



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PRC
Title : CRYSTALLOGRAPHIC REFINEMENT AT 2.3 ANGSTROMS RESOLUTION AND REFINED MODEL OF THE PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS
Authors : Deisenhofer, J.; Epp, O.; Miki, K.; Huber, R.; Michel, H.
Deposited on : 1988-02-04
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

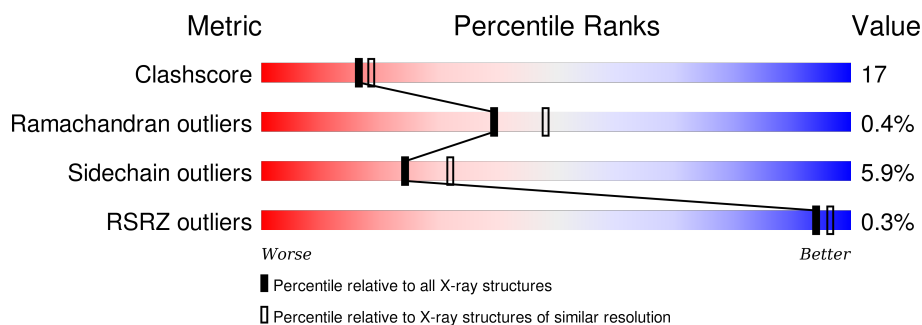
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	C	336	
2	L	273	
3	M	323	
4	H	258	

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
11	NS1	M	613	-	-	-	X
12	UQ1	L	614	-	-	X	X
13	LDA	H	616	-	-	-	X
6	SO4	H	622	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10288 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 PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	333	Total	C	N	O	S	54	0	1
			2603	1640	467	478	18			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	13	0	0
			2171	1459	350	355	7			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	26	0	0
			2555	1702	419	423	11			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	106	0	0
			2018	1292	344	380	2			

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

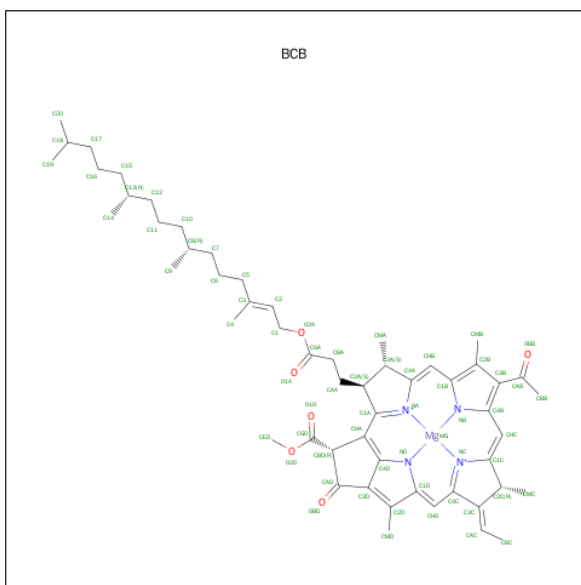
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



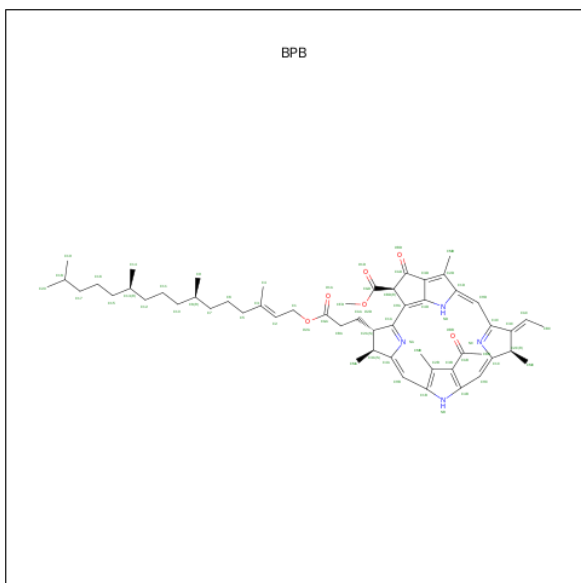
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



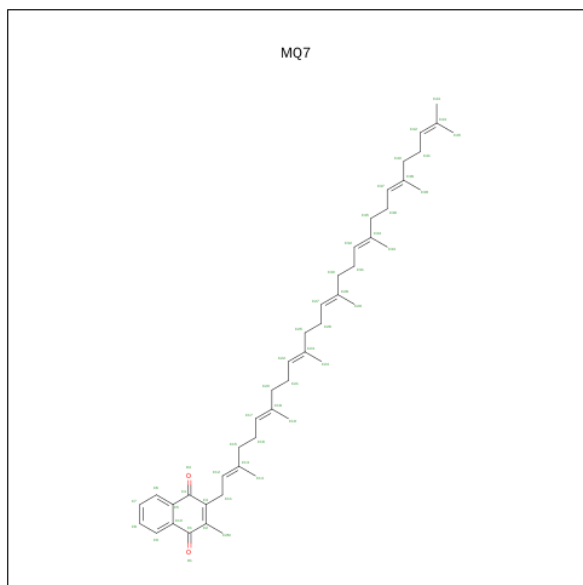
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	13	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_6$).



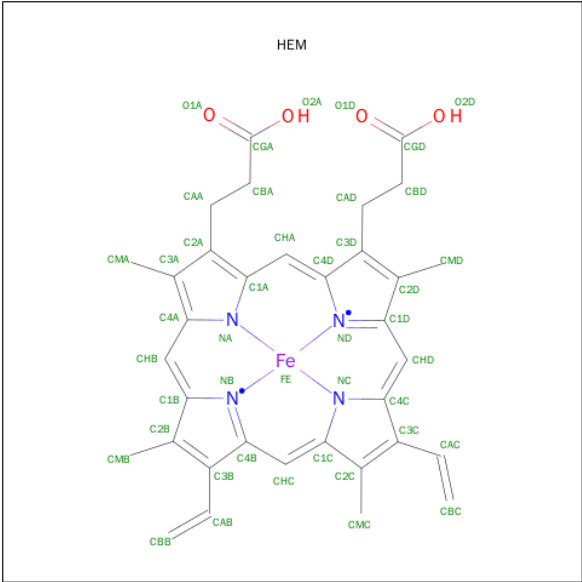
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	7	0
			65	55	4	6		
8	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



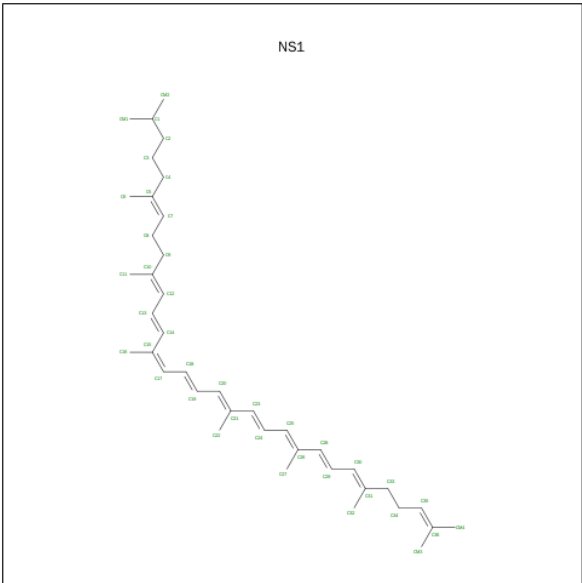
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	4	0
			48	46	2		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



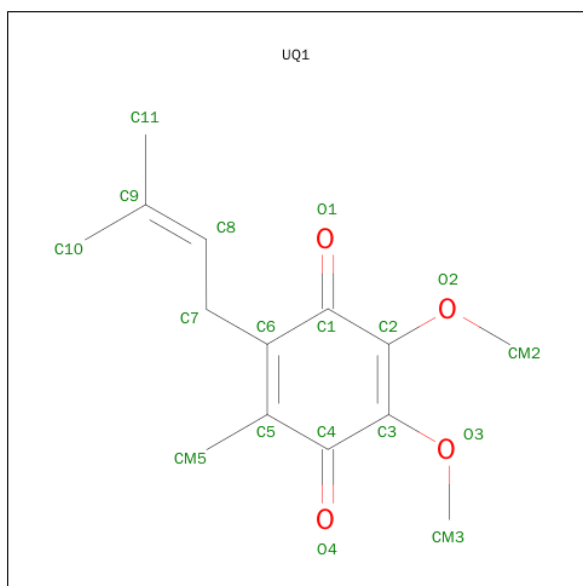
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is 15-TRANS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS1) (formula: C₄₀H₆₀).



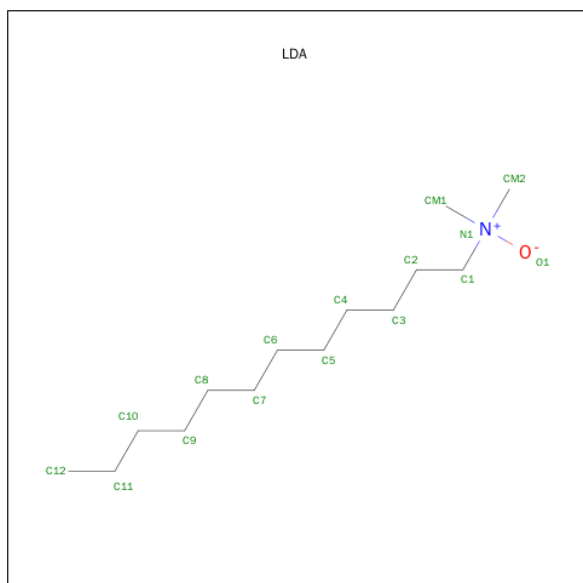
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C 40 40	14	0

- Molecule 12 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total C O 18 14 4	0	0

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	H	1	Total	C	N	O	6	0
			16	14	1	1		

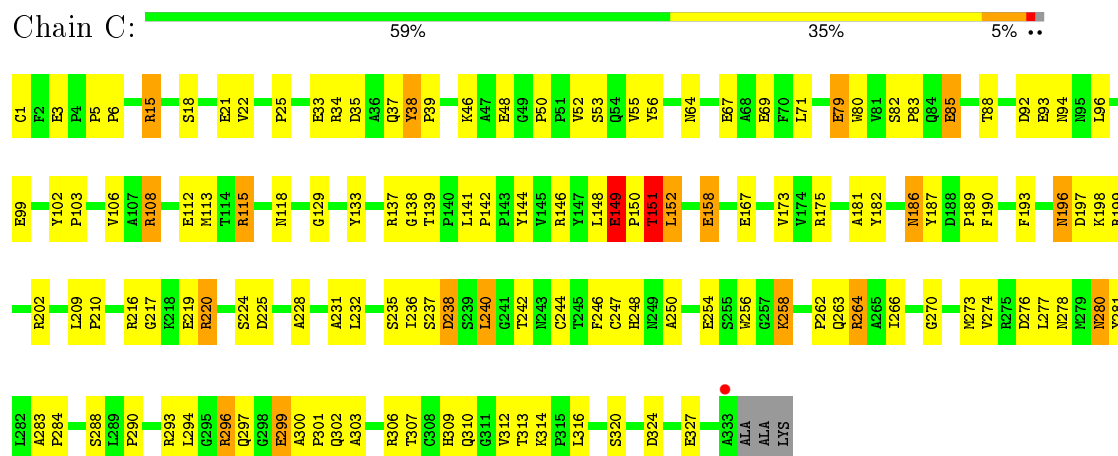
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	66	Total	O	0	0
			66	66		
14	H	41	Total	O	0	0
			41	41		
14	L	39	Total	O	0	0
			39	39		
14	M	55	Total	O	0	0
			55	55		

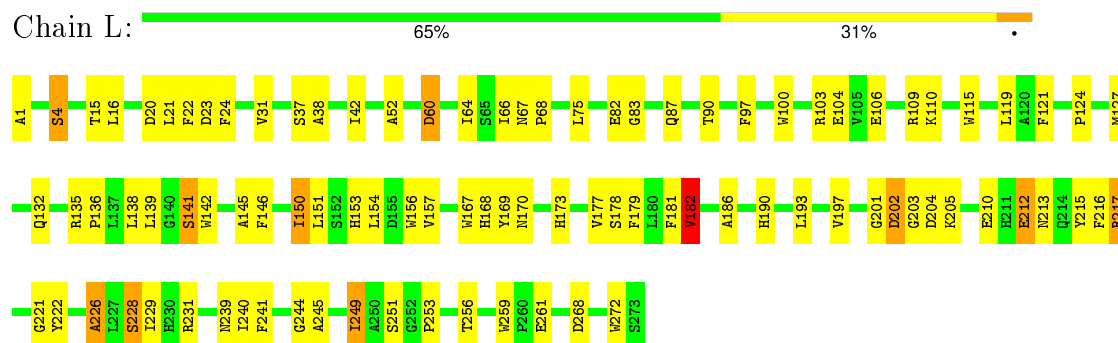
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

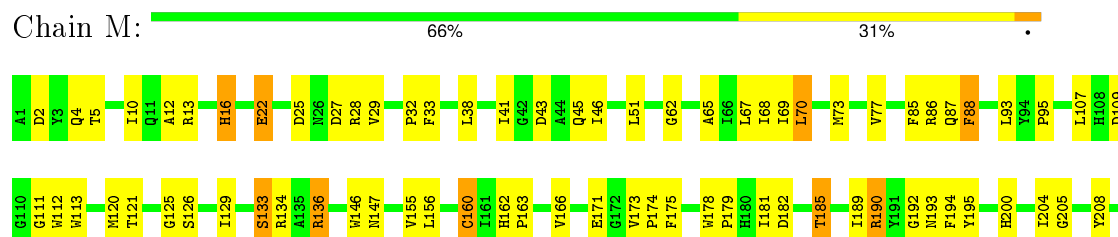
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

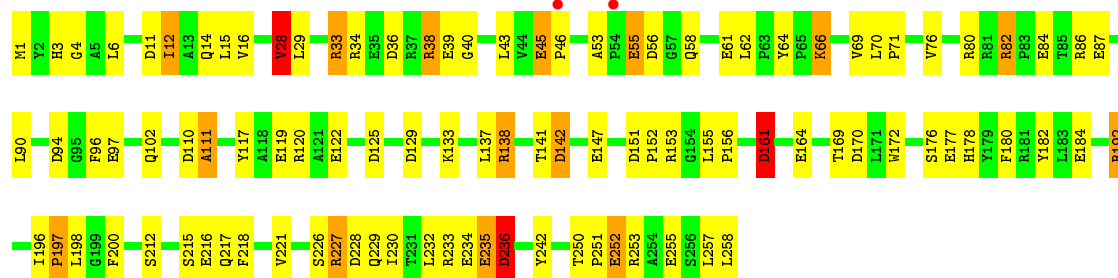


• Molecule 3: PHOTOSYNTHETIC REACTION CENTER





• Molecule 4: PHOTOSYNTHETIC REACTION CENTER



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.50 Å 223.50 Å 113.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.99-2.30) 75.5 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.193 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 95762 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10288	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: LDA, BPB, BCB, FE, MQ7, HEM, UQ1, NS1, FME, SO4

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	C	1.07	17/2670 (0.6%)	1.56	36/3639 (1.0%)
2	L	1.01	5/2259 (0.2%)	1.42	18/3084 (0.6%)
3	M	0.96	3/2659 (0.1%)	1.46	26/3637 (0.7%)
4	H	1.13	18/2055 (0.9%)	1.65	32/2807 (1.1%)
All	All	1.04	43/9643 (0.4%)	1.52	112/13167 (0.9%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	255	GLU	CD-OE2	9.06	1.35	1.25
1	C	299	GLU	CD-OE2	8.31	1.34	1.25
3	M	244	GLU	CD-OE2	8.03	1.34	1.25
2	L	261	GLU	CD-OE2	7.64	1.34	1.25
1	C	21	GLU	CD-OE2	7.48	1.33	1.25
4	H	177	GLU	CD-OE2	7.40	1.33	1.25
1	C	33	GLU	CD-OE2	7.39	1.33	1.25
1	C	158	GLU	CD-OE2	7.36	1.33	1.25
1	C	149	GLU	CD-OE2	7.18	1.33	1.25
4	H	234	GLU	CD-OE2	6.91	1.33	1.25
1	C	99	GLU	CD-OE2	6.86	1.33	1.25
4	H	122	GLU	CD-OE2	6.59	1.32	1.25
1	C	112	GLU	CD-OE2	6.56	1.32	1.25
4	H	164	GLU	CD-OE2	6.56	1.32	1.25
4	H	84	GLU	CD-OE2	6.54	1.32	1.25
1	C	167	GLU	CD-OE2	6.36	1.32	1.25
1	C	254	GLU	CD-OE1	-6.23	1.18	1.25
1	C	67	GLU	CD-OE2	6.16	1.32	1.25
4	H	119	GLU	CD-OE2	6.01	1.32	1.25
2	L	82	GLU	CD-OE2	5.94	1.32	1.25
4	H	252	GLU	CD-OE2	5.87	1.32	1.25
1	C	85	GLU	CD-OE2	5.82	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	GLU	CD-OE1	-5.77	1.19	1.25
1	C	79	GLU	CD-OE2	5.73	1.31	1.25
1	C	69	GLU	CD-OE2	5.71	1.31	1.25
4	H	61	GLU	CD-OE2	5.67	1.31	1.25
2	L	212	GLU	CD-OE2	5.58	1.31	1.25
1	C	3	GLU	CD-OE2	5.52	1.31	1.25
4	H	147	GLU	CD-OE2	5.48	1.31	1.25
4	H	87	GLU	CD-OE2	5.45	1.31	1.25
4	H	235	GLU	CD-OE2	5.40	1.31	1.25
2	L	104	GLU	CD-OE2	5.39	1.31	1.25
1	C	48	GLU	CD-OE2	5.37	1.31	1.25
4	H	216	GLU	CD-OE2	5.34	1.31	1.25
1	C	93	GLU	CD-OE2	5.32	1.31	1.25
3	M	22	GLU	CD-OE2	5.31	1.31	1.25
4	H	55	GLU	CD-OE2	5.22	1.31	1.25
4	H	97	GLU	CD-OE2	5.18	1.31	1.25
4	H	184	GLU	CD-OE2	5.10	1.31	1.25
3	M	232	GLU	CD-OE2	5.10	1.31	1.25
4	H	45	GLU	CD-OE2	5.04	1.31	1.25
4	H	39	GLU	CD-OE1	-5.03	1.20	1.25
2	L	210	GLU	CD-OE2	5.01	1.31	1.25

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	38	ARG	NE-CZ-NH2	-18.45	111.08	120.30
3	M	245	ARG	NE-CZ-NH2	-11.45	114.57	120.30
3	M	25	ASP	CB-CG-OD2	-10.22	109.10	118.30
4	H	153	ARG	NE-CZ-NH2	-9.86	115.37	120.30
4	H	153	ARG	NE-CZ-NH1	9.74	125.17	120.30
3	M	245	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	C	216	ARG	NE-CZ-NH1	9.51	125.05	120.30
3	M	239	ARG	NE-CZ-NH2	-9.45	115.58	120.30
3	M	27	ASP	CB-CG-OD2	-9.40	109.84	118.30
3	M	239	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	C	225	ASP	CB-CG-OD2	-9.02	110.18	118.30
2	L	231	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	C	108	ARG	NE-CZ-NH1	8.68	124.64	120.30
2	L	231	ARG	NE-CZ-NH2	-8.44	116.08	120.30
3	M	304	ASP	CB-CG-OD1	8.33	125.80	118.30
4	H	38	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	C	35	ASP	CB-CG-OD2	-8.03	111.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	236	ASP	CB-CG-OD1	7.97	125.47	118.30
2	L	215	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	C	220	ARG	NE-CZ-NH2	-7.79	116.41	120.30
3	M	25	ASP	CB-CG-OD1	7.76	125.28	118.30
3	M	190	ARG	NE-CZ-NH2	-7.59	116.51	120.30
4	H	161	ASP	CB-CG-OD2	-7.58	111.48	118.30
4	H	236	ASP	CB-CG-OD2	-7.47	111.58	118.30
2	L	20	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	C	313	THR	CA-CB-CG2	-7.38	102.07	112.40
1	C	264	ARG	NE-CZ-NH2	-7.24	116.68	120.30
3	M	160	CYS	CB-CA-C	-7.06	96.28	110.40
1	C	196	ASN	CB-CA-C	-7.05	96.29	110.40
1	C	225	ASP	CB-CG-OD1	7.03	124.63	118.30
1	C	324	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	C	115	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	L	23	ASP	CB-CG-OD1	6.88	124.50	118.30
4	H	62	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	C	115	ARG	NE-CZ-NH2	-6.77	116.91	120.30
3	M	251	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	146	ARG	NE-CZ-NH1	6.68	123.64	120.30
3	M	304	ASP	CB-CG-OD2	-6.64	112.33	118.30
3	M	43	ASP	CB-CG-OD2	-6.59	112.37	118.30
4	H	110	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	C	296	ARG	NE-CZ-NH1	6.49	123.55	120.30
3	M	85	PHE	CB-CA-C	6.39	123.18	110.40
2	L	215	TYR	CB-CG-CD1	6.35	124.81	121.00
2	L	60	ASP	CB-CG-OD2	-6.34	112.59	118.30
3	M	86	ARG	NE-CZ-NH1	6.31	123.45	120.30
3	M	230	ASP	CB-CG-OD2	-6.25	112.68	118.30
3	M	27	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	280	ASN	CB-CA-C	-6.21	97.99	110.40
1	C	197	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	L	23	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	149	GLU	N-CA-CB	6.12	121.62	110.60
1	C	216	ARG	NE-CZ-NH2	-6.07	117.27	120.30
3	M	134	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	L	202	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	C	224	SER	CB-CA-C	-5.96	98.78	110.10
2	L	204	ASP	CB-CG-OD2	-5.92	112.97	118.30
3	M	28	ARG	NE-CZ-NH2	-5.89	117.36	120.30
3	M	231	ARG	NE-CZ-NH2	-5.87	117.36	120.30
4	H	11	ASP	CB-CG-OD1	5.87	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	33	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	L	217	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	151	THR	CA-CB-CG2	-5.78	104.31	112.40
3	M	43	ASP	CB-CG-OD1	5.77	123.50	118.30
4	H	34	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	33	GLU	CB-CA-C	-5.75	98.89	110.40
4	H	151	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	46	LYS	N-CA-CB	5.68	120.83	110.60
1	C	300	ALA	CB-CA-C	-5.68	101.58	110.10
1	C	92	ASP	CB-CG-OD1	5.65	123.38	118.30
1	C	146	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	199	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	M	13	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	M	185	THR	CA-CB-CG2	-5.59	104.57	112.40
4	H	253	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	25	PRO	N-CA-CB	5.59	110.00	103.30
4	H	129	ASP	CA-CB-CG	-5.58	101.14	113.40
2	L	186	ALA	CB-CA-C	-5.57	101.75	110.10
2	L	268	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	324	ASP	CB-CG-OD1	5.51	123.26	118.30
3	M	190	ARG	NE-CZ-NH1	5.48	123.04	120.30
4	H	251	PRO	N-CA-CB	5.46	109.85	103.30
4	H	11	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	C	238	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	C	152	LEU	CB-CA-C	5.43	120.52	110.20
4	H	138	ARG	CB-CA-C	-5.40	99.60	110.40
1	C	220	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	139	THR	N-CA-CB	5.34	120.44	110.30
3	M	230	ASP	CB-CG-OD1	5.31	123.08	118.30
4	H	227	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	L	182	VAL	CB-CA-C	-5.29	101.34	111.40
4	H	64	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	92	ASP	CB-CG-OD2	-5.27	113.56	118.30
4	H	111	ALA	CB-CA-C	5.26	117.99	110.10
4	H	129	ASP	CB-CG-OD2	-5.25	113.58	118.30
2	L	60	ASP	CB-CG-OD1	5.23	123.01	118.30
4	H	14	GLN	CB-CA-C	-5.22	99.95	110.40
2	L	150	ILE	CA-CB-CG1	-5.20	101.12	111.00
4	H	94	ASP	CB-CG-OD2	-5.18	113.64	118.30
4	H	80	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	152	LEU	N-CA-CB	-5.17	100.06	110.40
4	H	28	VAL	CG1-CB-CG2	-5.15	102.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	34	ARG	NE-CZ-NH2	-5.15	117.72	120.30
4	H	161	ASP	CB-CG-OD1	5.15	122.93	118.30
4	H	192	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	L	226	ALA	N-CA-CB	-5.14	102.91	110.10
4	H	66	LYS	N-CA-CB	-5.12	101.39	110.60
2	L	90	THR	CA-CB-CG2	-5.11	105.25	112.40
1	C	237	SER	CB-CA-C	-5.09	100.43	110.10
1	C	296	ARG	NE-CZ-NH2	-5.07	117.76	120.30
3	M	109	ASP	CB-CG-OD1	5.04	122.83	118.30
4	H	197	PRO	N-CA-CB	5.04	109.34	103.30
4	H	141	THR	N-CA-CB	-5.02	100.77	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2603	0	2579	81	0
2	L	2171	0	2098	83	0
3	M	2555	0	2452	78	0
4	H	2018	0	2020	58	0
5	M	1	0	0	0	0
6	H	15	0	0	0	0
6	M	20	0	0	0	0
7	L	132	0	144	22	0
7	M	132	0	144	22	0
8	L	65	0	74	8	0
8	M	65	0	74	11	0
9	M	48	0	64	1	0
10	C	172	0	120	14	0
11	M	40	0	59	4	0
12	L	18	0	18	10	0
13	H	16	0	31	2	0
13	M	16	0	31	1	0
14	C	66	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H	41	0	0	1	0
14	L	39	0	0	3	0
14	M	55	0	0	3	0
All	All	10288	0	9908	321	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 17.

All (321) 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:M:120:MET:HE2	7:M:603:BCB:H172	1.41	1.00
3:M:136:ARG:HE	3:M:136:ARG:HA	1.31	0.93
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.90
8:L:606:BPB:HHC	8:L:606:BPB:HBBB	1.52	0.90
7:L:602:BCB:H61	7:L:604:BCB:HBB3	1.55	0.88
4:H:152:PRO:HA	4:H:155:LEU:CD1	2.04	0.86
3:M:318:LEU:HB3	3:M:319:PRO:HD2	1.57	0.86
3:M:275:MET:HG2	8:M:605:BPB:HBCA	1.58	0.84
7:L:604:BCB:HBB2	7:L:604:BCB:HHC	1.57	0.84
2:L:139:LEU:HD21	2:L:253:PRO:HD3	1.59	0.82
7:L:604:BCB:HMB2	8:L:606:BPB:HMBA	1.62	0.82
7:M:603:BCB:HBB3	7:M:603:BCB:HMB1	1.61	0.82
1:C:202:ARG:HG2	10:C:611:HEM:CGA	2.12	0.80
1:C:270:GLY:O	1:C:274:VAL:HG12	1.81	0.79
3:M:120:MET:HE3	7:M:603:BCB:H193	1.63	0.79
7:L:602:BCB:H61	7:L:604:BCB:CBB	2.13	0.79
2:L:190:HIS:HA	12:L:614:UQ1:O4	1.81	0.79
4:H:82:ARG:HG2	4:H:82:ARG:HH11	1.47	0.78
8:L:606:BPB:HHC	8:L:606:BPB:CBB	2.14	0.77
4:H:152:PRO:HA	4:H:155:LEU:HD11	1.67	0.77
2:L:181:PHE:HB3	8:M:605:BPB:HBBA	1.67	0.76
3:M:190:ARG:HD2	3:M:190:ARG:O	1.85	0.76
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.19	0.76
1:C:196:ASN:HB3	1:C:198:LYS:H	1.49	0.76
2:L:202:ASP:CG	2:L:203:GLY:H	1.90	0.74
8:M:605:BPB:H55	8:M:605:BPB:HMC	1.70	0.74
4:H:133:LYS:HG3	4:H:176:SER:HB2	1.69	0.73
3:M:185:THR:O	3:M:189:ILE:HG13	1.90	0.72
2:L:212:GLU:OE1	12:L:614:UQ1:HM33	1.90	0.72
1:C:148:LEU:HG	1:C:299:GLU:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:HD12	1:C:142:PRO:HD2	1.72	0.71
4:H:45:GLU:HB3	4:H:46:PRO:HD2	1.72	0.70
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.71	0.70
1:C:220:ARG:NH2	14:C:637:HOH:O	2.22	0.70
8:M:605:BPB:HBBB	8:M:605:BPB:HHC	1.73	0.70
4:H:55:GLU:HB3	4:H:58:GLN:HG3	1.73	0.70
4:H:138:ARG:NH1	4:H:228:ASP:OD1	2.25	0.70
3:M:5:THR:CG2	3:M:222:LEU:HB3	2.21	0.69
3:M:136:ARG:NE	3:M:136:ARG:HA	2.07	0.69
7:M:603:BCB:CBD	7:M:603:BCB:HAA2	2.23	0.68
7:L:602:BCB:C6	7:L:604:BCB:HBB3	2.23	0.68
8:L:606:BPB:HBB	3:M:208:TYR:CD2	2.28	0.68
7:M:603:BCB:HBD	7:M:603:BCB:HAA2	1.75	0.67
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.30	0.67
7:M:603:BCB:CBB	7:M:603:BCB:HMB1	2.24	0.67
7:M:601:BCB:CBB	11:M:613:NS1:H223	2.25	0.67
2:L:38:ALA:O	2:L:42:ILE:HG13	1.95	0.67
3:M:288:PHE:CD1	4:H:12:ILE:HD11	2.31	0.66
2:L:151:LEU:HD21	13:H:616:LDA:H111	1.78	0.66
2:L:151:LEU:CD2	13:H:616:LDA:H111	2.26	0.65
1:C:149:GLU:OE1	1:C:296:ARG:NH1	2.27	0.65
4:H:197:PRO:HG2	4:H:200:PHE:CD1	2.32	0.65
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.31	0.65
3:M:70:LEU:HD23	3:M:73:MET:CE	2.27	0.65
3:M:160:CYS:SG	11:M:613:NS1:H322	2.36	0.64
4:H:125:ASP:HB2	4:H:232:LEU:HD21	1.78	0.64
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.16	0.63
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.33	0.63
2:L:226:ALA:HA	12:L:614:UQ1:HM32	1.80	0.62
3:M:70:LEU:HD23	3:M:73:MET:HE2	1.79	0.62
4:H:218:PHE:O	4:H:221:VAL:HG23	1.99	0.62
4:H:250:THR:HG22	4:H:252:GLU:H	1.63	0.62
1:C:248:HIS:HB3	14:C:635:HOH:O	2.00	0.62
8:L:606:BPB:HBBA	3:M:208:TYR:HB3	1.82	0.61
2:L:226:ALA:O	2:L:229:ILE:HG22	2.01	0.61
1:C:278:ASN:OD1	1:C:302:GLN:HB3	2.00	0.61
2:L:22:PHE:HA	2:L:24:PHE:HE1	1.66	0.61
1:C:56:TYR:HB3	10:C:609:HEM:O2A	2.01	0.61
7:L:602:BCB:CBB	7:L:602:BCB:HMB1	2.31	0.61
2:L:124:PRO:HB2	7:L:602:BCB:H93	1.83	0.61
1:C:173:VAL:HB	3:M:87:GLN:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:611:HEM:HHA	10:C:611:HEM:HBA1	1.83	0.60
2:L:213:ASN:O	2:L:217:ARG:HG3	2.02	0.60
3:M:205:GLY:HA3	13:M:615:LDA:H121	1.84	0.60
1:C:247:CYS:HB2	10:C:611:HEM:C2C	2.36	0.60
7:M:601:BCB:OBB	7:M:601:BCB:HMB1	2.01	0.60
1:C:5:PRO:CB	1:C:6:PRO:HA	2.32	0.60
1:C:309:HIS:HE1	10:C:612:HEM:NA	1.99	0.60
1:C:102:TYR:CD1	1:C:103:PRO:HD3	2.37	0.60
2:L:178:SER:O	2:L:182:VAL:HG22	2.02	0.60
8:M:605:BPB:CBC	8:M:605:BPB:HMC	2.32	0.59
3:M:120:MET:CE	7:M:603:BCB:H193	2.32	0.59
7:M:601:BCB:HBB1	11:M:613:NS1:H223	1.83	0.59
1:C:108:ARG:NH1	10:C:609:HEM:O2D	2.35	0.59
1:C:15:ARG:HG2	14:L:629:HOH:O	2.03	0.59
7:L:602:BCB:NA	7:M:603:BCB:HBB2	2.18	0.59
2:L:154:LEU:HD23	2:L:154:LEU:N	2.18	0.59
2:L:139:LEU:HD21	2:L:253:PRO:CD	2.32	0.58
4:H:4:GLY:HA2	4:H:12:ILE:HD11	1.84	0.58
7:L:604:BCB:CBB	7:L:604:BCB:HHC	2.30	0.57
1:C:244:CYS:HA	10:C:611:HEM:HHC	1.86	0.57
4:H:86:ARG:NH2	4:H:111:ALA:O	2.38	0.57
3:M:227:PHE:HB2	3:M:242:ALA:HB2	1.87	0.57
3:M:258:ALA:HA	4:H:36:ASP:HB3	1.85	0.57
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.87	0.57
3:M:107:LEU:HD22	3:M:112:TRP:CE2	2.40	0.57
7:L:604:BCB:HMB2	8:L:606:BPB:CMB	2.33	0.56
2:L:216:PHE:CE2	12:L:614:UQ1:HM53	2.40	0.56
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.86	0.56
2:L:4:SER:HB3	4:H:40:GLY:HA2	1.85	0.56
3:M:93:LEU:HD21	3:M:113:TRP:HA	1.88	0.56
1:C:256:TRP:CH2	1:C:264:ARG:HG2	2.40	0.56
3:M:226:ARG:HG3	14:M:646:HOH:O	2.06	0.56
4:H:38:ARG:NH1	4:H:66:LYS:HB2	2.21	0.56
7:L:602:BCB:HBB3	7:L:602:BCB:HMB1	1.88	0.56
2:L:181:PHE:CD2	8:M:605:BPB:HBB	2.41	0.55
3:M:240:GLY:O	3:M:244:GLU:HG3	2.07	0.55
2:L:202:ASP:CG	2:L:203:GLY:N	2.59	0.55
4:H:137:LEU:HB2	4:H:170:ASP:OD2	2.06	0.55
2:L:179:PHE:HA	2:L:182:VAL:HG23	1.89	0.55
2:L:193:LEU:HD22	2:L:216:PHE:HE2	1.72	0.55
1:C:202:ARG:HG2	10:C:611:HEM:O2A	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:PRO:HG2	10:C:610:HEM:HBD1	1.87	0.55
3:M:162:HIS:O	3:M:166:VAL:HG22	2.07	0.55
1:C:244:CYS:HA	10:C:611:HEM:CHC	2.37	0.55
1:C:148:LEU:HD12	1:C:299:GLU:HB3	1.88	0.55
1:C:144:TYR:CD1	1:C:310:GLN:HG2	2.42	0.54
1:C:150:PRO:O	1:C:175:ARG:HD2	2.07	0.54
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.41	0.54
2:L:244:GLY:O	7:L:602:BCB:HED3	2.07	0.54
3:M:195:TYR:CZ	7:M:603:BCB:HMC2	2.42	0.54
2:L:170:ASN:HB2	2:L:259:TRP:CD1	2.43	0.53
7:L:602:BCB:C5	7:L:604:BCB:HBB3	2.38	0.53
2:L:181:PHE:CB	8:M:605:BPB:HBBA	2.38	0.53
4:H:155:LEU:HB3	4:H:156:PRO:HD2	1.90	0.53
4:H:82:ARG:HH11	4:H:82:ARG:CG	2.20	0.53
2:L:124:PRO:HB2	7:L:602:BCB:C9	2.39	0.53
2:L:193:LEU:HD22	2:L:216:PHE:CE2	2.43	0.53
4:H:70:LEU:HB3	4:H:71:PRO:HD2	1.91	0.53
3:M:318:LEU:HB3	3:M:319:PRO:CD	2.34	0.52
1:C:37:GLN:O	1:C:39:PRO:HD3	2.08	0.52
4:H:6:LEU:HD12	4:H:15:LEU:HD11	1.91	0.52
3:M:69:ILE:O	3:M:73:MET:HG3	2.09	0.52
2:L:153:HIS:O	2:L:157:VAL:HG23	2.10	0.52
3:M:195:TYR:CE2	7:M:603:BCB:HMC2	2.44	0.52
3:M:29:VAL:HG23	3:M:51:LEU:HD13	1.90	0.52
1:C:52:VAL:HA	1:C:55:VAL:HB	1.92	0.52
2:L:16:LEU:HB2	2:L:106:GLU:HG2	1.91	0.52
2:L:1:ALA:H2	4:H:43:LEU:HB3	1.74	0.52
2:L:138:LEU:HD12	2:L:249:ILE:CD1	2.40	0.52
2:L:127:MET:O	2:L:127:MET:HG3	2.10	0.52
4:H:192:ARG:NH1	4:H:221:VAL:O	2.43	0.51
2:L:168:HIS:CE1	7:L:602:BCB:HMC2	2.45	0.51
1:C:80:TRP:O	1:C:138:GLY:HA2	2.10	0.51
12:L:614:UQ1:C8	12:L:614:UQ1:HM51	2.39	0.51
2:L:150:ILE:HG13	14:L:633:HOH:O	2.10	0.51
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.92	0.51
1:C:22:VAL:HG12	2:L:256:THR:HB	1.92	0.51
1:C:96:LEU:O	10:C:609:HEM:HBA1	2.11	0.51
2:L:217:ARG:NH1	14:L:647:HOH:O	2.43	0.51
4:H:90:LEU:HD23	4:H:102:GLN:C	2.32	0.50
4:H:161:ASP:OD2	4:H:161:ASP:N	2.33	0.50
3:M:155:VAL:CG2	7:M:603:BCB:H62	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:21:LEU:HD23	2:L:22:PHE:CE2	2.46	0.50
3:M:212:LEU:HD23	3:M:212:LEU:C	2.32	0.50
1:C:309:HIS:HE1	10:C:612:HEM:C1A	2.29	0.50
2:L:167:TRP:NE1	2:L:173:HIS:CD2	2.79	0.50
1:C:238:ASP:OD1	1:C:306:ARG:NH2	2.45	0.50
2:L:60:ASP:O	2:L:64:ILE:HG13	2.10	0.50
3:M:155:VAL:HG21	7:M:603:BCB:H8	1.94	0.49
1:C:277:LEU:O	1:C:281:TYR:HB2	2.12	0.49
3:M:70:LEU:CD2	3:M:73:MET:HE3	2.42	0.49
4:H:196:ILE:HD12	4:H:242:TYR:CE1	2.48	0.49
4:H:152:PRO:CA	4:H:155:LEU:HD12	2.41	0.49
1:C:273:MET:O	1:C:277:LEU:HG	2.12	0.49
3:M:224:VAL:O	3:M:225:ALA:C	2.50	0.49
3:M:318:LEU:CB	3:M:319:PRO:HD2	2.35	0.48
1:C:15:ARG:NH2	14:C:667:HOH:O	2.45	0.48
3:M:51:LEU:HD12	3:M:51:LEU:N	2.28	0.48
3:M:162:HIS:HD2	14:M:626:HOH:O	1.96	0.48
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.48	0.48
12:L:614:UQ1:HM22	12:L:614:UQ1:O1	2.14	0.48
3:M:192:GLY:O	3:M:193:ASN:HB3	2.13	0.48
3:M:160:CYS:C	3:M:163:PRO:HD2	2.33	0.48
3:M:2:ASP:OD2	3:M:4:GLN:HB2	2.14	0.48
7:L:604:BCB:H192	7:L:604:BCB:H161	1.63	0.48
3:M:120:MET:CE	7:M:603:BCB:H172	2.28	0.48
4:H:133:LYS:HG3	4:H:176:SER:CB	2.40	0.47
3:M:5:THR:HG21	3:M:222:LEU:HB3	1.93	0.47
1:C:189:PRO:CB	1:C:232:LEU:HA	2.43	0.47
8:M:605:BPB:CBB	8:M:605:BPB:HHC	2.42	0.47
3:M:266:TRP:CH2	4:H:28:VAL:CG2	2.97	0.47
4:H:125:ASP:HB2	4:H:232:LEU:CD2	2.42	0.47
1:C:189:PRO:O	1:C:193:PHE:HB2	2.15	0.47
4:H:120:ARG:HB2	4:H:233:ARG:HA	1.97	0.47
4:H:70:LEU:HD11	4:H:76:VAL:HG23	1.96	0.47
3:M:234:GLU:HB2	14:H:632:HOH:O	2.14	0.47
4:H:226:SER:HB3	4:H:229:GLN:HG2	1.95	0.47
3:M:10:ILE:O	4:H:180:PHE:HD2	1.98	0.47
2:L:153:HIS:CE1	2:L:154:LEU:HD21	2.50	0.47
2:L:75:LEU:HA	2:L:75:LEU:HD23	1.70	0.47
2:L:249:ILE:O	2:L:253:PRO:HG2	2.15	0.47
4:H:138:ARG:NH1	4:H:227:ARG:NE	2.62	0.47
7:L:602:BCB:C3	7:L:604:BCB:HBB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:129:ILE:O	3:M:133:SER:HB3	2.15	0.46
4:H:142:ASP:OD2	4:H:142:ASP:N	2.40	0.46
2:L:135:ARG:NH2	2:L:251:SER:O	2.41	0.46
3:M:5:THR:HG22	3:M:222:LEU:HB3	1.96	0.46
1:C:262:PRO:O	1:C:266:ILE:HG12	2.14	0.46
1:C:181:ALA:O	1:C:182:TYR:HB2	2.15	0.46
1:C:240:LEU:HD23	1:C:240:LEU:N	2.30	0.46
4:H:45:GLU:HB3	4:H:46:PRO:CD	2.41	0.46
2:L:216:PHE:CD2	12:L:614:UQ1:H71	2.51	0.46
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.80	0.46
3:M:121:THR:HG23	3:M:156:LEU:HD21	1.98	0.46
4:H:161:ASP:OD1	4:H:215:SER:OG	2.33	0.46
2:L:205:LYS:HA	4:H:69:VAL:HG22	1.96	0.46
4:H:172:TRP:N	4:H:172:TRP:CD1	2.84	0.46
1:C:246:PHE:CE2	1:C:263:GLN:HG2	2.51	0.46
2:L:216:PHE:CE2	12:L:614:UQ1:CM5	2.98	0.45
1:C:276:ASP:O	1:C:280:ASN:HB2	2.16	0.45
2:L:245:ALA:O	2:L:249:ILE:HB	2.15	0.45
3:M:87:GLN:O	3:M:88:PHE:C	2.55	0.45
1:C:38:TYR:CD2	1:C:316:LEU:HD13	2.51	0.45
1:C:151:THR:O	1:C:152:LEU:HB2	2.17	0.45
1:C:309:HIS:O	1:C:310:GLN:C	2.54	0.45
1:C:242:THR:HA	14:C:675:HOH:O	2.17	0.45
2:L:193:LEU:HD12	2:L:193:LEU:HA	1.58	0.45
3:M:224:VAL:HG23	3:M:229:GLY:HA3	1.99	0.45
2:L:110:LYS:HB2	2:L:110:LYS:HE2	1.73	0.45
4:H:33:ARG:HD2	4:H:33:ARG:HA	1.90	0.45
4:H:197:PRO:HG2	4:H:200:PHE:HD1	1.76	0.45
8:M:605:BPB:CMC	8:M:605:BPB:H55	2.44	0.45
2:L:228:SER:HB3	3:M:41:ILE:O	2.17	0.45
8:L:606:BPB:CBB	3:M:208:TYR:CD2	2.98	0.45
1:C:137:ARG:HG3	1:C:310:GLN:HE22	1.82	0.45
2:L:240:ILE:HG22	2:L:241:PHE:CD1	2.52	0.44
3:M:155:VAL:HG22	7:M:603:BCB:H62	1.98	0.44
3:M:70:LEU:CD2	3:M:73:MET:CE	2.94	0.44
3:M:146:TRP:HA	3:M:146:TRP:CE3	2.52	0.44
8:M:605:BPB:H6A	8:M:605:BPB:H4	1.86	0.44
2:L:226:ALA:N	12:L:614:UQ1:HM21	2.32	0.44
1:C:56:TYR:HB3	10:C:609:HEM:CGA	2.48	0.44
3:M:38:LEU:CD2	3:M:46:ILE:HD11	2.47	0.44
2:L:121:PHE:O	2:L:124:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:601:BCB:HHC	7:M:601:BCB:HBB2	1.98	0.44
2:L:132:GLN:OE1	2:L:145:ALA:HB1	2.18	0.44
4:H:197:PRO:HG2	4:H:200:PHE:CE1	2.52	0.44
1:C:88:THR:O	1:C:88:THR:HG22	2.17	0.44
2:L:217:ARG:O	2:L:221:GLY:HA2	2.17	0.44
1:C:258:LYS:HD3	3:M:305:TYR:O	2.17	0.44
1:C:50:PRO:HG2	1:C:55:VAL:CG2	2.47	0.44
1:C:106:VAL:HG11	10:C:610:HEM:CAA	2.48	0.44
1:C:297:GLN:HB2	1:C:297:GLN:HE21	1.46	0.44
2:L:136:PRO:HB3	2:L:141:SER:O	2.18	0.44
1:C:299:GLU:N	1:C:299:GLU:OE2	2.41	0.43
2:L:135:ARG:HD3	2:L:135:ARG:HH11	1.69	0.43
1:C:118:ASN:OD1	1:C:129:GLY:HA2	2.17	0.43
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.00	0.43
3:M:173:VAL:HG12	3:M:174:PRO:O	2.18	0.43
1:C:228:ALA:O	1:C:231:ALA:HB3	2.18	0.43
4:H:16:VAL:O	4:H:16:VAL:HG12	2.19	0.43
7:M:601:BCB:HBB2	11:M:613:NS1:C22	2.48	0.43
2:L:239:ASN:HD22	2:L:239:ASN:HA	1.67	0.43
3:M:178:TRP:N	3:M:179:PRO:CD	2.81	0.43
2:L:37:SER:O	2:L:38:ALA:C	2.57	0.43
3:M:69:ILE:HD13	3:M:175:PHE:CD1	2.54	0.43
4:H:230:ILE:HD13	4:H:235:GLU:HG2	2.00	0.43
4:H:12:ILE:H	4:H:12:ILE:HG12	1.48	0.43
1:C:186:ASN:C	1:C:187:TYR:CD1	2.91	0.43
7:L:602:BCB:C4A	7:M:603:BCB:HBB2	2.49	0.43
7:M:601:BCB:C4A	7:M:601:BCB:CBA	2.97	0.43
1:C:186:ASN:ND2	14:C:649:HOH:O	2.51	0.43
2:L:83:GLY:O	2:L:87:GLN:HG3	2.19	0.43
8:M:605:BPB:H11A	8:M:605:BPB:H9	1.78	0.43
1:C:312:VAL:HG12	1:C:314:LYS:O	2.19	0.43
1:C:210:PRO:HB2	4:H:3:HIS:HD2	1.84	0.42
2:L:100:TRP:O	2:L:103:ARG:HB3	2.19	0.42
2:L:67:ASN:HB3	2:L:68:PRO:HD2	2.00	0.42
3:M:12:ALA:HB2	4:H:180:PHE:CE2	2.54	0.42
3:M:67:LEU:O	3:M:68:ILE:C	2.53	0.42
1:C:217:GLY:O	1:C:220:ARG:HB2	2.19	0.42
1:C:283:ALA:N	1:C:284:PRO:HD2	2.34	0.42
2:L:52:ALA:HB3	2:L:66:ILE:CD1	2.49	0.42
7:M:601:BCB:HBA1	7:M:601:BCB:C4A	2.50	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:115:TRP:CD1	2:L:115:TRP:N	2.88	0.42
4:H:1:FME:HB3	4:H:1:FME:HE2	1.84	0.42
1:C:102:TYR:O	1:C:103:PRO:C	2.58	0.42
3:M:259:THR:HG23	4:H:36:ASP:O	2.20	0.42
3:M:125:GLY:O	3:M:129:ILE:HG13	2.19	0.42
4:H:29:LEU:HD23	4:H:29:LEU:HA	1.82	0.42
2:L:229:ILE:HG13	2:L:229:ILE:O	2.20	0.42
3:M:289:VAL:HG21	3:M:292:TRP:CH2	2.55	0.42
1:C:79:GLU:O	1:C:83:PRO:HG3	2.19	0.41
3:M:293:TYR:O	3:M:297:VAL:HG23	2.19	0.41
2:L:156:TRP:O	2:L:157:VAL:C	2.57	0.41
2:L:201:GLY:O	2:L:202:ASP:HB3	2.20	0.41
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.55	0.41
7:L:602:BCB:H193	9:M:608:MQ7:H292	2.02	0.41
2:L:139:LEU:HA	2:L:139:LEU:HD23	1.81	0.41
2:L:229:ILE:HD13	12:L:614:UQ1:H8	2.02	0.41
4:H:4:GLY:HA2	4:H:12:ILE:CD1	2.49	0.41
3:M:62:GLY:O	3:M:65:ALA:HB3	2.21	0.41
3:M:282:ILE:HD13	3:M:282:ILE:HA	1.88	0.41
1:C:190:PHE:HE1	1:C:303:ALA:O	2.03	0.41
2:L:177:VAL:HG13	7:L:602:BCB:HMB3	2.02	0.41
4:H:117:TYR:HB2	4:H:236:ASP:HB3	2.02	0.41
3:M:95:PRO:HG2	14:M:629:HOH:O	2.20	0.41
1:C:236:ILE:O	1:C:240:LEU:HG	2.20	0.41
7:L:604:BCB:H13	7:L:604:BCB:H172	1.82	0.41
4:H:257:LEU:HA	4:H:257:LEU:HD23	1.72	0.41
1:C:102:TYR:CG	1:C:103:PRO:CD	2.96	0.41
3:M:231:ARG:HH22	4:H:235:GLU:CD	2.24	0.41
2:L:222:TYR:HD1	3:M:45:GLN:O	2.03	0.41
2:L:97:PHE:CZ	7:L:602:BCB:H112	2.55	0.41
2:L:169:TYR:OH	3:M:182:ASP:OD2	2.31	0.41
2:L:87:GLN:NE2	2:L:142:TRP:CD1	2.89	0.41
2:L:67:ASN:OD1	2:L:67:ASN:N	2.53	0.41
2:L:52:ALA:HB3	2:L:66:ILE:HD11	2.03	0.41
3:M:258:ALA:HB1	3:M:262:SER:OG	2.21	0.40
4:H:138:ARG:HG3	4:H:170:ASP:OD1	2.21	0.40
1:C:113:MET:HB2	1:C:281:TYR:CD1	2.56	0.40
3:M:16:HIS:HD2	3:M:32:PRO:HG3	1.85	0.40
3:M:312:THR:HA	3:M:313:PRO:HD2	1.90	0.40
2:L:241:PHE:CE2	8:L:606:BPB:H43	2.56	0.40
1:C:102:TYR:CE2	1:C:103:PRO:HD3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:TYR:O	1:C:307:THR:HG23	2.22	0.40
2:L:109:ARG:HD2	2:L:109:ARG:HH11	1.77	0.40
1:C:149:GLU:HB3	1:C:150:PRO:HD2	2.03	0.40
2:L:197:VAL:HG21	2:L:212:GLU:HG2	2.03	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	C	331/336 (98%)	306 (92%)	24 (7%)	1 (0%)	46	57
2	L	271/273 (99%)	252 (93%)	18 (7%)	1 (0%)	39	48
3	M	321/323 (99%)	300 (94%)	19 (6%)	2 (1%)	30	36
4	H	256/258 (99%)	239 (93%)	16 (6%)	1 (0%)	39	48
All	All	1179/1190 (99%)	1097 (93%)	77 (6%)	5 (0%)	39	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	22	GLU
4	H	53	ALA
3	M	88	PHE
1	C	250	ALA
2	L	31	VAL

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	C	281/282 (100%)	261 (93%)	20 (7%)	18	23
2	L	218/218 (100%)	210 (96%)	8 (4%)	41	55
3	M	249/249 (100%)	235 (94%)	14 (6%)	26	35
4	H	212/212 (100%)	197 (93%)	15 (7%)	18	23
All	All	960/961 (100%)	903 (94%)	57 (6%)	24	32

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	CYS
1	C	15	ARG
1	C	34	ARG
1	C	38	TYR
1	C	53	SER
1	C	64	ASN
1	C	94	ASN
1	C	115	ARG
1	C	149	GLU
1	C	151	THR
1	C	158	GLU
1	C	186	ASN
1	C	209	LEU
1	C	235	SER
1	C	240	LEU
1	C	258	LYS
1	C	288	SER
1	C	294	LEU
1	C	320	SER
1	C	327	GLU
2	L	4	SER
2	L	15	THR
2	L	119	LEU
2	L	141	SER
2	L	182	VAL
2	L	228	SER
2	L	249	ILE
2	L	272	TRP
3	M	16	HIS
3	M	33	PHE

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Mol	Chain	Res	Type
3	M	70	LEU
3	M	77	VAL
3	M	126	SER
3	M	133	SER
3	M	136	ARG
3	M	147	ASN
3	M	171	GLU
3	M	181	ILE
3	M	194	PHE
3	M	214	PHE
3	M	249	PHE
3	M	279	SER
4	H	12	ILE
4	H	28	VAL
4	H	56	ASP
4	H	82	ARG
4	H	96	PHE
4	H	142	ASP
4	H	161	ASP
4	H	169	THR
4	H	178	HIS
4	H	182	TYR
4	H	198	LEU
4	H	212	SER
4	H	217	GLN
4	H	236	ASP
4	H	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	ASN
1	C	297	GLN
1	C	302	GLN
1	C	310	GLN
2	L	144	HIS
2	L	183	ASN
2	L	214	GLN
2	L	239	ASN
4	H	3	HIS
4	H	225	GLN
4	H	229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
4	FME	H	1	4	8,9,10	0.88	1 (12%)	6,9,11	3.46	2 (33%)

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	FME	H	1	4	-	1/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	FME	CA-N	-2.13	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	O1-CN-N	-6.97	114.72	124.76
4	H	1	FME	CA-N-CN	-4.40	116.05	122.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	$\# Z > 2$
10	HEM	C	609	1	30,50,50	4.25	9 (30%)	24,82,82	3.23	9 (37%)
10	HEM	C	610	1	30,50,50	4.20	11 (36%)	24,82,82	3.39	11 (45%)
10	HEM	C	611	1	30,50,50	3.76	11 (36%)	24,82,82	3.08	10 (41%)
10	HEM	C	612	1	30,50,50	3.54	11 (36%)	24,82,82	2.71	9 (37%)
13	LDA	H	616	-	15,15,15	4.75	4 (26%)	16,17,17	1.20	2 (12%)
6	SO4	H	617	-	4,4,4	1.45	0	6,6,6	0.21	0
6	SO4	H	622	-	4,4,4	1.62	1 (25%)	6,6,6	0.20	0
6	SO4	H	623	-	4,4,4	1.47	0	6,6,6	0.26	0
7	BCB	L	602	2	56,74,74	1.58	6 (10%)	57,115,115	1.76	15 (26%)
7	BCB	L	604	2	56,74,74	1.53	6 (10%)	57,115,115	1.50	13 (22%)
8	BPB	L	606	-	63,70,70	1.38	7 (11%)	63,101,101	1.56	14 (22%)
12	UQ1	L	614	-	18,18,18	0.77	1 (5%)	22,25,25	1.07	3 (13%)
7	BCB	M	601	3	56,74,74	1.31	5 (8%)	57,115,115	1.63	13 (22%)
7	BCB	M	603	3	56,74,74	1.80	16 (28%)	57,115,115	1.86	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BPB	M	605	-	63,70,70	1.30	6 (9%)	63,101,101	1.39	7 (11%)
9	MQ7	M	608	-	49,49,49	1.41	6 (12%)	62,63,63	2.37	22 (35%)
11	NS1	M	613	-	39,39,39	2.65	12 (30%)	44,46,46	2.12	16 (36%)
13	LDA	M	615	-	15,15,15	4.97	4 (26%)	16,17,17	3.15	5 (31%)
6	SO4	M	618	-	4,4,4	1.16	0	6,6,6	0.29	0
6	SO4	M	619	-	4,4,4	1.20	0	6,6,6	0.23	0
6	SO4	M	620	-	4,4,4	0.91	0	6,6,6	0.15	0
6	SO4	M	621	-	4,4,4	1.60	0	6,6,6	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	C	609	1	-	0/10/54/54	0/0/8/8
10	HEM	C	610	1	-	0/10/54/54	0/0/8/8
10	HEM	C	611	1	-	0/10/54/54	0/0/8/8
10	HEM	C	612	1	-	0/10/54/54	0/0/8/8
13	LDA	H	616	-	-	0/13/13/13	0/0/0/0
6	SO4	H	617	-	-	0/0/0/0	0/0/0/0
6	SO4	H	622	-	-	0/0/0/0	0/0/0/0
6	SO4	H	623	-	-	0/0/0/0	0/0/0/0
7	BCB	L	602	2	-	0/37/137/137	0/0/9/9
7	BCB	L	604	2	-	0/37/137/137	0/0/9/9
8	BPB	L	606	-	-	0/46/105/105	0/1/6/6
12	UQ1	L	614	-	-	0/9/33/33	0/1/1/1
7	BCB	M	601	3	-	0/37/137/137	0/0/9/9
7	BCB	M	603	3	-	0/37/137/137	0/0/9/9
8	BPB	M	605	-	-	0/46/105/105	0/1/6/6
9	MQ7	M	608	-	-	0/41/61/61	0/2/2/2
11	NS1	M	613	-	-	0/43/43/43	0/0/0/0
13	LDA	M	615	-	-	0/13/13/13	0/0/0/0
6	SO4	M	618	-	-	0/0/0/0	0/0/0/0
6	SO4	M	619	-	-	0/0/0/0	0/0/0/0
6	SO4	M	620	-	-	0/0/0/0	0/0/0/0
6	SO4	M	621	-	-	0/0/0/0	0/0/0/0

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	615	LDA	O1-N1	-18.58	1.21	1.39
13	H	616	LDA	O1-N1	-17.56	1.22	1.39
10	C	609	HEM	C3B-C4B	-16.79	1.36	1.51
10	C	610	HEM	C3B-C4B	-14.89	1.38	1.51
10	C	611	HEM	C3B-C4B	-13.04	1.40	1.51
10	C	612	HEM	C3D-C4D	-11.10	1.37	1.51
10	C	610	HEM	C3D-C4D	-10.69	1.37	1.51
10	C	612	HEM	C3B-C4B	-10.22	1.42	1.51
10	C	611	HEM	C3D-C4D	-9.04	1.40	1.51
10	C	609	HEM	C2C-C1C	-8.98	1.35	1.52
10	C	610	HEM	C2C-C1C	-7.86	1.37	1.52
10	C	609	HEM	C3D-C4D	-7.57	1.41	1.51
10	C	611	HEM	C2C-C1C	-7.05	1.39	1.52
10	C	609	HEM	C2D-C3D	-6.82	1.34	1.54
10	C	612	HEM	C2C-C1C	-6.70	1.39	1.52
7	L	604	BCB	C2C-C1C	-6.60	1.46	1.51
10	C	611	HEM	C2D-C3D	-5.56	1.37	1.54
7	L	602	BCB	C4D-CHA	-5.56	1.38	1.45
10	C	610	HEM	C2D-C3D	-5.30	1.38	1.54
7	M	603	BCB	C4D-CHA	-4.92	1.38	1.45
7	L	602	BCB	C3D-CAD	-4.89	1.36	1.46
7	M	603	BCB	CAA-C2A	-4.60	1.44	1.54
7	L	604	BCB	O1A-CGA	-4.44	1.09	1.22
10	C	611	HEM	CAA-C2A	-4.20	1.44	1.52
10	C	610	HEM	C2D-C1D	-4.06	1.38	1.51
7	M	601	BCB	C4D-CHA	-4.01	1.40	1.45
8	L	606	BPB	O2D-CED	-3.85	1.35	1.45
7	M	601	BCB	O1D-CGD	-3.71	1.11	1.21
10	C	612	HEM	C2D-C1D	-3.67	1.39	1.51
9	M	608	MQ7	C10-C1	-3.64	1.41	1.48
10	C	610	HEM	CAA-C2A	-3.61	1.45	1.52
10	C	612	HEM	C2D-C3D	-3.59	1.43	1.54
7	L	602	BCB	O2D-CED	-3.58	1.36	1.45
7	L	604	BCB	C4D-CHA	-3.57	1.40	1.45
11	M	613	NS1	C14-C15	-3.53	1.38	1.45
9	M	608	MQ7	C10-C5	-3.52	1.35	1.40
10	C	610	HEM	C2B-C1B	-3.50	1.40	1.51
13	H	616	LDA	C1-N1	-3.43	1.45	1.51
7	M	603	BCB	O1A-CGA	-3.41	1.12	1.22
13	M	615	LDA	CM2-N1	-3.27	1.44	1.49
10	C	609	HEM	C2B-C1B	-3.22	1.41	1.51
10	C	611	HEM	C2B-C1B	-3.02	1.42	1.51
10	C	611	HEM	C2D-C1D	-3.00	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	609	HEM	C2D-C1D	-2.80	1.42	1.51
13	M	615	LDA	CM1-N1	-2.74	1.45	1.49
10	C	611	HEM	C3B-CAB	-2.74	1.46	1.51
7	L	602	BCB	CAC-C3C	-2.73	1.29	1.33
13	H	616	LDA	CM1-N1	-2.72	1.45	1.49
10	C	612	HEM	C2B-C1B	-2.69	1.43	1.51
13	H	616	LDA	CM2-N1	-2.58	1.45	1.49
9	M	608	MQ7	C6-C5	-2.56	1.35	1.39
7	L	604	BCB	C3D-C4D	-2.40	1.37	1.41
9	M	608	MQ7	C9-C10	-2.39	1.35	1.39
11	M	613	NS1	C2-C1	-2.36	1.33	1.51
7	M	603	BCB	C3D-CAD	-2.33	1.42	1.46
10	C	609	HEM	C4C-NC	-2.23	1.33	1.36
7	M	603	BCB	O1D-CGD	-2.23	1.15	1.21
8	L	606	BPB	CMA-C3A	-2.20	1.48	1.53
13	M	615	LDA	C1-N1	-2.20	1.47	1.51
7	M	603	BCB	C3B-C2B	-2.19	1.34	1.40
10	C	610	HEM	C3B-CAB	-2.17	1.47	1.51
7	M	603	BCB	C3B-CAB	-2.13	1.43	1.49
7	M	603	BCB	CAC-C3C	-2.11	1.30	1.33
7	M	603	BCB	CAA-CBA	-2.11	1.45	1.52
10	C	610	HEM	CMC-C2C	-2.08	1.48	1.53
7	M	603	BCB	O2D-CGD	-2.06	1.27	1.33
7	M	603	BCB	OBB-CAB	-2.06	1.15	1.22
8	M	605	BPB	C3B-C2B	-2.01	1.35	1.40
6	H	622	SO4	O1-S	2.00	1.54	1.47
9	M	608	MQ7	C12-C13	2.02	1.36	1.33
8	L	606	BPB	C5-C3	2.04	1.55	1.51
7	M	603	BCB	C5-C3	2.07	1.56	1.51
8	M	605	BPB	O2A-C1	2.10	1.52	1.46
12	L	614	UQ1	C7-C8	2.12	1.54	1.50
7	M	601	BCB	CBA-CGA	2.22	1.57	1.50
7	M	603	BCB	C4C-NC	2.22	1.41	1.37
11	M	613	NS1	C19-C18	2.24	1.41	1.35
11	M	613	NS1	C22-C21	2.25	1.55	1.50
7	M	601	BCB	C4C-C3C	2.27	1.49	1.45
8	M	605	BPB	CHC-C1C	2.27	1.43	1.37
7	M	603	BCB	OBD-CAD	2.30	1.25	1.22
7	M	603	BCB	CBC-CAC	2.31	1.59	1.49
7	L	604	BCB	O2A-C1	2.32	1.53	1.46
9	M	608	MQ7	C36-C37	2.41	1.57	1.50
8	L	606	BPB	C4C-C3C	2.48	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	612	HEM	FE-NC	2.49	2.05	1.95
11	M	613	NS1	C29-C28	2.51	1.41	1.34
7	M	601	BCB	C5-C3	2.53	1.57	1.51
10	C	612	HEM	C3B-CAB	2.54	1.56	1.51
8	L	606	BPB	CBC-CAC	2.57	1.60	1.49
7	L	602	BCB	C2C-C1C	2.79	1.54	1.51
10	C	612	HEM	C3C-CAC	2.85	1.56	1.51
10	C	611	HEM	FE-NC	3.02	2.07	1.95
8	M	605	BPB	C2-C3	3.05	1.38	1.33
8	L	606	BPB	CAA-C2A	3.13	1.60	1.54
7	L	604	BCB	C5-C3	3.14	1.58	1.51
11	M	613	NS1	C24-C23	3.18	1.42	1.34
10	C	611	HEM	CBB-CAB	3.37	1.48	1.29
10	C	611	HEM	CBC-CAC	3.66	1.50	1.29
8	M	605	BPB	C1-C2	3.72	1.61	1.49
7	L	602	BCB	C4C-C3C	3.74	1.51	1.45
10	C	609	HEM	CBB-CAB	3.82	1.51	1.29
11	M	613	NS1	C17-C15	3.84	1.40	1.35
10	C	612	HEM	CBC-CAC	3.89	1.51	1.29
8	L	606	BPB	C3B-C4B	4.04	1.46	1.41
10	C	610	HEM	CBC-CAC	4.10	1.53	1.29
10	C	609	HEM	CBC-CAC	4.18	1.53	1.29
10	C	610	HEM	CBB-CAB	4.25	1.53	1.29
11	M	613	NS1	C20-C21	4.36	1.41	1.35
8	M	605	BPB	C3B-C4B	4.52	1.47	1.41
10	C	612	HEM	CBB-CAB	4.56	1.55	1.29
11	M	613	NS1	C12-C10	4.75	1.39	1.34
7	M	603	BCB	C2C-C1C	5.16	1.56	1.51
11	M	613	NS1	C25-C26	5.33	1.42	1.35
11	M	613	NS1	C30-C31	7.29	1.42	1.34
11	M	613	NS1	C35-C36	7.30	1.54	1.32

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	610	HEM	C3C-CAC-CBC	-10.70	108.04	124.46
13	M	615	LDA	CM2-N1-CM1	-10.47	97.01	108.83
10	C	609	HEM	C3B-CAB-CBB	-9.65	109.66	124.46
9	M	608	MQ7	C11-C3-C4	-8.64	108.61	118.47
10	C	610	HEM	C3B-CAB-CBB	-7.46	113.01	124.46
10	C	611	HEM	C3B-CAB-CBB	-7.25	113.33	124.46
10	C	612	HEM	C3B-CAB-CBB	-6.52	114.45	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	609	HEM	C3C-CAC-CBC	-5.74	115.65	124.46
7	M	603	BCB	CAA-C2A-C1A	-5.43	93.32	112.47
9	M	608	MQ7	C21-C22-C23	-4.92	117.06	127.76
9	M	608	MQ7	C36-C37-C38	-4.87	117.17	127.76
11	M	613	NS1	C34-C35-C36	-4.60	110.04	127.73
7	L	602	BCB	CBC-CAC-C3C	-4.55	116.56	127.07
10	C	611	HEM	CAA-C2A-C3A	-4.15	117.16	129.00
11	M	613	NS1	CM4-C36-C35	-4.02	109.67	122.61
9	M	608	MQ7	O1-C1-C10	-4.00	114.83	121.55
8	M	605	BPB	C2C-C3C-C4C	-3.99	103.59	107.24
11	M	613	NS1	C8-C7-C5	-3.91	119.27	127.76
11	M	613	NS1	CM3-C36-C35	-3.89	110.09	122.61
7	M	603	BCB	CAA-CBA-CGA	-3.61	102.75	113.32
9	M	608	MQ7	C30-C31-C32	-3.50	102.53	111.69
9	M	608	MQ7	C39-C38-C37	-3.49	116.64	123.50
8	M	605	BPB	CBC-CAC-C3C	-3.47	119.06	127.07
7	M	603	BCB	O2D-CGD-O1D	-3.44	116.69	123.79
7	M	601	BCB	OBB-CAB-CBB	-3.22	112.41	120.13
7	L	602	BCB	C4-C3-C2	-3.21	117.21	123.50
8	M	605	BPB	OBB-CAB-CBB	-3.19	112.48	120.13
7	L	604	BCB	CMD-C2D-C1D	-3.16	123.14	128.36
9	M	608	MQ7	C2M-C2-C1	-3.16	111.15	116.27
7	L	604	BCB	C16-C15-C13	-3.11	105.16	115.49
8	L	606	BPB	CHD-C1D-ND	-3.02	119.03	124.66
9	M	608	MQ7	C31-C32-C33	-2.97	121.31	127.76
8	L	606	BPB	CED-O2D-CGD	-2.91	109.16	115.99
10	C	609	HEM	CBD-CAD-C3D	-2.86	105.24	113.55
8	L	606	BPB	CBD-CHA-C4D	-2.85	105.27	108.46
7	M	601	BCB	CAA-CBA-CGA	-2.82	105.06	113.32
7	M	601	BCB	O2D-CGD-O1D	-2.81	118.00	123.79
7	L	602	BCB	C11-C10-C8	-2.80	106.19	115.49
7	L	602	BCB	OBD-CAD-CBD	-2.80	121.72	125.94
10	C	610	HEM	C2C-C1C-NC	-2.78	105.53	110.21
11	M	613	NS1	C18-C17-C15	-2.72	123.27	127.20
7	M	603	BCB	C4-C3-C2	-2.68	118.23	123.50
7	L	604	BCB	C4-C3-C2	-2.67	118.27	123.50
11	M	613	NS1	C13-C14-C15	-2.66	118.48	126.32
7	L	602	BCB	CHD-C4C-C3C	-2.65	121.60	129.02
7	L	602	BCB	C14-C13-C15	-2.64	100.91	111.08
9	M	608	MQ7	O4-C4-C3	-2.63	116.53	120.58
7	M	603	BCB	O2A-CGA-O1A	-2.62	116.73	123.49
13	M	615	LDA	C9-C8-C7	-2.62	101.02	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	613	NS1	C27-C26-C25	-2.60	119.06	122.90
7	L	604	BCB	OBD-CAD-CBD	-2.60	122.02	125.94
8	L	606	BPB	C7-C6-C5	-2.56	105.49	113.06
7	M	601	BCB	C6-C7-C8	-2.56	107.00	115.49
8	L	606	BPB	CMA-C3A-C2A	-2.56	103.04	114.35
7	M	603	BCB	CHD-C4C-C3C	-2.53	121.95	129.02
7	M	601	BCB	CAA-C2A-C1A	-2.53	103.56	112.47
7	M	603	BCB	C11-C10-C8	-2.46	107.32	115.49
9	M	608	MQ7	C16-C17-C18	-2.41	122.51	127.76
7	L	602	BCB	CAA-CBA-CGA	-2.40	106.28	113.32
8	L	606	BPB	CBC-CAC-C3C	-2.39	121.54	127.07
7	M	601	BCB	C7-C6-C5	-2.38	106.03	113.06
9	M	608	MQ7	C24-C23-C22	-2.37	118.84	123.50
8	M	605	BPB	CBD-CHA-C4D	-2.37	105.80	108.46
9	M	608	MQ7	C34-C33-C32	-2.37	118.85	123.50
7	M	603	BCB	CMD-C2D-C1D	-2.36	124.46	128.36
7	L	604	BCB	C11-C12-C13	-2.36	107.67	115.49
7	M	603	BCB	OBB-CAB-CBB	-2.31	114.60	120.13
7	L	602	BCB	C3B-C4B-NB	-2.30	105.85	110.50
8	L	606	BPB	C2C-C3C-C4C	-2.28	105.16	107.24
7	M	603	BCB	C7-C6-C5	-2.26	106.38	113.06
7	L	602	BCB	CED-O2D-CGD	-2.26	110.69	115.99
11	M	613	NS1	C22-C21-C20	-2.22	119.62	122.90
11	M	613	NS1	C19-C18-C17	-2.22	118.48	123.39
7	M	601	BCB	OBD-CAD-CBD	-2.21	122.60	125.94
8	L	606	BPB	C14-C13-C12	-2.15	102.79	111.08
7	M	601	BCB	C5-C3-C2	-2.15	116.97	121.05
10	C	611	HEM	CMA-C3A-C2A	-2.15	120.74	125.24
7	M	603	BCB	CAA-C2A-C3A	-2.14	107.06	113.22
11	M	613	NS1	C6-C5-C7	-2.13	119.31	123.50
7	L	604	BCB	CHD-C4C-C3C	-2.13	123.06	129.02
9	M	608	MQ7	C11-C12-C13	-2.12	123.11	126.70
11	M	613	NS1	C24-C23-C21	-2.11	120.10	126.32
12	L	614	UQ1	CM5-C5-C6	-2.10	119.60	124.10
8	L	606	BPB	O2D-CGD-O1D	-2.09	119.48	123.79
7	M	603	BCB	OBD-CAD-CBD	-2.08	122.80	125.94
10	C	610	HEM	C1D-CHD-C4C	-2.07	122.35	125.82
13	M	615	LDA	C6-C5-C4	-2.06	103.88	114.53
8	L	606	BPB	C9-C8-C10	-2.06	103.16	111.08
7	L	604	BCB	OBB-CAB-CBB	-2.06	115.20	120.13
7	M	601	BCB	CGD-CBD-CAD	-2.05	103.68	110.62
11	M	613	NS1	CM4-C36-CM3	-2.05	109.61	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	614	UQ1	C7-C8-C9	-2.04	119.30	127.16
9	M	608	MQ7	C25-C26-C27	-2.04	106.36	111.69
7	M	601	BCB	C11-C10-C8	-2.03	108.74	115.49
13	H	616	LDA	O1-N1-C1	-2.03	107.99	110.27
10	C	609	HEM	C4B-CHC-C1C	-2.03	122.43	125.82
8	L	606	BPB	OBD-CAD-C3D	2.01	133.79	128.37
12	L	614	UQ1	C11-C9-C10	2.02	119.60	114.64
9	M	608	MQ7	C2M-C2-C3	2.03	128.44	124.10
10	C	612	HEM	CBA-CAA-C2A	2.03	116.17	112.53
7	L	604	BCB	O2A-CGA-CBA	2.07	118.20	111.90
7	L	604	BCB	CMB-C2B-C3B	2.08	129.15	125.09
7	L	602	BCB	O2A-CGA-CBA	2.09	118.27	111.90
7	L	602	BCB	CAA-C2A-C1A	2.13	119.99	112.47
7	L	602	BCB	CMB-C2B-C3B	2.18	129.35	125.09
8	M	605	BPB	O1D-CGD-CBD	2.18	127.75	124.62
11	M	613	NS1	C14-C15-C17	2.22	122.55	118.98
7	L	604	BCB	OBB-CAB-C3B	2.22	123.52	120.00
8	L	606	BPB	C2D-C1D-ND	2.26	113.12	109.73
7	L	602	BCB	CMD-C2D-C3D	2.27	129.52	125.09
7	M	603	BCB	O1D-CGD-CBD	2.30	127.91	124.62
8	M	605	BPB	C4D-C3D-CAD	2.31	109.67	105.51
10	C	611	HEM	CMD-C2D-C3D	2.33	124.65	114.35
13	M	615	LDA	CM2-N1-C1	2.35	117.34	109.77
10	C	612	HEM	CAA-CBA-CGA	2.38	117.11	112.75
7	M	603	BCB	CMB-C2B-C3B	2.39	129.75	125.09
10	C	610	HEM	CBD-CAD-C3D	2.42	120.59	113.55
7	M	603	BCB	O2D-CGD-CBD	2.50	114.72	111.30
10	C	610	HEM	CMD-C2D-C3D	2.50	125.41	114.35
7	L	604	BCB	CED-O2D-CGD	2.55	121.98	115.99
7	M	601	BCB	C6-C5-C3	2.58	118.14	112.48
10	C	612	HEM	CMD-C2D-C3D	2.73	126.42	114.35
8	M	605	BPB	OBB-CAB-C3B	2.78	124.41	120.00
9	M	608	MQ7	C14-C13-C15	2.80	119.68	115.41
8	L	606	BPB	CAA-C2A-C1A	2.82	122.42	112.47
7	M	603	BCB	CMD-C2D-C3D	2.85	130.66	125.09
11	M	613	NS1	C6-C5-C4	2.87	119.79	115.41
10	C	609	HEM	CAD-C3D-C2D	2.88	121.49	113.22
9	M	608	MQ7	C29-C28-C30	2.90	119.84	115.41
7	L	602	BCB	O1D-CGD-CBD	2.97	128.88	124.62
13	H	616	LDA	O1-N1-CM2	2.98	113.04	109.05
9	M	608	MQ7	O1-C1-C2	2.99	124.00	120.27
10	C	611	HEM	C2D-C3D-C4D	3.01	106.60	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	604	BCB	C4-C3-C5	3.06	120.08	115.41
7	M	603	BCB	O2A-CGA-CBA	3.09	121.30	111.90
11	M	613	NS1	C11-C10-C9	3.22	120.33	115.41
10	C	609	HEM	C2D-C3D-C4D	3.23	106.97	101.50
10	C	609	HEM	CMB-C2B-C3B	3.25	124.65	116.53
10	C	610	HEM	C2D-C3D-C4D	3.25	107.01	101.50
7	L	604	BCB	CMD-C2D-C3D	3.29	131.53	125.09
9	M	608	MQ7	C9-C10-C5	3.30	123.00	119.26
10	C	610	HEM	CMC-C2C-C3C	3.37	124.93	116.53
7	M	601	BCB	O2D-CGD-CBD	3.40	115.96	111.30
10	C	612	HEM	CAD-C3D-C4D	3.45	124.62	112.47
9	M	608	MQ7	C24-C23-C25	3.47	120.71	115.41
10	C	612	HEM	CMB-C2B-C3B	3.56	125.41	116.53
10	C	611	HEM	CAD-C3D-C2D	3.62	123.62	113.22
10	C	610	HEM	CAD-C3D-C2D	3.76	124.02	113.22
10	C	611	HEM	CMC-C2C-C3C	3.80	126.02	116.53
10	C	610	HEM	CMB-C2B-C3B	4.00	126.51	116.53
7	M	603	BCB	C4-C3-C5	4.05	121.59	115.41
9	M	608	MQ7	C34-C33-C35	4.12	121.71	115.41
10	C	610	HEM	CAD-C3D-C4D	4.16	127.15	112.47
10	C	612	HEM	CBD-CAD-C3D	4.18	125.73	113.55
8	L	606	BPB	O1D-CGD-CBD	4.32	130.82	124.62
13	M	615	LDA	O1-N1-C1	4.42	115.25	110.27
9	M	608	MQ7	C39-C38-C40	4.50	122.28	115.41
7	L	602	BCB	C4-C3-C5	4.61	122.45	115.41
7	M	601	BCB	C4-C3-C5	4.74	122.64	115.41
11	M	613	NS1	C19-C20-C21	4.85	134.21	127.20
10	C	611	HEM	CAD-C3D-C4D	4.88	129.69	112.47
10	C	609	HEM	CAD-C3D-C4D	5.23	130.93	112.47
10	C	612	HEM	CMC-C2C-C3C	5.26	129.67	116.53
10	C	611	HEM	CMB-C2B-C3B	5.29	129.74	116.53
10	C	612	HEM	CAD-C3D-C2D	5.59	129.30	113.22
10	C	609	HEM	CMC-C2C-C3C	5.86	131.15	116.53
10	C	611	HEM	CAA-C2A-C1A	6.48	134.04	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	609	HEM	4	0
10	C	610	HEM	2	0
10	C	611	HEM	6	0
10	C	612	HEM	2	0
13	H	616	LDA	2	0
7	L	602	BCB	16	0
7	L	604	BCB	11	0
8	L	606	BPB	8	0
12	L	614	UQ1	10	0
7	M	601	BCB	7	0
7	M	603	BCB	15	0
8	M	605	BPB	11	0
9	M	608	MQ7	1	0
11	M	613	NS1	4	0
13	M	615	LDA	1	0

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, 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	C	333/336 (99%)	-0.99	1 (0%) 94 96	7, 21, 46, 73	17 (5%)
2	L	273/273 (100%)	-1.12	0 100 100	6, 16, 36, 53	6 (2%)
3	M	323/323 (100%)	-1.05	0 100 100	4, 18, 41, 58	8 (2%)
4	H	250/258 (96%)	-0.91	2 (0%) 87 90	8, 23, 51, 78	17 (6%)
All	All	1179/1190 (99%)	-1.02	3 (0%) 94 96	4, 19, 44, 78	48 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	46	PRO	3.8
4	H	54	PRO	3.3
1	C	333	ALA	3.1

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	FME	H	1	10/11	0.98	0.06	-	21,32,41,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
12	UQ1	L	614	18/18	0.84	0.57	46.70	19,26,29,30	18
6	SO4	H	622	5/5	0.92	0.22	11.58	73,74,85,89	0
13	LDA	H	616	16/16	0.91	0.17	7.37	0,27,42,46	6
11	NS1	M	613	40/40	0.96	0.11	4.14	0,25,39,49	14
8	BPB	M	605	65/65	0.96	0.10	1.48	0,21,62,71	7
10	HEM	C	611	43/43	0.99	0.09	0.94	5,16,25,38	0
6	SO4	M	618	5/5	1.00	0.07	0.63	22,23,35,37	0
10	HEM	C	610	43/43	0.99	0.09	0.61	3,21,29,37	0
8	BPB	L	606	65/65	0.99	0.07	0.54	3,10,19,22	0
6	SO4	H	617	5/5	0.98	0.07	0.53	47,50,59,61	0
10	HEM	C	612	43/43	0.98	0.08	0.25	3,22,31,46	0
10	HEM	C	609	43/43	0.99	0.08	0.20	7,22,32,36	0
7	BCB	L	602	66/66	0.99	0.07	0.05	3,10,19,21	0
13	LDA	M	615	16/16	0.97	0.07	-0.17	17,25,36,37	0
9	MQ7	M	608	48/48	0.98	0.06	-0.49	0,10,20,32	4
7	BCB	L	604	66/66	0.98	0.06	-0.52	3,10,27,35	0
7	BCB	M	603	66/66	0.99	0.06	-0.62	3,10,20,21	0
7	BCB	M	601	66/66	0.98	0.06	-1.15	0,12,40,61	13
5	FE	M	607	1/1	1.00	0.04	-1.20	19,19,19,19	0
6	SO4	M	620	5/5	0.99	0.05	-1.25	31,34,40,41	0
6	SO4	H	623	5/5	0.94	0.13	-	58,59,62,64	5
6	SO4	M	619	5/5	0.99	0.11	-	39,43,50,59	0
6	SO4	M	621	5/5	0.97	0.20	-	68,78,81,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.