	A	793	PRO	O-C-N	-5.43	114.02	122.70
2	B	70	ALA	N-CA-CB	-5.40	102.54	110.10
1	A	736	CYS	N-CA-CB	5.39	120.31	110.60
3	C	185	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	A	617	THR	CA-CB-CG2	-5.39	104.85	112.40
3	C	191	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	A	426	ALA	O-C-N	5.37	131.29	122.70
3	C	94	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	A	562	SER	O-C-N	5.35	131.26	122.70
1	A	75	ILE	O-C-N	-5.35	114.15	122.70
1	A	59	LEU	CB-CA-C	-5.34	100.06	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5	THR	OG1-CB-CG2	5.34	122.28	110.00
1	A	242	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	302	VAL	CA-CB-CG1	-5.32	102.92	110.90
1	A	301	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	554	CYS	O-C-N	5.32	131.21	122.70
3	C	69	MET	CG-SD-CE	5.30	108.68	100.20
1	A	329	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	A	331	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	1005	TYR	CG-CD1-CE1	5.25	125.50	121.30
1	A	578	TYR	CB-CG-CD2	5.24	124.14	121.00
2	B	80	MET	CG-SD-CE	-5.23	91.83	100.20
1	A	936	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	314	ASP	CB-CG-OD1	-5.21	113.62	118.30
1	A	798	ILE	O-C-N	-5.20	114.38	122.70
2	B	183	ALA	N-CA-CB	5.20	117.37	110.10
1	A	180	PHE	CB-CG-CD2	-5.19	117.17	120.80
3	C	174	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	A	437	MET	CG-SD-CE	5.17	108.47	100.20
3	C	199	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	554	CYS	N-CA-CB	5.16	119.90	110.60
1	A	316	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	B	208	TYR	CB-CG-CD2	5.15	124.09	121.00
1	A	734	SER	O-C-N	-5.14	114.48	122.70
2	B	138	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	150	GLU	OE1-CD-OE2	5.12	129.45	123.30
1	A	332	GLN	CG-CD-OE1	-5.12	111.35	121.60
1	A	951	ALA	N-CA-CB	-5.12	102.93	110.10
1	A	613	ARG	CG-CD-NE	-5.12	101.05	111.80
1	A	410	LEU	CA-C-O	-5.12	109.35	120.10
1	A	580	VAL	CG1-CB-CG2	-5.12	102.72	110.90
1	A	647	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	A	924	GLU	OE1-CD-OE2	5.11	129.44	123.30
1	A	96	ALA	N-CA-CB	5.11	117.26	110.10
3	C	200	TRP	CA-CB-CG	-5.09	104.02	113.70
1	A	949	ALA	N-CA-CB	-5.09	102.98	110.10
2	B	276	TYR	O-C-N	-5.08	114.58	122.70
1	A	201	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	A	549	VAL	CA-CB-CG1	-5.07	103.30	110.90
2	B	206	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	B	120	GLN	CG-CD-OE1	-5.05	111.51	121.60
2	B	4	GLU	OE1-CD-OE2	5.04	129.35	123.30
3	C	128	LEU	CB-CG-CD1	-5.04	102.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	104	GLU	OE1-CD-OE2	5.04	129.35	123.30
1	A	603	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	130	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7719	0	7457	102	0
2	B	2207	0	2140	30	0
3	C	1783	0	1836	67	0
4	A	8	0	0	0	0
4	B	32	0	0	0	0
5	A	94	0	43	5	0
6	A	1	0	0	0	0
7	B	70	0	83	4	0
8	C	86	0	60	3	0
9	C	19	0	21	1	0
10	A	1493	0	0	27	0
10	B	410	0	0	11	0
10	C	81	0	0	9	0
All	All	14003	0	11640	196	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 8.

All (196) 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:830:GLU:HG3	1:A:832:MET:HE2	1.40	0.98
1:A:356:HIS:HD2	1:A:358:ARG:H	1.11	0.89
1:A:869:ASN:HB3	1:A:872:VAL:HG23	1.58	0.85
1:A:224:ASN:HD22	1:A:403:THR:H	1.21	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:HIS:HD2	3:C:102:LYS:H	1.25	0.84
3:C:201:TYR:HB3	10:C:1844:HOH:O	1.77	0.83
1:A:830:GLU:CG	1:A:832:MET:HE2	2.10	0.82
3:C:213:SER:HA	10:C:1896:HOH:O	1.81	0.80
1:A:307:ASN:HB3	1:A:832:MET:HE3	1.63	0.78
3:C:15:ARG:HG2	3:C:183:MET:HE3	1.67	0.77
1:A:197:HIS:HD2	1:A:200:THR:OG1	1.70	0.75
1:A:876:GLU:HG3	10:A:1897:HOH:O	1.85	0.75
1:A:830:GLU:HG3	1:A:832:MET:CE	2.16	0.74
3:C:101:HIS:CD2	3:C:102:LYS:H	2.06	0.73
1:A:359:CYS:HB3	10:A:1667:HOH:O	1.88	0.72
2:B:279:ILE:HD13	3:C:97:LYS:HA	1.71	0.71
3:C:101:HIS:CD2	3:C:102:LYS:HG3	2.25	0.71
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.73	0.71
3:C:112:GLY:HA3	9:C:811:HQO:H132	1.71	0.71
2:B:283:LYS:HD2	2:B:284:GLU:H	1.58	0.68
3:C:86:ILE:HB	3:C:87:PRO:HD3	1.76	0.68
3:C:193:ALA:HB1	3:C:201:TYR:HB2	1.76	0.67
1:A:196:SEC:SE	10:A:1476:HOH:O	2.61	0.67
3:C:84:LYS:HB3	10:C:1932:HOH:O	1.94	0.67
1:A:356:HIS:CD2	1:A:358:ARG:H	2.04	0.66
3:C:11:LYS:HG2	3:C:13:ILE:HG22	1.80	0.64
1:A:412:TRP:CZ3	1:A:425:MET:HG3	2.34	0.63
3:C:176:VAL:HG11	10:C:1990:HOH:O	1.99	0.63
1:A:84:HIS:HE1	1:A:634:GLN:OE1	1.82	0.62
3:C:7:ILE:HG13	3:C:188:VAL:HG23	1.81	0.62
1:A:125:SER:OG	1:A:128:GLU:HG3	1.99	0.62
1:A:781:ARG:HA	1:A:798:ILE:HD11	1.82	0.62
1:A:193:ALA:HA	1:A:451:ILE:HD11	1.82	0.61
1:A:630:GLY:O	1:A:631:ARG:HB2	2.00	0.61
1:A:476:VAL:HG22	10:A:1532:HOH:O	2.01	0.59
1:A:622:GLU:OE1	1:A:648:ASN:HB2	2.02	0.59
3:C:5:LYS:HG2	3:C:6:MET:SD	2.43	0.59
3:C:198:PRO:HA	10:C:1844:HOH:O	2.03	0.59
1:A:820:THR:HB	1:A:821:PRO:HD2	1.85	0.59
2:B:68:ASN:HA	2:B:69:PRO:C	2.23	0.59
1:A:224:ASN:HD21	1:A:795:ARG:HH22	1.51	0.58
2:B:258:LYS:HG3	10:B:970:HOH:O	2.02	0.58
3:C:4:SER:OG	3:C:190:ARG:NH2	2.34	0.58
3:C:202:ARG:HA	3:C:205:GLU:OE1	2.04	0.57
3:C:91:ASN:O	3:C:95:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ILE:HD13	10:A:1476:HOH:O	2.05	0.56
1:A:896:ARG:HH22	5:A:1017:MGD:H15	1.53	0.56
1:A:199:PRO:HG2	1:A:413:THR:HB	1.88	0.56
1:A:415:HIS:HD2	10:A:1100:HOH:O	1.88	0.56
3:C:79:ASN:HA	3:C:114:LYS:HG2	1.88	0.56
3:C:86:ILE:N	3:C:87:PRO:CD	2.69	0.55
3:C:101:HIS:HD2	3:C:102:LYS:HG3	1.68	0.55
3:C:204:ILE:O	3:C:208:GLU:HB2	2.06	0.55
2:B:176:VAL:HG22	2:B:184:ILE:CG2	2.37	0.55
1:A:989:ASN:ND2	5:A:1017:MGD:H192	2.04	0.55
1:A:327:ASP:OD1	1:A:327:ASP:C	2.44	0.55
3:C:188:VAL:HG11	3:C:192:TRP:CZ3	2.43	0.54
1:A:961:ASN:HB3	10:A:1697:HOH:O	2.07	0.54
1:A:542:ASN:O	1:A:546:GLU:HG3	2.08	0.54
1:A:786:ILE:HG12	10:A:1720:HOH:O	2.08	0.54
3:C:202:ARG:O	3:C:206:LYS:HD2	2.08	0.54
1:A:411:GLY:O	1:A:415:HIS:HE1	1.90	0.54
3:C:190:ARG:O	3:C:194:LYS:HG3	2.08	0.54
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.38	0.53
1:A:854:GLU:HB3	1:A:1009:LEU:HD12	1.91	0.53
1:A:648:ASN:HB3	10:A:1872:HOH:O	2.09	0.52
1:A:384:LYS:HA	10:A:1708:HOH:O	2.09	0.52
3:C:190:ARG:NH1	3:C:201:TYR:OH	2.39	0.52
3:C:93:VAL:O	3:C:97:LYS:HG3	2.10	0.52
1:A:351:ASP:HB3	10:A:1667:HOH:O	2.08	0.51
3:C:127:LEU:HD21	3:C:159:GLY:N	2.25	0.51
3:C:190:ARG:O	3:C:193:ALA:HB3	2.11	0.51
1:A:135:LYS:HE2	10:A:1791:HOH:O	2.09	0.51
1:A:163:MET:HG2	1:A:553:PHE:HB2	1.92	0.51
3:C:199:ARG:O	3:C:203:GLU:HG2	2.10	0.51
1:A:832:MET:SD	10:A:1596:HOH:O	2.60	0.51
1:A:509:MET:SD	10:A:2292:HOH:O	2.60	0.50
3:C:86:ILE:N	3:C:87:PRO:HD2	2.27	0.50
3:C:105:ASP:HB2	10:C:1672:HOH:O	2.12	0.50
1:A:885:LYS:HE3	10:A:2493:HOH:O	2.11	0.50
1:A:493:ASP:CB	1:A:821:PRO:HG2	2.42	0.50
3:C:22:VAL:HG22	8:C:810:HEM:CHC	2.41	0.50
1:A:122:GLN:HG2	10:A:2081:HOH:O	2.11	0.50
1:A:200:THR:HA	1:A:422:ILE:HD13	1.93	0.50
1:A:307:ASN:HB3	1:A:832:MET:CE	2.35	0.50
1:A:817:ALA:HB1	1:A:818:PRO:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ASP:HB3	10:A:1885:HOH:O	2.11	0.49
2:B:266:ILE:HG21	7:B:812:CDL:H771	1.95	0.49
2:B:266:ILE:HD13	7:B:812:CDL:H751	1.94	0.49
1:A:164:LEU:HB3	1:A:557:PHE:CD1	2.48	0.49
1:A:633:LEU:HD12	1:A:633:LEU:N	2.27	0.49
3:C:15:ARG:HA	3:C:183:MET:CE	2.42	0.49
1:A:126:TRP:CZ2	1:A:647:ARG:HG3	2.48	0.48
1:A:412:TRP:HZ3	1:A:425:MET:HG3	1.77	0.48
2:B:185:HIS:CD2	10:B:949:HOH:O	2.66	0.48
1:A:53:CYS:HA	1:A:447:GLY:O	2.14	0.48
2:B:110:LYS:HE3	10:B:1125:HOH:O	2.13	0.48
2:B:176:VAL:HG22	2:B:184:ILE:HG22	1.95	0.48
1:A:360:VAL:HG13	1:A:836:PHE:HB2	1.96	0.47
1:A:34:GLN:HA	10:B:933:HOH:O	2.15	0.47
1:A:224:ASN:HD22	1:A:403:THR:N	2.01	0.47
1:A:961:ASN:OD1	1:A:966:GLN:OE1	2.31	0.47
1:A:370:ARG:HD2	10:A:2279:HOH:O	2.15	0.47
1:A:410:LEU:HA	1:A:413:THR:OG1	2.15	0.47
2:B:235:GLU:HG3	10:B:1038:HOH:O	2.15	0.47
1:A:202:ALA:O	1:A:206:PRO:HG2	2.14	0.47
3:C:208:GLU:HB3	3:C:209:ALA:H	1.48	0.47
3:C:160:ILE:O	3:C:164:HIS:HD2	1.98	0.46
1:A:199:PRO:HB2	1:A:413:THR:HG22	1.96	0.46
2:B:10:LYS:HB2	2:B:120:GLN:HB3	1.96	0.46
3:C:101:HIS:CD2	3:C:102:LYS:N	2.78	0.46
1:A:645:GLU:HA	10:A:1919:HOH:O	2.16	0.46
3:C:95:VAL:HG13	3:C:100:GLU:HB3	1.97	0.46
1:A:84:HIS:CD2	1:A:86:VAL:H	2.34	0.46
1:A:513:TYR:HE2	10:A:2292:HOH:O	1.99	0.46
2:B:269:PHE:O	2:B:273:ILE:HD12	2.16	0.46
2:B:8:ILE:HD12	2:B:119:ILE:HD12	1.98	0.45
1:A:775:ARG:HD3	1:A:812:ASP:HA	1.98	0.45
2:B:185:HIS:HE1	10:B:891:HOH:O	1.99	0.45
1:A:224:ASN:HD21	1:A:795:ARG:NH2	2.14	0.45
3:C:170:MET:HG2	8:C:810:HEM:CAB	2.46	0.45
3:C:216:GLY:O	3:C:217:ILE:C	2.55	0.45
3:C:87:PRO:HG2	10:C:1672:HOH:O	2.16	0.45
3:C:176:VAL:O	3:C:179:SER:OG	2.27	0.45
1:A:781:ARG:O	1:A:781:ARG:HG3	2.16	0.45
2:B:285:VAL:CG2	3:C:191:ARG:HH11	2.30	0.45
3:C:15:ARG:HG2	3:C:183:MET:CE	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:LEU:O	3:C:57:HIS:C	2.53	0.45
1:A:673:GLU:HB3	1:A:674:PRO:HD3	1.98	0.44
2:B:197:GLU:HG3	10:B:1199:HOH:O	2.16	0.44
1:A:343:ASP:HA	1:A:349:LYS:HE2	1.98	0.44
1:A:989:ASN:HD21	5:A:1017:MGD:H192	1.63	0.44
2:B:29:GLU:OE1	2:B:223:HIS:HE1	1.99	0.44
3:C:79:ASN:HD22	3:C:114:LYS:HA	1.81	0.44
2:B:152:LYS:HG2	10:B:917:HOH:O	2.16	0.44
3:C:214:GLU:HA	3:C:214:GLU:OE1	2.18	0.44
3:C:175:TRP:CE3	3:C:176:VAL:HG23	2.52	0.44
3:C:11:LYS:HG3	3:C:12:PHE:N	2.33	0.44
1:A:54:SER:OG	1:A:629:SER:HB2	2.17	0.44
1:A:108:LEU:HD12	1:A:583:ASP:O	2.17	0.43
7:B:812:CDL:H432	3:C:25:PHE:CD1	2.53	0.43
3:C:10:THR:HA	10:C:1035:HOH:O	2.18	0.43
3:C:181:LYS:HD2	3:C:185:GLU:OE1	2.18	0.43
3:C:123:MET:HA	3:C:123:MET:CE	2.49	0.43
1:A:126:TRP:CE2	1:A:647:ARG:HG3	2.54	0.43
2:B:283:LYS:HD3	3:C:177:LYS:HB2	2.00	0.43
3:C:15:ARG:HA	3:C:183:MET:HE2	2.00	0.43
3:C:212:GLU:HB2	10:C:1767:HOH:O	2.19	0.43
1:A:937:ARG:HH11	1:A:937:ARG:HD2	1.59	0.43
3:C:44:THR:HB	3:C:50:PRO:HG3	2.01	0.43
3:C:62:ILE:HD13	3:C:62:ILE:HA	1.74	0.43
1:A:135:LYS:HG3	10:A:1574:HOH:O	2.18	0.43
1:A:217:TRP:CH2	1:A:445:LEU:HD22	2.53	0.43
1:A:257:VAL:HG23	1:A:269:ALA:HB2	2.01	0.42
3:C:166:ILE:HD11	8:C:810:HEM:HBC2	2.01	0.42
2:B:78:THR:HG23	10:B:1204:HOH:O	2.18	0.42
1:A:229:MET:HG3	1:A:258:VAL:HB	1.99	0.42
1:A:197:HIS:CD2	1:A:200:THR:OG1	2.61	0.42
1:A:205:ALA:HB3	1:A:206:PRO:HD3	2.00	0.42
1:A:410:LEU:HD11	5:A:1018:MGD:S12	2.60	0.42
1:A:984:LYS:HE3	10:A:1726:HOH:O	2.20	0.42
1:A:566:LYS:HA	10:A:1251:HOH:O	2.19	0.42
1:A:312:VAL:HG21	1:A:363:LEU:HD12	2.01	0.42
1:A:359:CYS:SG	1:A:362:ASN:ND2	2.93	0.42
2:B:20:PRO:HD2	10:B:935:HOH:O	2.20	0.42
2:B:102:HIS:O	2:B:223:HIS:HD2	2.03	0.42
3:C:160:ILE:HD13	3:C:160:ILE:HA	1.76	0.42
3:C:205:GLU:HA	3:C:208:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:CYS:HB3	1:A:238:PRO:HG2	2.02	0.42
1:A:460:LEU:O	1:A:461:SER:C	2.58	0.42
2:B:245:LYS:HE3	2:B:245:LYS:HB3	1.78	0.42
1:A:242:ARG:O	1:A:242:ARG:HG2	2.20	0.41
3:C:159:GLY:O	3:C:163:ILE:HG13	2.20	0.41
1:A:772:PRO:HG2	1:A:775:ARG:HD2	2.03	0.41
2:B:55:ILE:HD13	2:B:55:ILE:HG21	1.85	0.41
1:A:193:ALA:HB3	1:A:460:LEU:HD21	2.01	0.41
1:A:633:LEU:HD23	10:A:1689:HOH:O	2.21	0.41
3:C:17:CYS:SG	3:C:70:PHE:HD2	2.42	0.41
1:A:415:HIS:CD2	10:A:1100:HOH:O	2.70	0.41
2:B:285:VAL:HG12	2:B:288:ASP:H	1.84	0.41
1:A:214:THR:HG21	1:A:435:MET:HE1	2.03	0.41
1:A:451:ILE:HG21	10:A:1476:HOH:O	2.21	0.41
2:B:206:ARG:HH11	2:B:206:ARG:HD3	1.73	0.41
2:B:266:ILE:CG2	7:B:812:CDL:H771	2.51	0.41
1:A:896:ARG:HE	5:A:1018:MGD:H15	1.64	0.41
1:A:224:ASN:ND2	1:A:402:ARG:HA	2.36	0.41
2:B:279:ILE:HG22	2:B:280:GLY:O	2.21	0.41
3:C:15:ARG:NH1	3:C:184:ILE:O	2.54	0.41
3:C:211:LYS:HA	3:C:211:LYS:HD3	1.86	0.41
1:A:400:PRO:HA	10:A:1709:HOH:O	2.21	0.40
1:A:956:ARG:HH11	1:A:956:ARG:HD2	1.55	0.40
2:B:185:HIS:HD2	10:B:907:HOH:O	2.04	0.40
1:A:356:HIS:HA	1:A:357:PRO:HD2	1.91	0.40
1:A:198:GLY:N	1:A:199:PRO:CD	2.85	0.40
1:A:511:SER:OG	1:A:735:SER:HB3	2.21	0.40
3:C:88:TRP:CZ2	3:C:95:VAL:HG11	2.56	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	979/1015 (96%)	949 (97%)	29 (3%)	1 (0%)	51	81
2	B	287/294 (98%)	280 (98%)	7 (2%)	0	100	100
3	C	214/217 (99%)	206 (96%)	6 (3%)	2 (1%)	17	46
All	All	1480/1526 (97%)	1435 (97%)	42 (3%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	208	GLU
1	A	838	ILE
3	C	198	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	815/837 (97%)	805 (99%)	10 (1%)	71	92
2	B	238/243 (98%)	225 (94%)	13 (6%)	21	52
3	C	188/189 (100%)	183 (97%)	5 (3%)	44	78
All	All	1241/1269 (98%)	1213 (98%)	28 (2%)	50	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	101	TYR
1	A	344	GLU
1	A	557	PHE
1	A	648	ASN
1	A	790	PRO
1	A	843	GLU
1	A	855	THR
1	A	937	ARG
1	A	954	THR

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Mol	Chain	Res	Type
2	B	51	GLU
2	B	67	ASP
2	B	68	ASN
2	B	69	PRO
2	B	113	PRO
2	B	160	CYS
2	B	162	LEU
2	B	178	THR
2	B	229	HIS
2	B	235	GLU
2	B	245	LYS
2	B	285	VAL
2	B	289	GLU
3	C	101	HIS
3	C	105	ASP
3	C	189	SER
3	C	205	GLU
3	C	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	191	ASN
1	A	197	HIS
1	A	224	ASN
1	A	332	GLN
1	A	341	GLN
1	A	356	HIS
1	A	362	ASN
1	A	415	HIS
1	A	479	GLN
1	A	689	GLN
1	A	865	ASN
1	A	966	GLN
1	A	989	ASN
2	B	185	HIS
2	B	223	HIS
3	C	79	ASN
3	C	101	HIS
3	C	164	HIS
3	C	196	HIS

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)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SF4	B	808	2	0,12,12	-	-	-		
4	SF4	B	805	2	0,12,12	-	-	-		
7	CDL	B	812	-	69,69,99	2.89	20 (28%)	75,81,111	2.66	17 (22%)
4	SF4	B	807	2	0,12,12	-	-	-		
5	MGD	A	1017	6	41,52,52	2.16	8 (19%)	40,81,81	2.50	13 (32%)
8	HEM	C	809	3	41,50,50	1.52	4 (9%)	45,82,82	1.23	5 (11%)
8	HEM	C	810	3	41,50,50	1.57	7 (17%)	45,82,82	1.73	9 (20%)
5	MGD	A	1018	6	41,52,52	2.31	8 (19%)	40,81,81	2.22	15 (37%)
4	SF4	A	1016	1	0,12,12	-	-	-		
9	HQO	C	811	-	20,20,20	2.96	9 (45%)	18,26,26	3.56	7 (38%)
4	SF4	B	806	2	0,12,12	-	-	-		

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	SF4	B	808	2	-	-	0/6/5/5
4	SF4	B	805	2	-	-	0/6/5/5
7	CDL	B	812	-	-	41/80/80/110	-
4	SF4	B	807	2	-	-	0/6/5/5
5	MGD	A	1017	6	-	8/18/66/66	0/6/6/6
8	HEM	C	809	3	-	4/12/54/54	-
8	HEM	C	810	3	-	3/12/54/54	-
5	MGD	A	1018	6	-	5/18/66/66	0/6/6/6
4	SF4	A	1016	1	-	-	0/6/5/5
9	HQO	C	811	-	-	2/7/7/7	0/2/2/2
4	SF4	B	806	2	-	-	0/6/5/5

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	812	CDL	OB8-CB6	-15.23	1.10	1.45
5	A	1018	MGD	O3A-C10	-10.41	1.04	1.44
5	A	1017	MGD	O3A-C10	-10.00	1.06	1.44
7	B	812	CDL	OA6-CA5	8.44	1.58	1.34
9	C	811	HQO	C11-C3	7.71	1.71	1.50
7	B	812	CDL	OB6-CB5	7.19	1.54	1.34
9	C	811	HQO	O1-C1	6.30	1.53	1.36
7	B	812	CDL	PA1-OA3	5.50	1.70	1.50
7	B	812	CDL	C51-CB5	5.24	1.66	1.50
8	C	809	HEM	C3C-C2C	-4.76	1.33	1.40
5	A	1018	MGD	C5-C6	-4.16	1.39	1.47
8	C	810	HEM	C3C-C2C	-4.06	1.34	1.40
9	C	811	HQO	O4-N1	-4.00	1.32	1.38
7	B	812	CDL	OA8-CA7	3.82	1.44	1.33
5	A	1017	MGD	C5-C6	-3.81	1.39	1.47
5	A	1018	MGD	C23-C14	-3.68	1.50	1.53
5	A	1018	MGD	O11-C11	-3.56	1.39	1.43
8	C	809	HEM	C3C-CAC	3.50	1.55	1.47
5	A	1017	MGD	C21-N22	3.47	1.39	1.35
8	C	810	HEM	C3C-CAC	3.42	1.54	1.47
5	A	1018	MGD	O5'-C5'	-3.33	1.32	1.44
9	C	811	HQO	C8-C9	3.26	1.44	1.36
9	C	811	HQO	C3-N1	3.24	1.42	1.36
7	B	812	CDL	PB2-OB3	3.21	1.62	1.50
7	B	812	CDL	OB8-CB7	-3.18	1.24	1.33
5	A	1018	MGD	C14-N15	-3.12	1.42	1.46
9	C	811	HQO	C2-C3	3.12	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	810	HEM	CAB-C3B	3.05	1.55	1.47
5	A	1017	MGD	C5'-C4'	-2.94	1.42	1.51
7	B	812	CDL	PB2-OB4	2.88	1.68	1.55
7	B	812	CDL	C79-C78	2.86	1.73	1.49
9	C	811	HQO	C7-C6	2.84	1.43	1.36
7	B	812	CDL	C11-CA5	2.83	1.59	1.50
7	B	812	CDL	OB6-CB4	-2.81	1.39	1.46
9	C	811	HQO	C2-C1	2.74	1.43	1.37
5	A	1017	MGD	O5'-C5'	-2.72	1.34	1.44
5	A	1017	MGD	O11-C11	-2.67	1.40	1.43
8	C	809	HEM	CAB-C3B	2.60	1.54	1.47
7	B	812	CDL	CA3-CA4	-2.60	1.42	1.50
8	C	809	HEM	C1A-NA	2.57	1.41	1.36
7	B	812	CDL	C39-C38	-2.57	1.37	1.51
7	B	812	CDL	C12-C11	2.51	1.61	1.52
7	B	812	CDL	C42-C41	-2.49	1.37	1.51
7	B	812	CDL	CB3-CB4	2.43	1.58	1.50
7	B	812	CDL	C52-C51	2.39	1.61	1.52
7	B	812	CDL	C19-C18	-2.37	1.34	1.51
7	B	812	CDL	PA1-OA5	2.34	1.68	1.59
8	C	810	HEM	CAA-C2A	2.33	1.55	1.52
5	A	1017	MGD	C14-N15	-2.24	1.43	1.46
9	C	811	HQO	C8-C7	2.24	1.43	1.38
8	C	810	HEM	CAD-C3D	2.20	1.57	1.51
5	A	1018	MGD	PB-O1B	-2.15	1.43	1.50
5	A	1018	MGD	C5'-C4'	-2.10	1.45	1.51
5	A	1017	MGD	C16-C21	2.05	1.42	1.38
8	C	810	HEM	O1A-CGA	2.05	1.28	1.22
8	C	810	HEM	CMC-C2C	2.01	1.56	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	812	CDL	OB6-CB5-C51	13.32	140.21	111.50
9	C	811	HQO	C11-C3-C2	10.85	139.33	120.74
5	A	1017	MGD	O11-C23-C14	8.49	114.63	108.96
7	B	812	CDL	C52-C51-CB5	-7.21	87.41	113.62
5	A	1018	MGD	O4'-C1'-C2'	-7.10	96.55	106.93
7	B	812	CDL	CA6-CA4-CA3	-6.89	95.49	111.79
7	B	812	CDL	CB6-OB8-CB7	-6.77	92.04	117.12
9	C	811	HQO	C13-C11-C3	-6.37	97.03	113.82
7	B	812	CDL	OB7-CB5-C51	-6.08	100.01	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	811	HQO	O1-C1-C10	5.69	123.41	116.31
5	A	1017	MGD	C19-N20-C21	5.57	123.48	113.43
5	A	1018	MGD	C19-N20-C21	5.07	122.58	113.43
7	B	812	CDL	OA6-CA5-OA7	-4.75	112.22	123.70
8	C	810	HEM	CMA-C3A-C4A	-4.43	121.65	128.46
5	A	1017	MGD	O4'-C1'-C2'	-4.42	100.47	106.93
8	C	810	HEM	O2A-CGA-O1A	4.29	133.98	123.30
8	C	810	HEM	C4B-CHC-C1C	3.86	127.65	122.56
5	A	1017	MGD	O5'-C5'-C4'	3.82	122.14	108.99
5	A	1017	MGD	N2-C2-N3	3.77	127.08	119.74
7	B	812	CDL	OB8-CB7-OB9	3.76	133.09	123.59
5	A	1018	MGD	O17-C17-C16	-3.75	118.65	127.24
5	A	1017	MGD	O17-C17-N18	-3.65	113.12	120.12
7	B	812	CDL	OB6-CB5-OB7	-3.65	114.89	123.70
5	A	1017	MGD	O6-C6-N1	3.62	124.92	120.65
7	B	812	CDL	CB6-CB4-CB3	-3.44	103.66	111.79
8	C	810	HEM	CMA-C3A-C2A	3.43	131.41	124.94
8	C	809	HEM	CMA-C3A-C4A	-3.42	123.20	128.46
9	C	811	HQO	C2-C3-N1	3.41	122.69	118.94
5	A	1018	MGD	O11-C23-C14	-3.36	106.72	108.96
7	B	812	CDL	CA4-OA6-CA5	-3.14	110.07	117.79
5	A	1018	MGD	N18-C19-N20	-3.08	117.58	123.32
9	C	811	HQO	C2-C1-C10	-3.02	116.93	120.52
8	C	809	HEM	O2D-CGD-O1D	3.02	130.83	123.30
7	B	812	CDL	CA6-OA8-CA7	-2.96	106.16	117.12
8	C	810	HEM	O1D-CGD-CBD	-2.87	113.85	123.08
7	B	812	CDL	OA6-CA5-C11	2.83	117.59	111.50
8	C	809	HEM	O1D-CGD-CBD	-2.81	114.05	123.08
5	A	1018	MGD	C19-N18-C17	-2.80	119.99	125.10
5	A	1018	MGD	O6-C6-N1	-2.80	117.34	120.65
7	B	812	CDL	O1-C1-CA2	-2.75	99.92	109.56
8	C	810	HEM	O1A-CGA-CBA	-2.75	114.26	123.08
7	B	812	CDL	CB4-OB6-CB5	-2.75	111.03	117.79
9	C	811	HQO	C12-C13-C11	-2.70	103.25	113.76
8	C	810	HEM	CMC-C2C-C3C	2.68	129.70	124.68
5	A	1018	MGD	O5'-C5'-C4'	2.66	118.14	108.99
7	B	812	CDL	OA4-PA1-OA3	-2.49	99.94	112.24
5	A	1017	MGD	N18-C19-N20	-2.39	118.86	123.32
5	A	1018	MGD	N2-C2-N3	2.27	124.16	119.74
5	A	1018	MGD	C16-C17-N18	2.25	119.01	112.31
8	C	809	HEM	CMA-C3A-C2A	2.22	129.12	124.94
5	A	1018	MGD	O4'-C4'-C5'	2.21	116.63	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	810	HEM	CBA-CAA-C2A	-2.19	108.89	112.62
5	A	1017	MGD	N2-C2-N1	-2.18	112.07	116.71
7	B	812	CDL	OB9-CB7-C71	-2.17	115.26	123.73
5	A	1018	MGD	C23-C14-C13	-2.17	105.67	110.53
7	B	812	CDL	OB2-PB2-OB3	-2.16	100.64	109.07
5	A	1017	MGD	C5'-C4'-C3'	-2.15	107.12	115.18
5	A	1017	MGD	PA-O3A-C10	-2.14	109.15	121.68
5	A	1017	MGD	O4'-C4'-C5'	2.09	116.25	109.37
5	A	1018	MGD	N19-C19-N18	2.08	121.14	116.71
5	A	1018	MGD	O11-C23-N22	-2.07	106.44	108.57
8	C	809	HEM	C4C-CHD-C1D	2.07	125.29	122.56
5	A	1017	MGD	C23-C14-C13	-2.04	105.95	110.53
9	C	811	HQO	C9-C10-C1	-2.04	119.41	122.21
8	C	810	HEM	CAD-C3D-C2D	2.03	131.65	127.88
5	A	1018	MGD	C17-C16-N15	2.01	122.16	116.76

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1017	MGD	PA-O3B-PB-O5'
5	A	1017	MGD	C5'-O5'-PB-O1B
5	A	1017	MGD	C10-O3A-PA-O1A
7	B	812	CDL	CA3-OA5-PA1-OA3
7	B	812	CDL	CA3-OA5-PA1-OA4
7	B	812	CDL	CB2-OB2-PB2-OB3
7	B	812	CDL	CB3-OB5-PB2-OB2
7	B	812	CDL	CB3-OB5-PB2-OB3
7	B	812	CDL	CB3-OB5-PB2-OB4
7	B	812	CDL	C11-CA5-OA6-CA4
7	B	812	CDL	CB2-C1-CA2-OA2
7	B	812	CDL	CA7-C31-C32-C33
7	B	812	CDL	O1-C1-CA2-OA2
7	B	812	CDL	CA3-OA5-PA1-OA2
7	B	812	CDL	CB2-OB2-PB2-OB5
9	C	811	HQO	C3-C11-C13-C12
7	B	812	CDL	OB7-CB5-OB6-CB4
7	B	812	CDL	O1-C1-CB2-OB2
7	B	812	CDL	C36-C37-C38-C39
7	B	812	CDL	C37-C38-C39-C40
8	C	809	HEM	C2B-C3B-CAB-CBB
7	B	812	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
8	C	809	HEM	C4B-C3B-CAB-CBB
7	B	812	CDL	OB9-CB7-OB8-CB6
8	C	810	HEM	C3D-CAD-CBD-CGD
7	B	812	CDL	C71-C72-C73-C74
7	B	812	CDL	CA2-C1-CB2-OB2
9	C	811	HQO	C13-C12-C14-C15
7	B	812	CDL	CB3-CB4-CB6-OB8
7	B	812	CDL	CB5-C51-C52-C53
7	B	812	CDL	CA5-C11-C12-C13
7	B	812	CDL	C73-C74-C75-C76
7	B	812	CDL	C1-CA2-OA2-PA1
7	B	812	CDL	OB5-CB3-CB4-OB6
7	B	812	CDL	C17-C18-C19-C20
7	B	812	CDL	C41-C42-C43-C44
5	A	1018	MGD	PA-O3B-PB-O5'
7	B	812	CDL	C71-CB7-OB8-CB6
7	B	812	CDL	OA5-CA3-CA4-OA6
7	B	812	CDL	OB6-CB4-CB6-OB8
5	A	1017	MGD	C5'-O5'-PB-O3B
5	A	1017	MGD	C10-O3A-PA-O3B
5	A	1018	MGD	C10-O3A-PA-O3B
5	A	1017	MGD	C10-O3A-PA-O2A
5	A	1018	MGD	C10-O3A-PA-O1A
7	B	812	CDL	OA5-CA3-CA4-CA6
7	B	812	CDL	C39-C40-C41-C42
7	B	812	CDL	CA2-OA2-PA1-OA5
7	B	812	CDL	C52-C53-C54-C55
7	B	812	CDL	C15-C16-C17-C18
7	B	812	CDL	OA7-CA5-OA6-CA4
5	A	1017	MGD	O3A-C10-C11-O11
5	A	1018	MGD	O3A-C10-C11-O11
7	B	812	CDL	C32-C31-CA7-OA8
8	C	809	HEM	CAA-CBA-CGA-O2A
8	C	810	HEM	CAA-CBA-CGA-O1A
7	B	812	CDL	C52-C51-CB5-OB6
7	B	812	CDL	OB5-CB3-CB4-CB6
5	A	1017	MGD	O4'-C4'-C5'-O5'
8	C	809	HEM	CAA-CBA-CGA-O1A
5	A	1018	MGD	C5'-O5'-PB-O1B
7	B	812	CDL	C12-C11-CA5-OA7
8	C	810	HEM	CAA-CBA-CGA-O2A

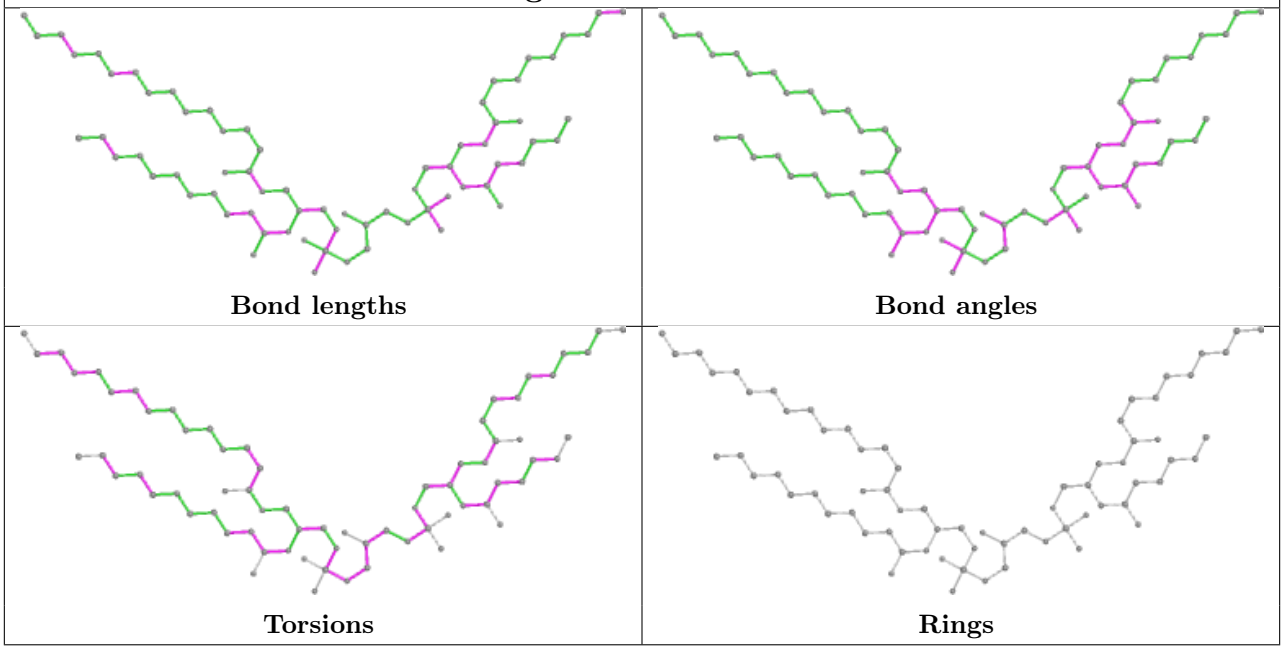
There are no ring outliers.

5 monomers are involved in 13 short contacts:

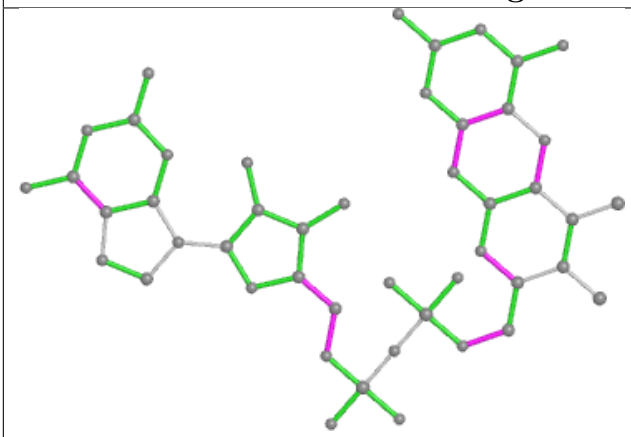
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	812	CDL	4	0
5	A	1017	MGD	3	0
8	C	810	HEM	3	0
5	A	1018	MGD	2	0
9	C	811	HQO	1	0

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

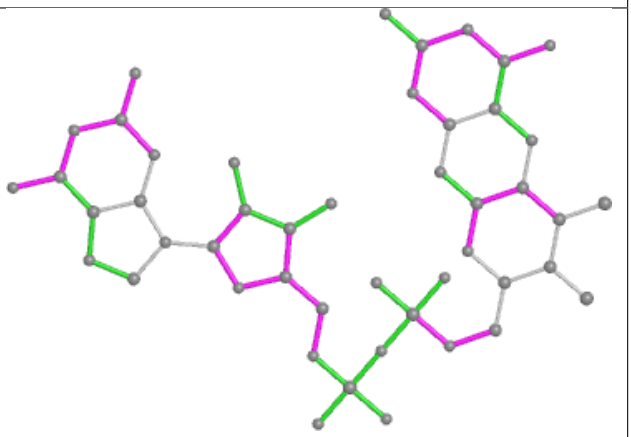
Ligand CDL B 812



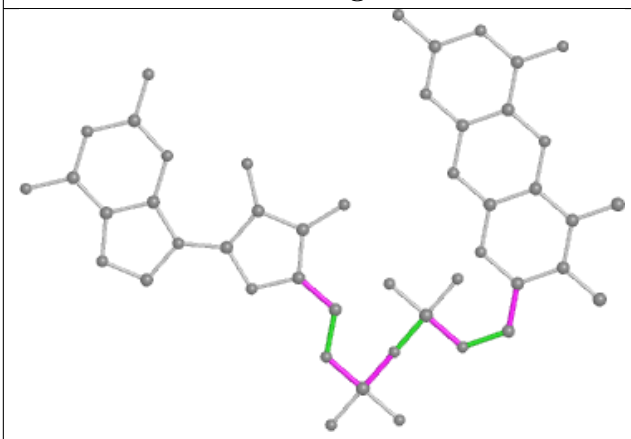
Ligand MGD A 1017



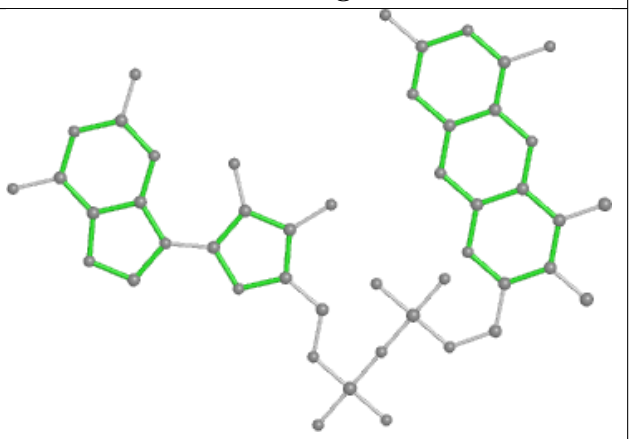
Bond lengths



Bond angles

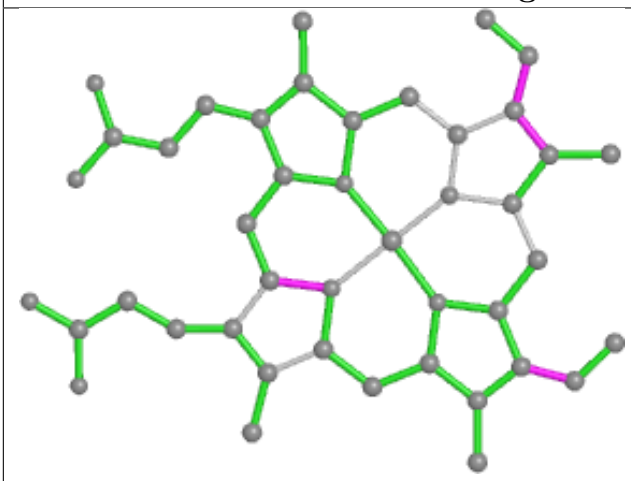


Torsions

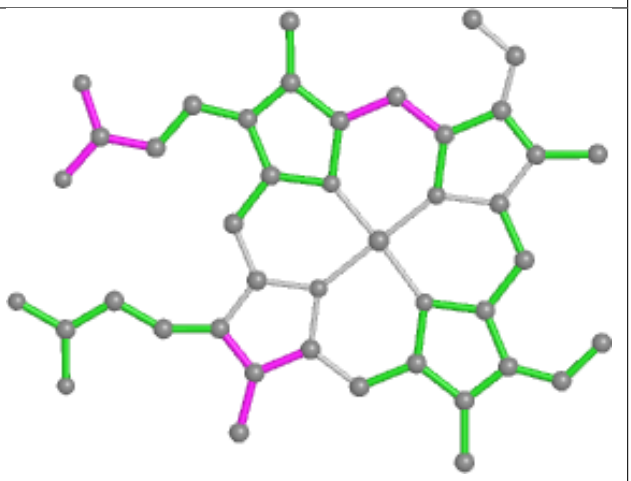


Rings

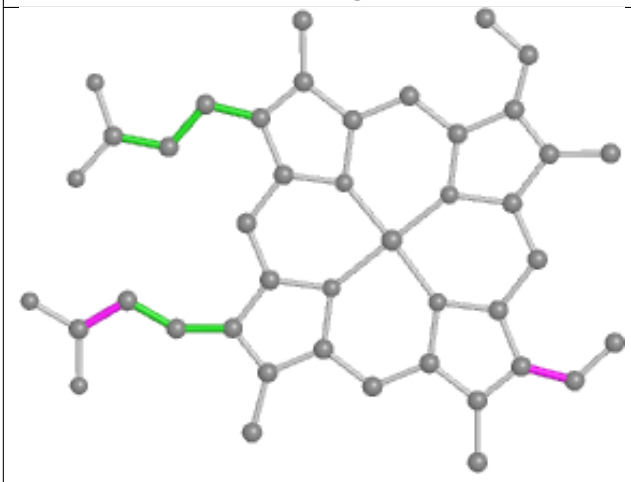
Ligand HEM C 809



Bond lengths



Bond angles



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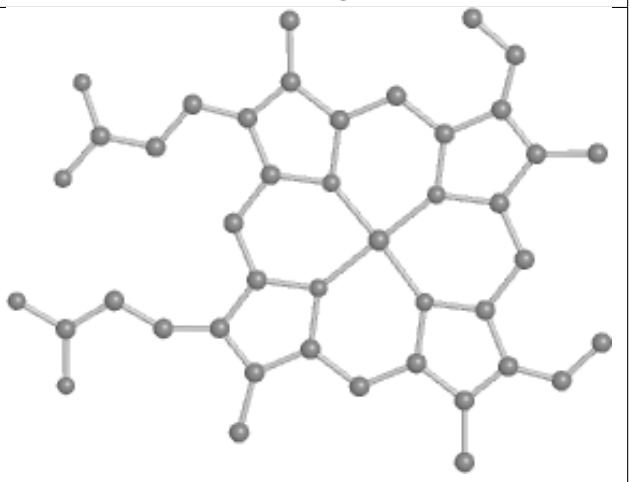
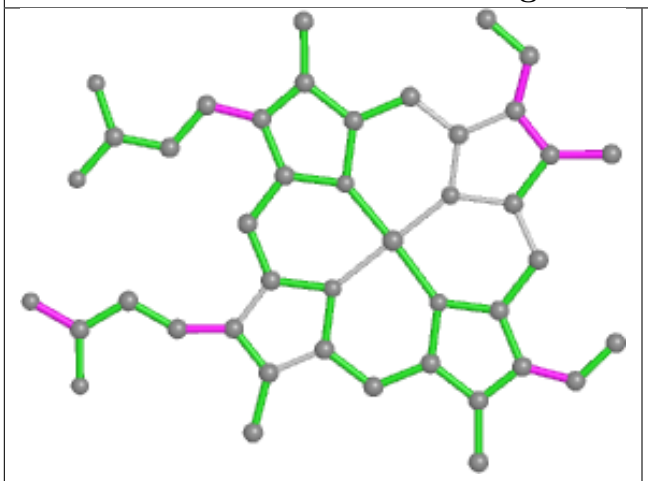
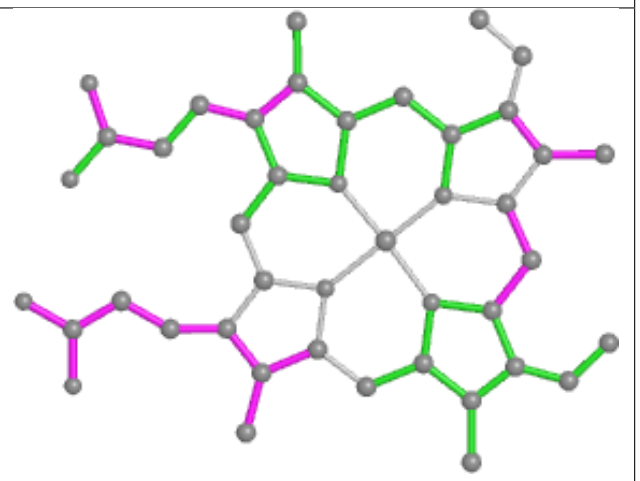


Rings

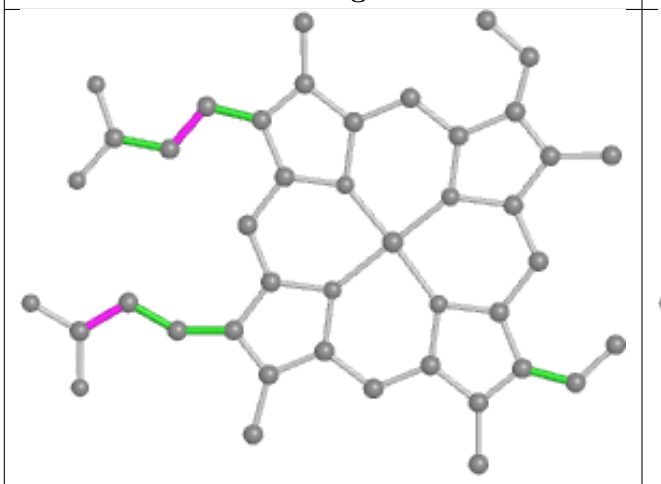
Ligand HEM C 810



Bond lengths



Bond angles



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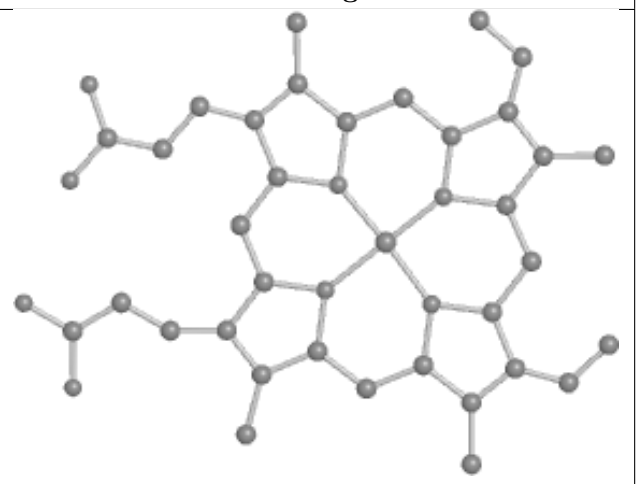
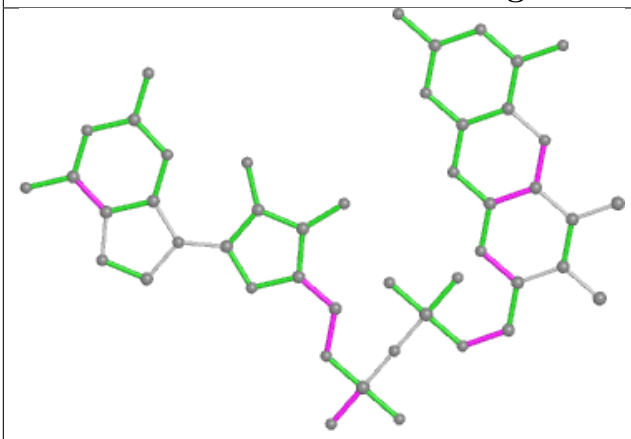
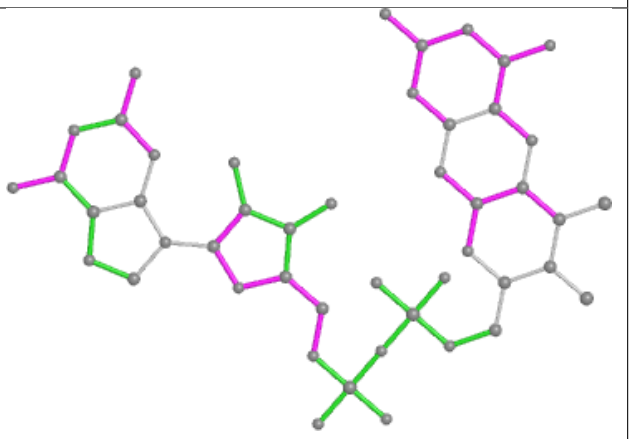


Rings

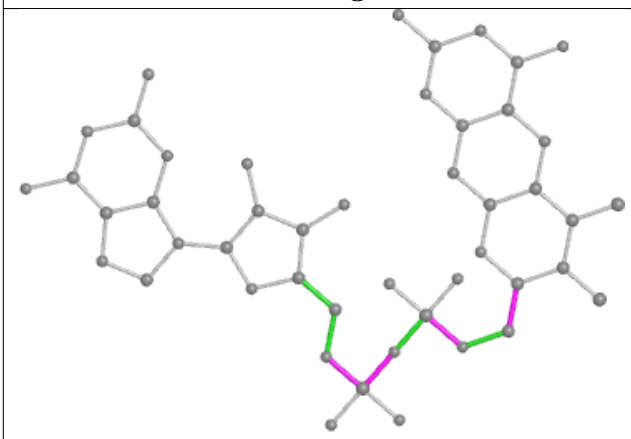
Ligand MGD A 1018



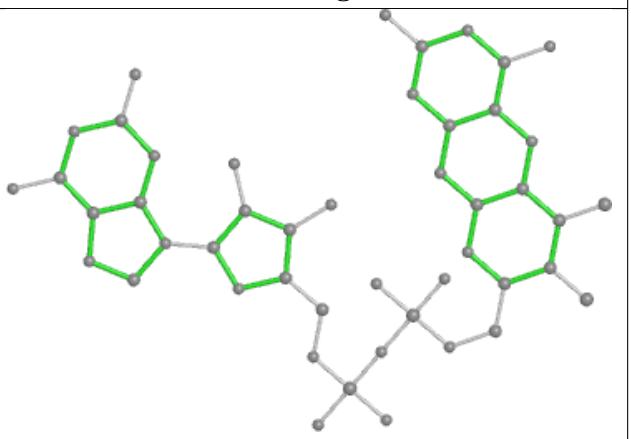
Bond lengths



Bond angles

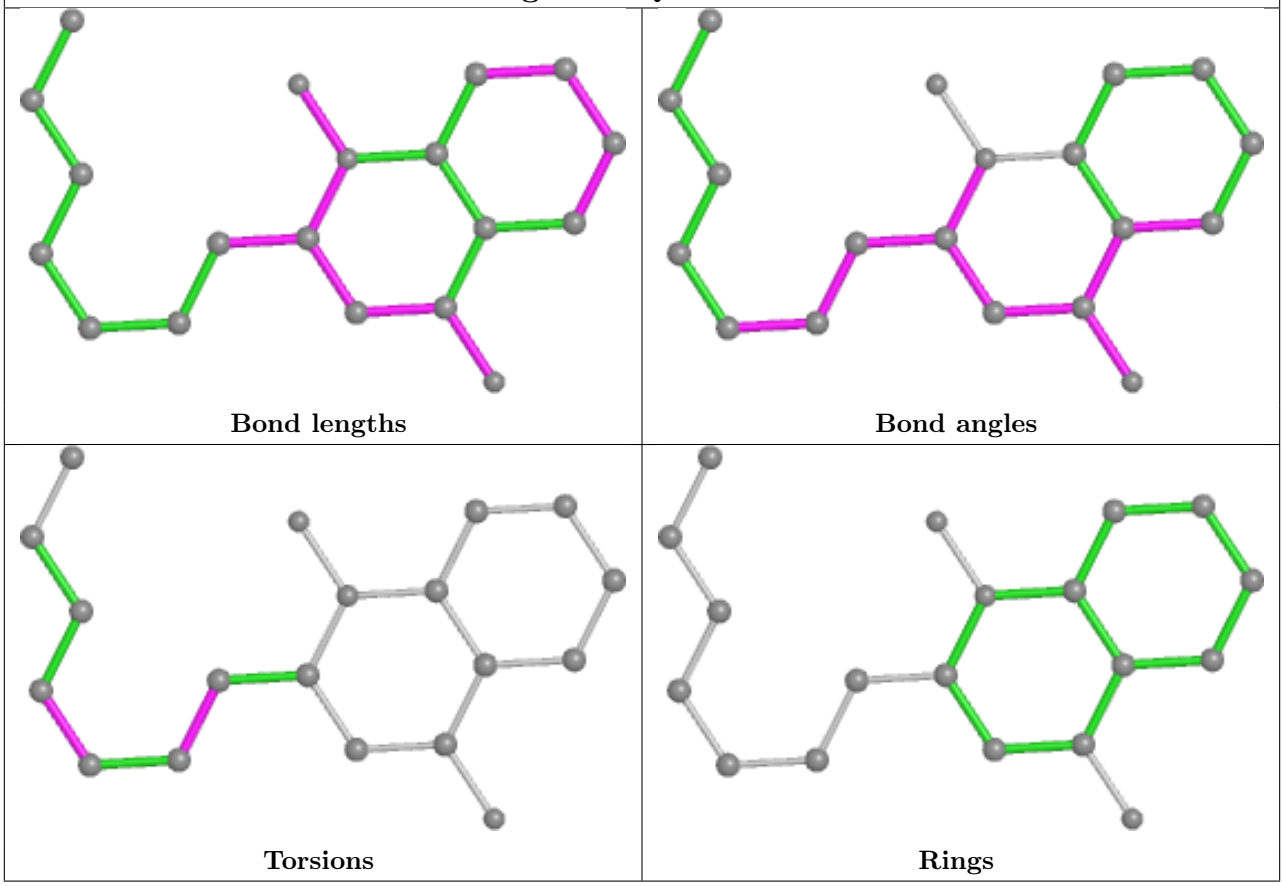


Torsions



Rings

Ligand HQO C 811



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.