



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:35 AM UTC

PDB ID : 5L05 / pdb_00005l05
Title : Crystal structure of catalase-peroxidase KATG of burkholderia pseudomallei treated with INH
Authors : Loewen, P.C.
Deposited on : 2016-07-26
Resolution : 1.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

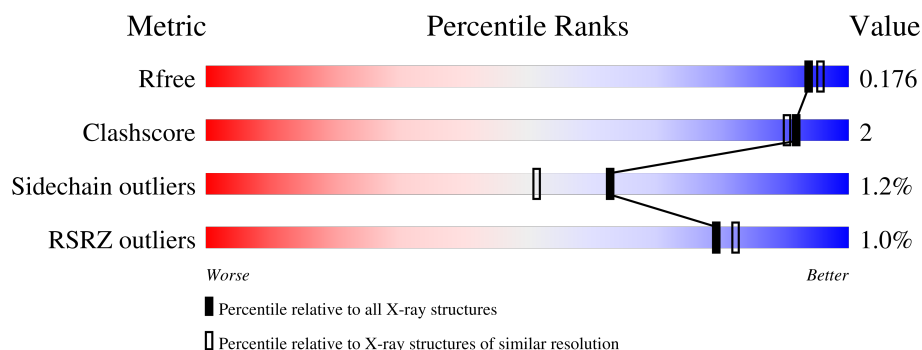
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	% 85% 12% ..
1	B	728	% 84% 13% ..

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
2	HP5	A	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HP5	B	801	X	-	-	-
5	MPD	A	805	-	X	-	-

2 Entry composition [i](#)

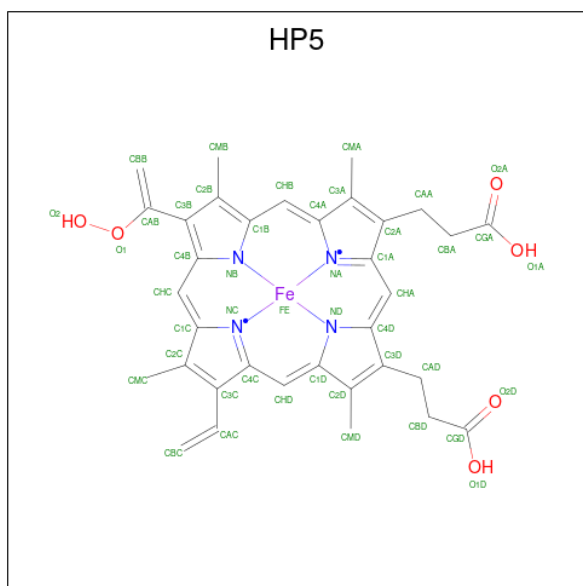
There are 6 unique types of molecules in this entry. The entry contains 13066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	5	0
			5534	3496	987	1037	14			
1	B	713	Total	C	N	O	S	0	5	0
			5534	3496	987	1037	14			

- Molecule 2 is Peroxidized Heme Form 2 (CCD ID: HP5) (formula: $C_{34}H_{32}FeN_4O_6$).

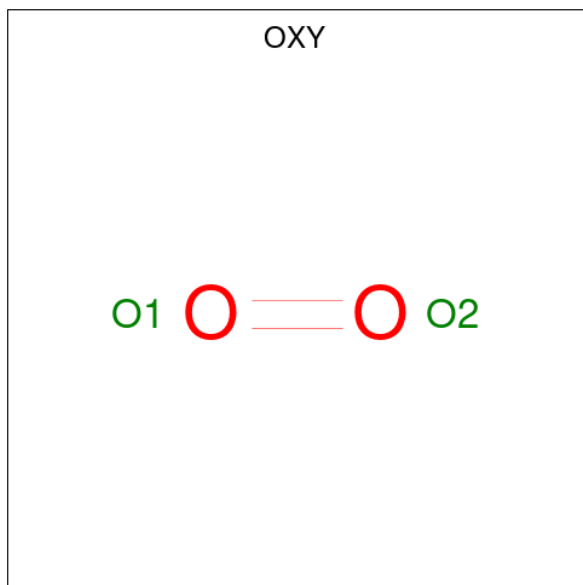


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			45	34	1	4	6		
2	B	1	Total	C	Fe	N	O	0	0
			45	34	1	4	6		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

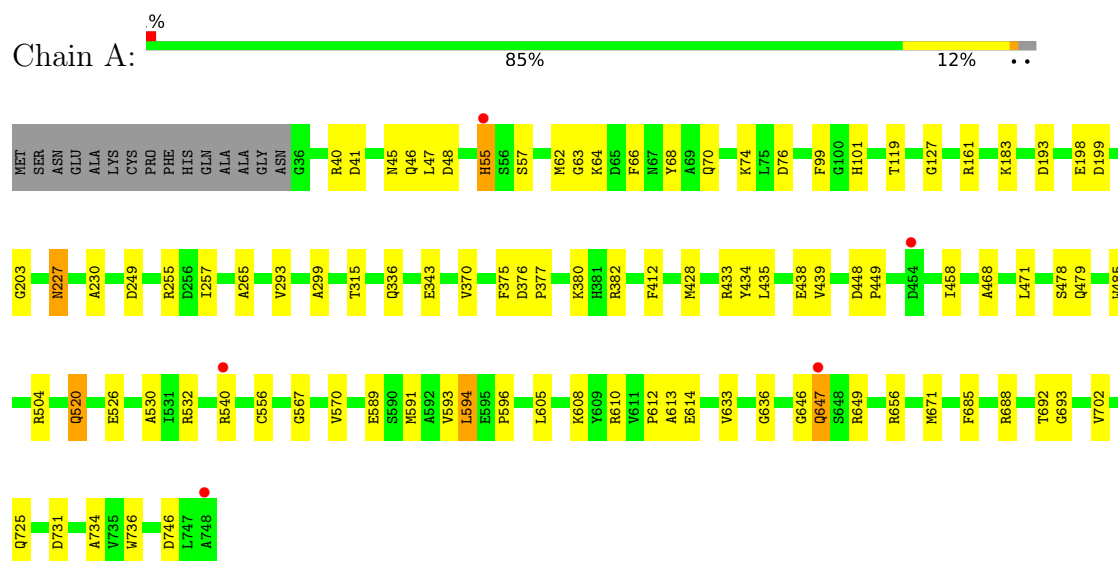
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	945	Total	O	0	0
			945	945		
6	B	933	Total	O	0	0
			933	933		

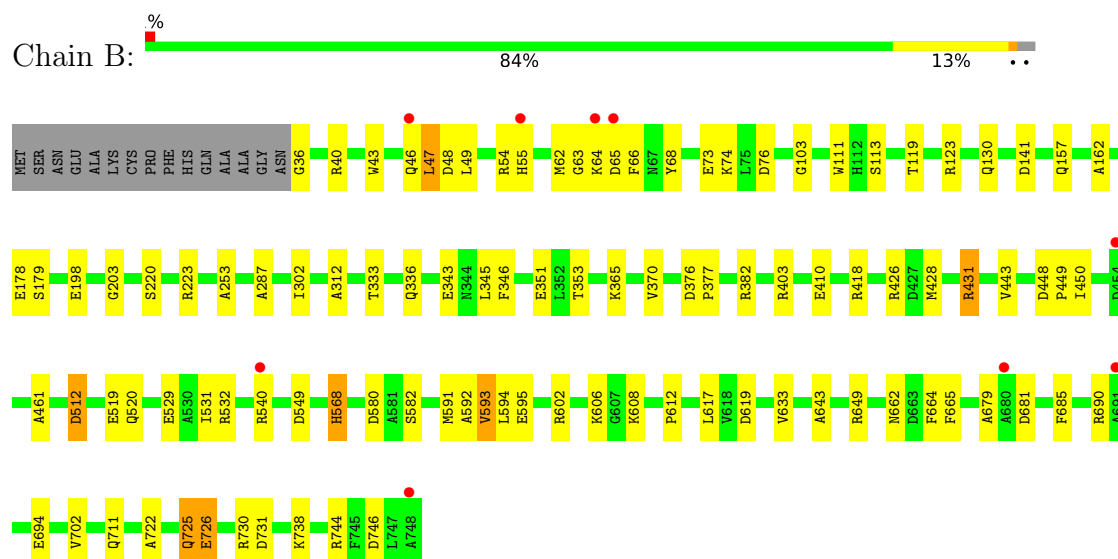
3 Residue-property plots [i](#)

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

• Molecule 1: Catalase-peroxidase



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.94Å 115.62Å 175.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 1.70 18.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (18.00-1.70) 98.9 (18.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.145 , 0.176 (Not available) , 0.176	Depositor DCC
R_{free} test set	22115 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13066	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, NA, OXY, HP5

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	1.82	76/5691 (1.3%)	1.41	23/7736 (0.3%)
1	B	1.78	71/5691 (1.2%)	1.39	27/7736 (0.3%)
All	All	1.80	147/11382 (1.3%)	1.40	50/15472 (0.3%)

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	532	ARG	CD-NE	-11.31	1.30	1.46
1	B	63	GLY	N-CA	11.12	1.60	1.45
1	A	382	ARG	CZ-NH1	8.81	1.45	1.32
1	A	63	GLY	N-CA	8.42	1.56	1.45
1	B	532	ARG	NE-CZ	-8.41	1.23	1.33
1	B	512	ASP	CG-OD2	8.25	1.41	1.25
1	B	540	ARG	C-O	8.23	1.34	1.23
1	B	382	ARG	CZ-NH1	7.97	1.44	1.32
1	A	375	PHE	C-O	-7.93	1.14	1.24
1	A	532	ARG	CZ-NH2	-7.74	1.23	1.33
1	A	377	PRO	C-O	-7.58	1.13	1.24
1	A	540	ARG	C-O	7.45	1.33	1.23
1	A	725	GLN	CD-NE2	7.40	1.48	1.33
1	B	73	GLU	CD-OE2	7.39	1.39	1.25
1	A	435	LEU	N-CA	-7.38	1.37	1.45
1	A	74	LYS	CA-C	7.20	1.62	1.52
1	A	47	LEU	CB-CG	-7.19	1.39	1.53
1	B	450	ILE	CA-CB	-6.96	1.48	1.54
1	B	593	VAL	CA-C	-6.92	1.43	1.52
1	A	376	ASP	N-CA	6.91	1.54	1.46
1	A	45	ASN	C-O	-6.90	1.14	1.24
1	A	532	ARG	NE-CZ	-6.86	1.25	1.33
1	B	665	PHE	C-N	-6.81	1.25	1.33
1	B	47	LEU	CB-CG	-6.80	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	681	ASP	CA-C	6.67	1.60	1.52
1	B	592	ALA	CA-C	-6.64	1.43	1.52
1	A	193	ASP	N-CA	6.57	1.54	1.45
1	A	68	TYR	N-CA	6.56	1.54	1.46
1	A	183	LYS	CA-CB	6.54	1.61	1.53
1	A	692	THR	CA-C	-6.53	1.44	1.52
1	B	746	ASP	C-O	-6.53	1.15	1.24
1	A	448	ASP	N-CA	6.52	1.52	1.46
1	B	370	VAL	C-O	-6.48	1.16	1.24
1	B	612	PRO	CA-C	6.47	1.60	1.52
1	A	556	CYS	CA-C	6.43	1.61	1.52
1	A	299	ALA	CA-C	-6.37	1.44	1.52
1	A	734	ALA	N-CA	-6.36	1.38	1.46
1	B	449	PRO	CA-C	6.35	1.60	1.52
1	B	730	ARG	CZ-NH1	6.33	1.41	1.32
1	A	199	ASP	C-O	6.31	1.31	1.24
1	A	448	ASP	CA-CB	6.30	1.58	1.52
1	A	530	ALA	N-CA	6.28	1.54	1.46
1	B	376	ASP	N-CA	6.21	1.54	1.46
1	A	471	LEU	CA-C	6.16	1.60	1.52
1	A	725	GLN	CG-CD	6.15	1.67	1.52
1	B	568	HIS	CA-C	6.14	1.60	1.52
1	B	582	SER	N-CA	6.13	1.53	1.45
1	B	162	ALA	CA-C	6.12	1.61	1.52
1	A	370	VAL	C-O	-6.05	1.17	1.24
1	B	606	LYS	N-CA	6.05	1.54	1.46
1	A	520	GLN	CA-C	6.03	1.60	1.52
1	A	485	TRP	N-CA	5.99	1.53	1.46
1	B	103	GLY	CA-C	5.99	1.58	1.52
1	B	223	ARG	CG-CD	-5.95	1.34	1.52
1	A	647	GLN	CG-CD	5.94	1.66	1.52
1	A	702	VAL	C-O	5.93	1.31	1.24
1	B	730	ARG	CZ-NH2	5.93	1.41	1.33
1	A	736	TRP	N-CA	5.92	1.53	1.46
1	B	580	ASP	CG-OD2	5.91	1.36	1.25
1	B	722	ALA	C-N	-5.90	1.25	1.33
1	B	443	VAL	CA-C	-5.90	1.45	1.52
1	B	694	GLU	CA-C	5.83	1.60	1.52
1	B	68	TYR	N-CA	5.82	1.53	1.46
1	B	738	LYS	N-CA	-5.80	1.39	1.46
1	A	343	GLU	N-CA	5.77	1.53	1.46
1	A	458	ILE	CA-CB	-5.75	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	GLN	CD-OE1	5.75	1.34	1.23
1	B	461	ALA	CA-C	5.74	1.60	1.52
1	B	685	PHE	N-CA	-5.73	1.38	1.45
1	A	438	GLU	CD-OE2	5.72	1.36	1.25
1	A	613	ALA	CA-CB	-5.72	1.44	1.53
1	A	41	ASP	C-O	5.70	1.30	1.24
1	B	690	ARG	CD-NE	-5.67	1.38	1.46
1	A	636	GLY	N-CA	5.67	1.52	1.45
1	B	410	GLU	CD-OE2	5.67	1.36	1.25
1	B	679	ALA	N-CA	5.66	1.53	1.46
1	B	36	GLY	N-CA	5.65	1.54	1.45
1	A	203	GLY	CA-C	5.64	1.58	1.51
1	A	656	ARG	CA-CB	-5.62	1.45	1.53
1	B	602	ARG	CZ-NH2	-5.62	1.26	1.33
1	A	646	GLY	C-O	-5.61	1.16	1.23
1	B	418	ARG	CZ-NH2	-5.61	1.26	1.33
1	B	336	GLN	CA-C	-5.60	1.45	1.52
1	A	434	TYR	CA-C	-5.58	1.45	1.52
1	A	688	ARG	CA-C	-5.55	1.46	1.52
1	B	74	LYS	CA-C	5.54	1.60	1.52
1	B	111	TRP	CA-C	5.54	1.59	1.52
1	A	127	GLY	C-O	5.53	1.30	1.24
1	A	161	ARG	NE-CZ	5.51	1.39	1.33
1	A	66	PHE	C-O	-5.50	1.17	1.23
1	A	693	GLY	C-O	5.50	1.31	1.24
1	B	664	PHE	CA-C	5.50	1.59	1.52
1	A	746	ASP	C-O	-5.47	1.17	1.24
1	A	596	PRO	CA-CB	-5.47	1.48	1.54
1	B	203	GLY	N-CA	5.46	1.50	1.45
1	A	570	VAL	CA-C	-5.45	1.46	1.52
1	B	73	GLU	CA-CB	5.42	1.63	1.53
1	B	365	LYS	C-O	5.41	1.30	1.23
1	A	315	THR	C-O	-5.40	1.17	1.24
1	B	343	GLU	C-O	5.39	1.30	1.24
1	A	101	HIS	C-O	-5.39	1.17	1.23
1	B	312	ALA	N-CA	5.38	1.53	1.46
1	A	99	PHE	CA-CB	5.35	1.62	1.53
1	A	526	GLU	C-O	5.33	1.30	1.24
1	B	253	ALA	C-O	5.31	1.30	1.24
1	B	726	GLU	CG-CD	5.31	1.65	1.52
1	A	227	ASN	C-O	5.31	1.31	1.24
1	B	157	GLN	CA-C	-5.30	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	VAL	N-CA	5.28	1.52	1.46
1	A	230	ALA	CA-C	-5.24	1.46	1.53
1	B	130	GLN	CA-C	5.24	1.59	1.52
1	B	731	ASP	C-O	5.23	1.30	1.24
1	A	257	ILE	CA-CB	5.23	1.60	1.54
1	B	113	SER	CA-C	5.23	1.59	1.52
1	B	448	ASP	C-O	5.22	1.26	1.23
1	A	567	GLY	C-O	-5.21	1.17	1.24
1	B	448	ASP	N-CA	5.20	1.50	1.46
1	B	619	ASP	CG-OD1	-5.20	1.15	1.25
1	B	65	ASP	CB-CG	5.20	1.65	1.52
1	A	692	THR	N-CA	5.19	1.52	1.46
1	B	725	GLN	CD-OE1	5.19	1.33	1.23
1	B	377	PRO	C-O	-5.17	1.16	1.24
1	A	468	ALA	N-CA	5.17	1.52	1.46
1	A	594	LEU	N-CA	-5.16	1.39	1.46
1	B	643	ALA	N-CA	-5.15	1.39	1.46
1	A	449	PRO	CA-C	5.14	1.58	1.52
1	B	431	ARG	CD-NE	5.13	1.53	1.46
1	B	54	ARG	CA-C	-5.13	1.46	1.53
1	B	179	SER	C-O	5.12	1.30	1.24
1	B	220	SER	N-CA	5.12	1.52	1.45
1	A	685	PHE	N-CA	-5.12	1.39	1.46
1	A	731	ASP	N-CA	-5.12	1.39	1.46
1	A	433	ARG	N-CA	-5.11	1.39	1.46
1	A	612	PRO	CA-C	5.10	1.58	1.52
1	A	734	ALA	C-O	5.09	1.30	1.24
1	A	688	ARG	CZ-NH2	-5.09	1.26	1.33
1	A	614	GLU	C-O	5.08	1.30	1.24
1	B	531	ILE	C-O	5.07	1.29	1.24
1	B	287	ALA	CA-CB	-5.07	1.45	1.53
1	B	353	THR	CA-C	5.06	1.59	1.52
1	A	449	PRO	N-CA	-5.06	1.40	1.47
1	B	410	GLU	CG-CD	5.06	1.64	1.52
1	A	249	ASP	CA-C	5.06	1.59	1.52
1	B	450	ILE	CB-CG1	5.04	1.63	1.53
1	A	671	MET	CA-C	5.04	1.59	1.52
1	B	549	ASP	CG-OD1	5.04	1.34	1.25
1	A	76	ASP	CA-C	5.01	1.59	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-16.89	104.00	119.20
1	A	532	ARG	NE-CZ-NH1	11.29	132.79	121.50
1	B	46	GLN	N-CA-C	-8.84	99.12	110.53
1	A	532	ARG	CD-NE-CZ	7.45	134.83	124.40
1	A	46	GLN	N-CA-C	-7.38	99.60	110.52
1	B	62	MET	CA-C-N	-7.03	111.03	121.01
1	B	62	MET	C-N-CA	-7.03	111.03	121.01
1	B	450	ILE	CA-CB-CG1	-6.86	98.73	110.40
1	B	529	GLU	N-CA-C	-6.85	103.87	111.82
1	A	479	GLN	N-CA-C	6.70	118.59	111.28
1	A	62	MET	CA-C-N	-6.54	112.56	121.06
1	A	62	MET	C-N-CA	-6.54	112.56	121.06
1	B	54	ARG	CG-CD-NE	-6.47	97.76	112.00
1	B	345	LEU	O-C-N	6.35	128.85	122.12
1	A	47	LEU	N-CA-CB	-6.34	100.48	110.06
1	A	48	ASP	N-CA-C	6.21	119.30	107.75
1	A	520	GLN	CB-CG-CD	6.15	123.06	112.60
1	B	633	VAL	CG1-CB-CG2	-6.04	97.52	110.80
1	A	439	VAL	N-CA-C	5.98	114.81	108.95
1	B	123	ARG	NE-CZ-NH1	5.96	127.45	121.50
1	B	43	TRP	CA-C-N	-5.89	113.68	120.04
1	B	43	TRP	C-N-CA	-5.89	113.68	120.04
1	B	595	GLU	O-C-N	5.88	126.53	121.30
1	A	127	GLY	N-CA-C	5.82	121.07	114.67
1	B	450	ILE	CB-CA-C	5.69	116.84	110.52
1	B	76	ASP	OD1-CG-OD2	5.64	136.43	122.90
1	B	333	THR	O-C-N	5.63	125.96	121.17
1	B	351	GLU	CB-CG-CD	-5.57	103.13	112.60
1	A	198	GLU	CG-CD-OE1	5.51	131.09	118.40
1	A	46	GLN	CB-CG-CD	5.50	121.95	112.60
1	B	76	ASP	CB-CG-OD2	-5.48	105.79	118.40
1	B	428	MET	CA-CB-CG	-5.46	103.19	114.10
1	B	46	GLN	CA-CB-CG	5.42	124.94	114.10
1	B	66	PHE	CA-C-N	-5.41	115.18	122.86
1	B	66	PHE	C-N-CA	-5.41	115.18	122.86
1	A	428	MET	CA-CB-CG	-5.38	103.33	114.10
1	B	48	ASP	N-CA-C	5.34	117.68	107.75
1	A	380	LYS	CB-CG-CD	5.32	123.53	111.30
1	B	529	GLU	CB-CG-CD	5.28	121.58	112.60
1	B	365	LYS	O-C-N	5.28	129.42	122.93
1	A	57	SER	N-CA-C	-5.24	105.99	112.38
1	B	74	LYS	CB-CA-C	-5.24	101.35	110.09
1	A	70	GLN	CA-CB-CG	5.19	124.48	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	744	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	B	198	GLU	CG-CD-OE1	5.17	130.29	118.40
1	A	478	SER	N-CA-C	5.09	116.83	111.28
1	A	412	PHE	CA-CB-CG	5.07	118.86	113.80
1	A	605	LEU	CB-CA-C	-5.05	102.37	110.14
1	A	46	GLN	CB-CA-C	5.03	118.64	109.83
1	A	633	VAL	CG1-CB-CG2	-5.00	99.79	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5534	0	5363	13	0
1	B	5534	0	5363	20	0
2	A	45	0	0	0	0
2	B	45	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	16	0	28	1	0
5	B	8	0	14	0	0
6	A	945	0	0	9	0
6	B	933	0	0	11	0
All	All	13066	0	10768	34	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 2.

All (34) 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:B:520:GLN:HG3	6:B:1177:HOH:O	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119[B]:THR:HG21	6:A:1115:HOH:O	1.65	0.96
1:A:520:GLN:HG3	6:A:983:HOH:O	1.73	0.89
5:A:804:MPD:O2	5:A:804:MPD:O4	1.85	0.87
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.59	0.85
1:B:119[B]:THR:HG23	6:B:1153:HOH:O	1.87	0.74
1:A:589:GLU:HG2	6:A:1287:HOH:O	1.90	0.72
1:B:512:ASP:OD1	6:B:902:HOH:O	2.10	0.70
1:B:519:GLU:OE1	6:B:903:HOH:O	2.11	0.68
1:A:336:GLN:HG2	6:A:1551:HOH:O	1.95	0.65
1:A:647:GLN:HG2	6:A:1396:HOH:O	1.98	0.64
1:A:55:HIS:CE1	6:A:1098:HOH:O	2.55	0.59
1:B:591:MET:SD	1:B:594:LEU:HD12	2.45	0.57
1:B:55:HIS:NE2	6:B:909:HOH:O	2.32	0.57
1:B:711[A]:GLN:NE2	6:B:912:HOH:O	2.36	0.56
1:B:568:HIS:ND1	1:B:726:GLU:OE1	2.38	0.56
1:B:119[B]:THR:HG21	6:B:1681:HOH:O	2.07	0.54
1:A:255:ARG:HD2	6:A:1624:HOH:O	2.08	0.54
1:B:178:GLU:OE1	6:B:905:HOH:O	2.19	0.50
1:A:593:VAL:HG13	6:A:988:HOH:O	2.12	0.49
1:B:662:ASN:H	1:B:725:GLN:HE22	1.59	0.49
1:B:49:LEU:HD12	1:B:711[B]:GLN:CD	2.39	0.47
1:A:591:MET:SD	1:A:594:LEU:HD12	2.55	0.47
1:B:512:ASP:HB2	6:B:1466:HOH:O	2.15	0.46
1:A:504:ARG:HD2	6:A:1038:HOH:O	2.15	0.46
1:B:346:PHE:CZ	1:B:403[A]:ARG:HG2	2.51	0.45
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.86	0.44
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.49	0.43
1:A:591:MET:HE2	1:A:591:MET:HB2	1.75	0.43
1:B:591:MET:HB2	1:B:591:MET:HE2	1.83	0.42
1:B:617:LEU:HD22	1:B:702:VAL:HG13	2.02	0.42
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	2.01	0.42
1:B:431:ARG:HD3	6:B:1583:HOH:O	2.20	0.41
1:B:47:LEU:HB2	6:B:1235:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	555/561 (99%)	548 (99%)	7 (1%)	61	48
1	B	555/561 (99%)	549 (99%)	6 (1%)	65	54
All	All	1110/1122 (99%)	1097 (99%)	13 (1%)	63	51

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	55	HIS
1	A	64	LYS
1	A	227	ASN
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	64	LYS
1	B	141	ASP
1	B	302	ILE
1	B	608	LYS
1	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	568	HIS
1	B	336	GLN
1	B	725	GLN
1	B	737	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
5	MPD	A	804	-	7,7,7	0.64	0	9,10,10	1.51	2 (22%)
2	HP5	B	801	1,6	52,52,52	2.65	23 (44%)	65,85,85	8.70	31 (47%)
5	MPD	A	805	-	7,7,7	0.94	0	9,10,10	1.67	4 (44%)
4	OXY	B	803	-	1,1,1	0.57	0	-	-	-
2	HP5	A	801	1,6	52,52,52	2.67	18 (34%)	65,85,85	8.17	24 (36%)
5	MPD	B	804	-	7,7,7	0.88	1 (14%)	9,10,10	2.05	3 (33%)
4	OXY	A	803	-	1,1,1	0.40	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
5	MPD	A	804	-	-	3/5/5/5	-
2	HP5	B	801	1,6	1/1/4/9	3/12/58/58	-
5	MPD	A	805	-	-	5/5/5/5	-
2	HP5	A	801	1,6	1/1/4/9	2/12/58/58	-
5	MPD	B	804	-	-	2/5/5/5	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HP5	FE-NA	6.66	2.15	1.94
2	B	801	HP5	C4A-NA	6.00	1.50	1.40
2	A	801	HP5	C4D-C3D	-5.79	1.35	1.45
2	B	801	HP5	FE-NB	5.71	2.14	1.95
2	A	801	HP5	FE-NB	5.58	2.13	1.95
2	B	801	HP5	FE-ND	5.48	2.13	1.95
2	B	801	HP5	CHC-C4B	-4.96	1.28	1.39
2	A	801	HP5	C1B-NB	4.91	1.48	1.39
2	A	801	HP5	C4A-C3A	-4.79	1.34	1.44
2	B	801	HP5	C1D-ND	-4.52	1.31	1.39
2	B	801	HP5	C4D-C3D	-4.48	1.37	1.45
2	B	801	HP5	C4D-ND	4.47	1.48	1.39
2	A	801	HP5	CHC-C4B	-4.39	1.29	1.39
2	A	801	HP5	CHA-C1A	-4.34	1.29	1.39
2	B	801	HP5	C4A-C3A	-4.28	1.35	1.44
2	A	801	HP5	C4B-NB	4.27	1.47	1.39
2	A	801	HP5	O1-CAB	4.23	1.54	1.36
2	A	801	HP5	FE-NC	4.03	2.07	1.94
2	B	801	HP5	C1A-C2A	-3.94	1.38	1.45
2	A	801	HP5	FE-ND	3.89	2.08	1.95
2	A	801	HP5	CHB-C1B	-3.70	1.31	1.39
2	B	801	HP5	FE-NA	3.70	2.06	1.94
2	B	801	HP5	CHA-C4D	-3.67	1.31	1.38
2	B	801	HP5	O1-CAB	3.66	1.51	1.36
2	A	801	HP5	CMC-C2C	-3.57	1.43	1.50
2	B	801	HP5	FE-NC	3.28	2.05	1.94
2	B	801	HP5	CHD-C1D	3.12	1.44	1.38
2	A	801	HP5	CHC-C1C	-3.05	1.32	1.38
2	A	801	HP5	C1A-C2A	-2.99	1.40	1.45
2	B	801	HP5	C4B-NB	2.75	1.44	1.39
2	B	801	HP5	CHB-C4A	-2.66	1.33	1.38
2	A	801	HP5	O2A-CGA	2.59	1.30	1.22
2	B	801	HP5	O2-O1	2.44	1.52	1.46
2	B	801	HP5	C1B-NB	2.39	1.44	1.39
2	B	801	HP5	CBB-CAB	-2.35	1.25	1.31
2	A	801	HP5	C1C-C2C	-2.33	1.39	1.44
2	B	801	HP5	CAD-C3D	-2.24	1.45	1.51
2	B	801	HP5	O2A-CGA	2.21	1.29	1.22
2	B	801	HP5	CBA-CGA	2.12	1.55	1.50
5	B	804	MPD	C3-C2	-2.11	1.47	1.54
2	B	801	HP5	C3B-C2B	-2.03	1.35	1.42
2	A	801	HP5	C3C-C4C	2.00	1.48	1.44

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HP5	CHA-C4D-ND	-27.03	95.02	124.45
2	A	801	HP5	CHA-C1A-NA	-24.43	98.13	124.42
2	B	801	HP5	CHA-C4D-ND	-24.38	97.91	124.45
2	B	801	HP5	CHC-C1C-NC	-23.88	94.83	124.37
2	B	801	HP5	CHA-C1A-NA	-23.11	99.55	124.42
2	B	801	HP5	CHB-C4A-NA	-21.98	97.18	124.37
2	A	801	HP5	C4D-CHA-C1A	21.69	172.12	126.02
2	B	801	HP5	C4D-CHA-C1A	21.47	171.66	126.02
2	B	801	HP5	C4B-CHC-C1C	19.17	171.34	126.25
2	B	801	HP5	C1B-CHB-C4A	18.99	170.91	126.25
2	B	801	HP5	CHA-C4D-C3D	18.64	154.30	124.86
2	A	801	HP5	CHA-C1A-C2A	18.62	151.93	124.77
2	A	801	HP5	C1B-CHB-C4A	18.43	169.58	126.25
2	A	801	HP5	CHB-C4A-NA	-18.21	101.84	124.37
2	A	801	HP5	CHC-C1C-NC	-17.91	102.21	124.37
2	A	801	HP5	C4B-CHC-C1C	17.56	167.55	126.25
2	A	801	HP5	CHA-C4D-C3D	15.30	149.02	124.86
2	B	801	HP5	CHA-C1A-C2A	14.32	145.65	124.77
2	B	801	HP5	CHB-C1B-NB	-13.92	98.61	123.86
2	B	801	HP5	CHC-C4B-NB	-12.95	100.38	123.86
2	A	801	HP5	CHC-C4B-NB	-12.49	101.21	123.86
2	A	801	HP5	CHB-C1B-NB	-12.39	101.40	123.86
2	B	801	HP5	CHB-C1B-C2B	9.00	153.55	127.43
2	B	801	HP5	CHB-C4A-C3A	8.70	151.68	126.95
2	B	801	HP5	CMB-C2B-C1B	-8.51	112.45	125.42
2	A	801	HP5	CHB-C1B-C2B	8.03	150.73	127.43
2	A	801	HP5	CMB-C2B-C1B	-7.42	114.13	125.42
2	B	801	HP5	C3C-C2C-C1C	-7.07	101.10	106.41
2	A	801	HP5	CHB-C4A-C3A	6.90	146.55	126.95
2	B	801	HP5	CHC-C1C-C2C	6.64	145.82	126.95
2	A	801	HP5	CHC-C1C-C2C	6.44	145.25	126.95
2	B	801	HP5	C2C-C1C-NC	6.35	117.14	109.84
2	B	801	HP5	C4A-NA-C1A	-5.87	98.25	105.21
2	B	801	HP5	C1C-NC-C4C	-5.77	98.37	105.21
2	B	801	HP5	CHC-C4B-C3B	5.38	153.11	131.72
2	A	801	HP5	C3D-C4D-ND	4.78	114.94	110.32
2	A	801	HP5	CHC-C4B-C3B	4.78	150.72	131.72
2	B	801	HP5	C3C-C4C-NC	4.73	112.86	109.47
5	B	804	MPD	O4-C4-C3	-4.36	93.99	111.35
2	B	801	HP5	C2A-C1A-NA	4.34	114.55	110.35
2	A	801	HP5	CMB-C2B-C3B	3.92	138.04	125.67
2	B	801	HP5	CAD-C3D-C2D	3.72	134.84	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HP5	CMA-C3A-C4A	-3.72	119.22	125.03
2	B	801	HP5	CMB-C2B-C3B	3.71	137.36	125.67
2	B	801	HP5	CAA-CBA-CGA	-3.64	104.02	113.67
2	B	801	HP5	CAD-C3D-C4D	-3.36	118.02	124.85
2	A	801	HP5	O2A-CGA-CBA	-3.27	112.71	123.09
5	A	804	MPD	O2-C2-C1	-3.24	97.90	107.99
2	B	801	HP5	CMC-C2C-C3C	3.12	135.97	128.43
2	B	801	HP5	C3D-C4D-ND	-3.09	107.34	110.32
2	A	801	HP5	O1A-CGA-CBA	2.90	123.15	114.00
2	B	801	HP5	C4A-C3A-C2A	2.83	109.95	106.98
5	A	805	MPD	C5-C4-C3	2.81	124.75	111.67
2	A	801	HP5	CHD-C1D-ND	2.81	127.52	124.45
2	A	801	HP5	O2D-CGD-CBD	-2.67	114.62	123.09
2	A	801	HP5	CAA-CBA-CGA	-2.63	106.70	113.67
5	B	804	MPD	O2-C2-C3	-2.42	100.21	109.27
5	A	804	MPD	O2-C2-CM	2.34	115.27	107.99
2	B	801	HP5	O2A-CGA-CBA	-2.32	115.74	123.09
2	A	801	HP5	C2C-C1C-NC	2.26	112.43	109.84
5	A	805	MPD	C1-C2-C3	2.25	119.89	110.20
5	A	805	MPD	O4-C4-C3	-2.21	102.55	111.35
5	A	805	MPD	CM-C2-C1	-2.06	106.02	110.63
5	B	804	MPD	CM-C2-C1	2.01	115.12	110.63

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	HP5	ND
2	B	801	HP5	ND

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	805	MPD	C1-C2-C3-C4
5	A	805	MPD	C2-C3-C4-C5
5	A	805	MPD	O2-C2-C3-C4
5	B	804	MPD	O2-C2-C3-C4
5	A	804	MPD	CM-C2-C3-C4
5	A	805	MPD	CM-C2-C3-C4
5	B	804	MPD	C2-C3-C4-C5
2	A	801	HP5	CAA-CBA-CGA-O1A
2	A	801	HP5	CAA-CBA-CGA-O2A
2	B	801	HP5	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	801	HP5	CAA-CBA-CGA-O1A
5	A	804	MPD	C2-C3-C4-O4
5	A	805	MPD	C2-C3-C4-O4
5	A	804	MPD	C1-C2-C3-C4
2	B	801	HP5	CAD-CBD-CGD-O1D

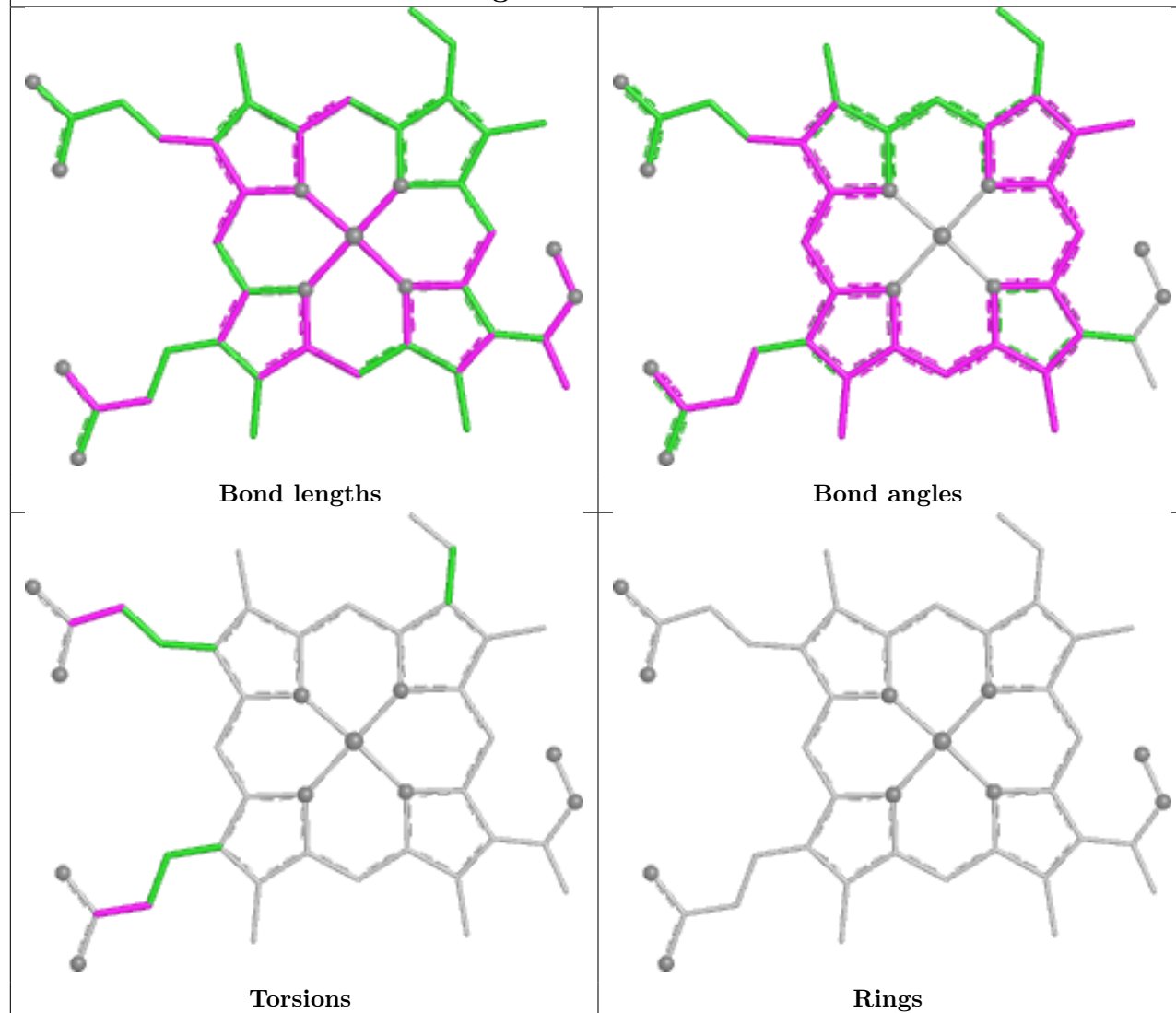
There are no ring outliers.

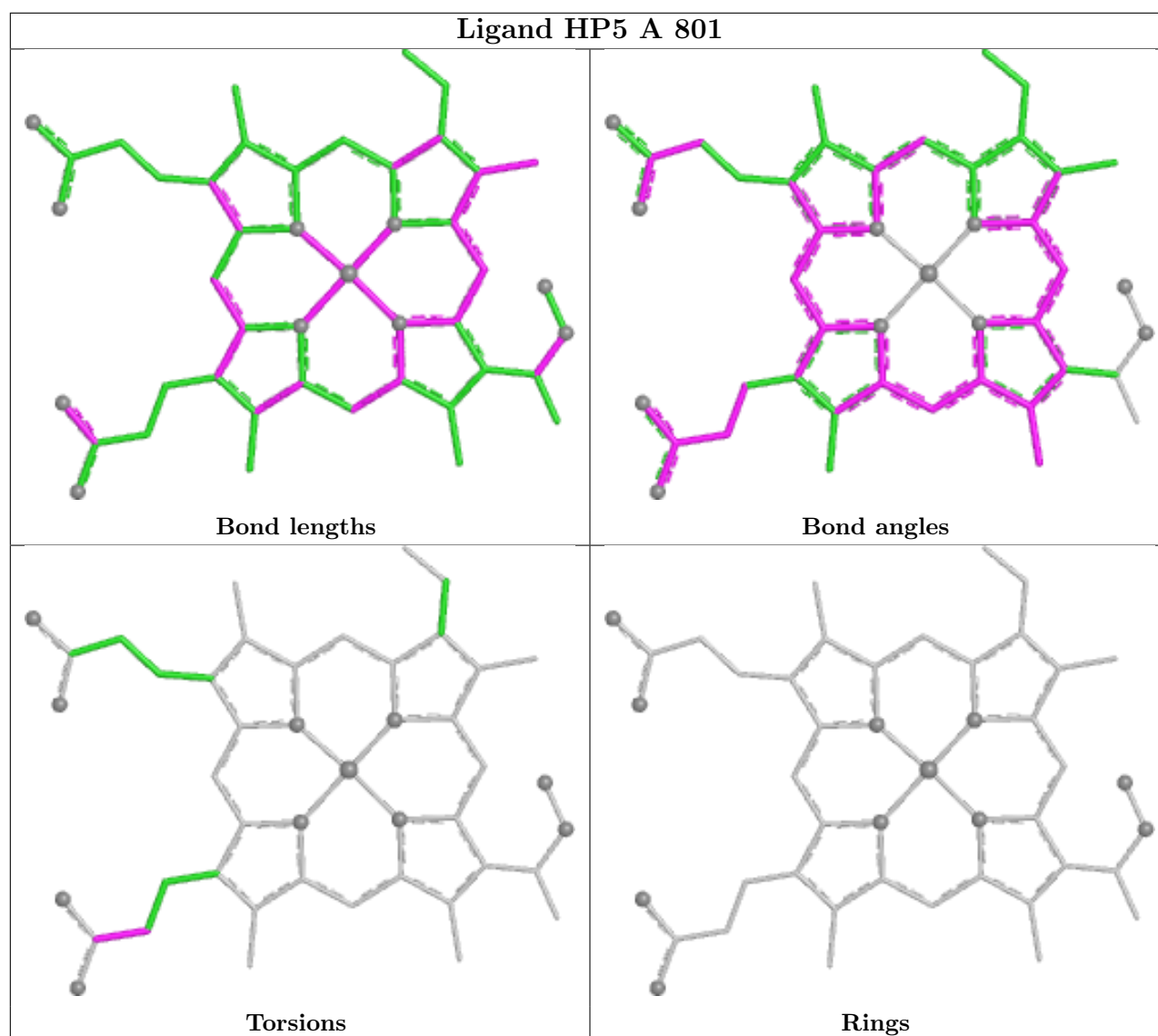
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	MPD	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HP5 B 801





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	A	713/728 (97%)	-0.44	5 (0%) 84 86	8, 18, 36, 78	5 (0%)
1	B	713/728 (97%)	-0.49	9 (1%) 75 79	9, 18, 35, 77	5 (0%)
All	All	1426/1456 (97%)	-0.46	14 (0%) 79 82	8, 18, 36, 78	10 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	4.7
1	B	748	ALA	4.1
1	B	55	HIS	3.1
1	B	65	ASP	2.9
1	B	64	LYS	2.6
1	A	454	ASP	2.5
1	B	680	ALA	2.5
1	B	540	ARG	2.3
1	A	55	HIS	2.3
1	B	454	ASP	2.2
1	B	46	GLN	2.1
1	A	540	ARG	2.1
1	A	647	GLN	2.0
1	B	691	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

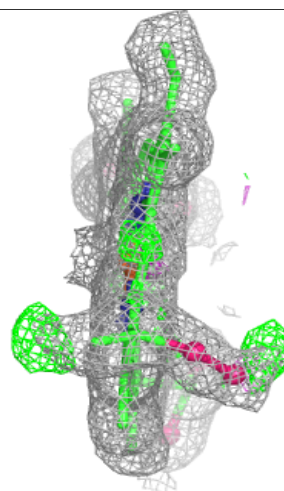
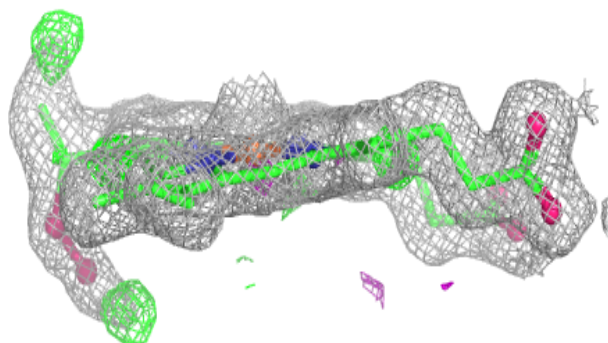
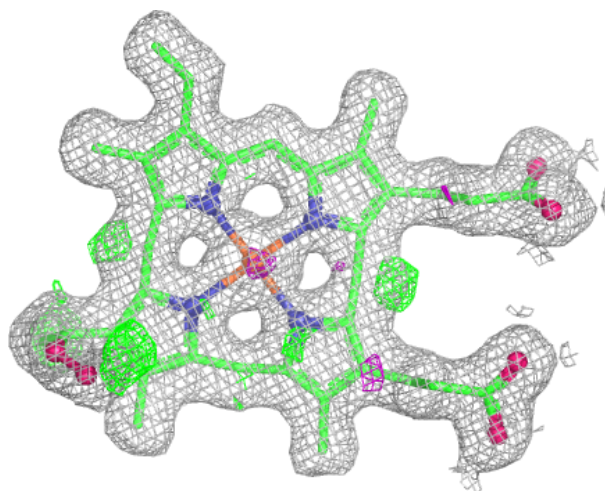
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MPD	B	804	8/8	0.86	0.14	50,56,60,65	0
5	MPD	A	804	8/8	0.88	0.12	47,55,70,74	0
4	OXY	B	803	2/2	0.90	0.22	31,31,31,32	0
5	MPD	A	805	8/8	0.91	0.11	35,40,51,54	0
4	OXY	A	803	2/2	0.91	0.23	33,33,33,41	0
3	NA	A	802	1/1	0.99	0.07	15,15,15,15	0
2	HP5	A	801	45/45	0.99	0.05	12,15,22,33	2
2	HP5	B	801	45/45	0.99	0.05	12,13,20,27	2
3	NA	B	802	1/1	1.00	0.06	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

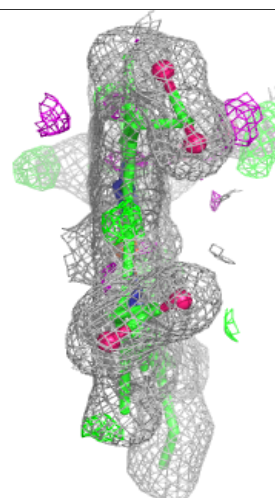
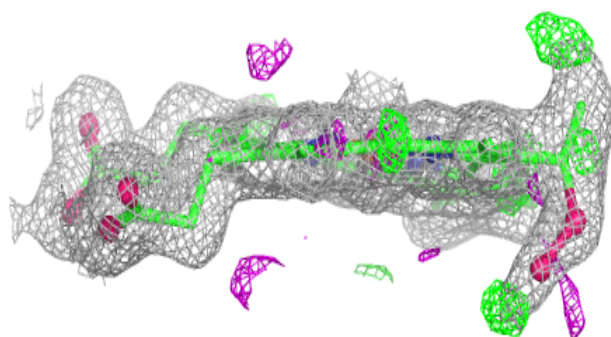
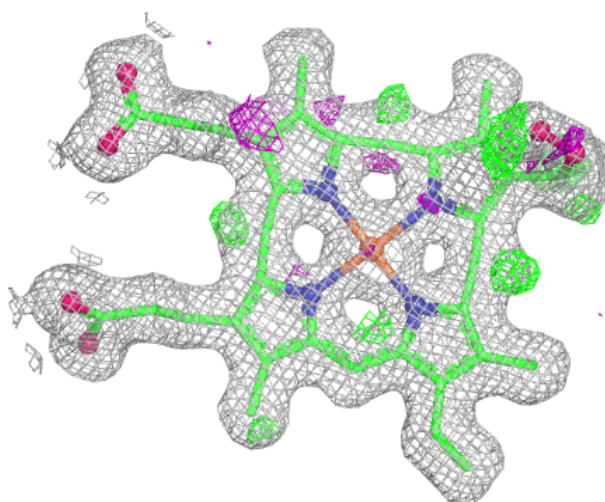
Electron density around HP5 A 801:

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



Electron density around HP5 B 801:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.