



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:31 AM EDT

PDB ID : 6BZI / pdb_00006bzi
Title : Crystal structure of halogenase PltM in complex with ethyl mercury and mercury
Authors : Pang, A.H.; Garneau-Tsodikova, S.; Tsodikov, O.V.
Deposited on : 2017-12-24
Resolution : 2.40 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

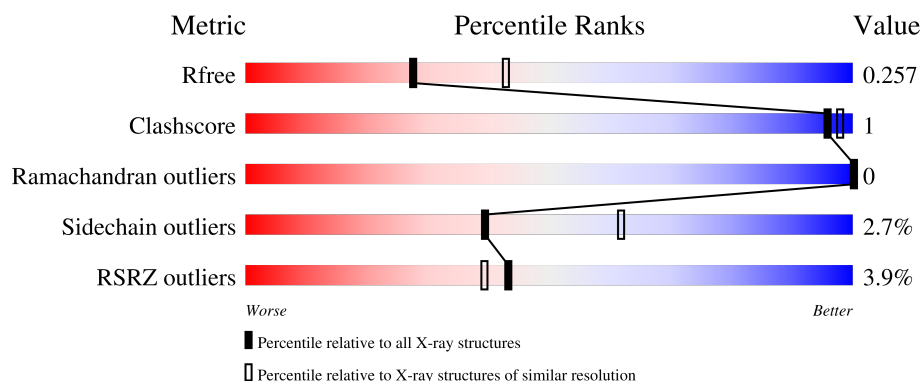
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

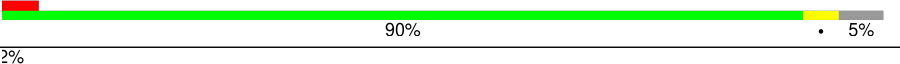
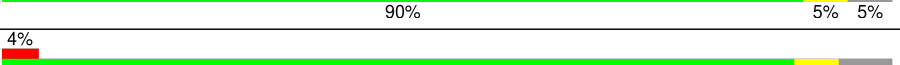
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	522	 3% 89% 5% 7%
1	B	522	 4% 90% 5% 5%
1	C	522	 2% 90% 5% 5%
1	D	522	 4% 89% 5% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16117 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 Halogenase PltM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3844	2455	677	701	11			
1	B	495	Total	C	N	O	S	0	2	0
			3925	2505	694	713	13			
1	C	496	Total	C	N	O	S	0	1	0
			3922	2504	694	712	12			
1	D	493	Total	C	N	O	S	0	2	0
			3904	2491	691	709	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q4KCZ3
A	-18	GLY	-	expression tag	UNP Q4KCZ3
A	-17	SER	-	expression tag	UNP Q4KCZ3
A	-16	SER	-	expression tag	UNP Q4KCZ3
A	-15	HIS	-	expression tag	UNP Q4KCZ3
A	-14	HIS	-	expression tag	UNP Q4KCZ3
A	-13	HIS	-	expression tag	UNP Q4KCZ3
A	-12	HIS	-	expression tag	UNP Q4KCZ3
A	-11	HIS	-	expression tag	UNP Q4KCZ3
A	-10	HIS	-	expression tag	UNP Q4KCZ3
A	-9	SER	-	expression tag	UNP Q4KCZ3
A	-8	SER	-	expression tag	UNP Q4KCZ3
A	-7	GLY	-	expression tag	UNP Q4KCZ3
A	-6	LEU	-	expression tag	UNP Q4KCZ3
A	-5	VAL	-	expression tag	UNP Q4KCZ3
A	-4	PRO	-	expression tag	UNP Q4KCZ3
A	-3	ARG	-	expression tag	UNP Q4KCZ3
A	-2	GLY	-	expression tag	UNP Q4KCZ3
A	-1	SER	-	expression tag	UNP Q4KCZ3
A	0	HIS	-	expression tag	UNP Q4KCZ3
B	-19	MET	-	initiating methionine	UNP Q4KCZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q4KCZ3
B	-17	SER	-	expression tag	UNP Q4KCZ3
B	-16	SER	-	expression tag	UNP Q4KCZ3
B	-15	HIS	-	expression tag	UNP Q4KCZ3
B	-14	HIS	-	expression tag	UNP Q4KCZ3
B	-13	HIS	-	expression tag	UNP Q4KCZ3
B	-12	HIS	-	expression tag	UNP Q4KCZ3
B	-11	HIS	-	expression tag	UNP Q4KCZ3
B	-10	HIS	-	expression tag	UNP Q4KCZ3
B	-9	SER	-	expression tag	UNP Q4KCZ3
B	-8	SER	-	expression tag	UNP Q4KCZ3
B	-7	GLY	-	expression tag	UNP Q4KCZ3
B	-6	LEU	-	expression tag	UNP Q4KCZ3
B	-5	VAL	-	expression tag	UNP Q4KCZ3
B	-4	PRO	-	expression tag	UNP Q4KCZ3
B	-3	ARG	-	expression tag	UNP Q4KCZ3
B	-2	GLY	-	expression tag	UNP Q4KCZ3
B	-1	SER	-	expression tag	UNP Q4KCZ3
B	0	HIS	-	expression tag	UNP Q4KCZ3
C	-19	MET	-	initiating methionine	UNP Q4KCZ3
C	-18	GLY	-	expression tag	UNP Q4KCZ3
C	-17	SER	-	expression tag	UNP Q4KCZ3
C	-16	SER	-	expression tag	UNP Q4KCZ3
C	-15	HIS	-	expression tag	UNP Q4KCZ3
C	-14	HIS	-	expression tag	UNP Q4KCZ3
C	-13	HIS	-	expression tag	UNP Q4KCZ3
C	-12	HIS	-	expression tag	UNP Q4KCZ3
C	-11	HIS	-	expression tag	UNP Q4KCZ3
C	-10	HIS	-	expression tag	UNP Q4KCZ3
C	-9	SER	-	expression tag	UNP Q4KCZ3
C	-8	SER	-	expression tag	UNP Q4KCZ3
C	-7	GLY	-	expression tag	UNP Q4KCZ3
C	-6	LEU	-	expression tag	UNP Q4KCZ3
C	-5	VAL	-	expression tag	UNP Q4KCZ3
C	-4	PRO	-	expression tag	UNP Q4KCZ3
C	-3	ARG	-	expression tag	UNP Q4KCZ3
C	-2	GLY	-	expression tag	UNP Q4KCZ3
C	-1	SER	-	expression tag	UNP Q4KCZ3
C	0	HIS	-	expression tag	UNP Q4KCZ3
D	-19	MET	-	initiating methionine	UNP Q4KCZ3
D	-18	GLY	-	expression tag	UNP Q4KCZ3
D	-17	SER	-	expression tag	UNP Q4KCZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q4KCZ3
D	-15	HIS	-	expression tag	UNP Q4KCZ3
D	-14	HIS	-	expression tag	UNP Q4KCZ3
D	-13	HIS	-	expression tag	UNP Q4KCZ3
D	-12	HIS	-	expression tag	UNP Q4KCZ3
D	-11	HIS	-	expression tag	UNP Q4KCZ3
D	-10	HIS	-	expression tag	UNP Q4KCZ3
D	-9	SER	-	expression tag	UNP Q4KCZ3
D	-8	SER	-	expression tag	UNP Q4KCZ3
D	-7	GLY	-	expression tag	UNP Q4KCZ3
D	-6	LEU	-	expression tag	UNP Q4KCZ3
D	-5	VAL	-	expression tag	UNP Q4KCZ3
D	-4	PRO	-	expression tag	UNP Q4KCZ3
D	-3	ARG	-	expression tag	UNP Q4KCZ3
D	-2	GLY	-	expression tag	UNP Q4KCZ3
D	-1	SER	-	expression tag	UNP Q4KCZ3
D	0	HIS	-	expression tag	UNP Q4KCZ3

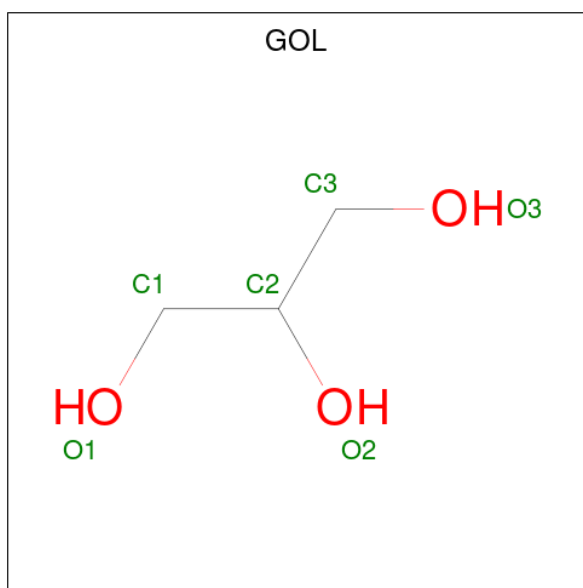
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

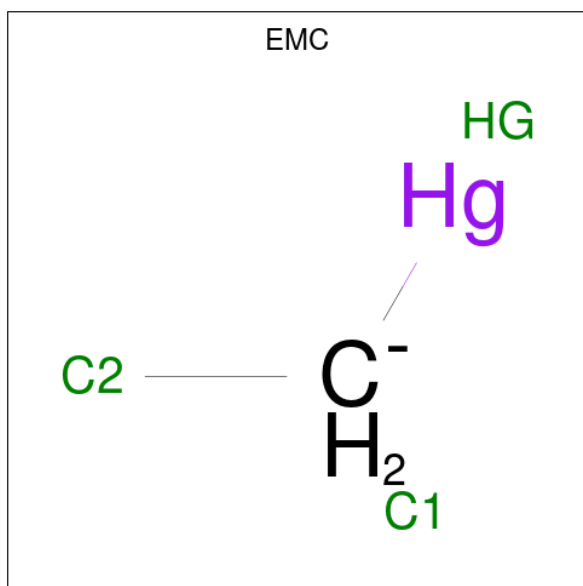
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total Hg 7 7	0	0
3	B	8	Total Hg 8 8	0	0
3	C	4	Total Hg 4 4	0	0
3	D	6	Total Hg 6 6	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is ETHYL MERCURY ION (CCD ID: EMC) (formula: C_2H_5Hg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Hg 3 2 1	0	0
5	B	1	Total C Hg 3 2 1	0	0
5	B	1	Total C Hg 3 2 1	0	0
5	C	1	Total C Hg 3 2 1	0	0
5	C	1	Total C Hg 3 2 1	0	0
5	C	1	Total C Hg 3 2 1	0	0
5	D	1	Total C Hg 3 2 1	0	0
5	D	1	Total C Hg 3 2 1	0	0

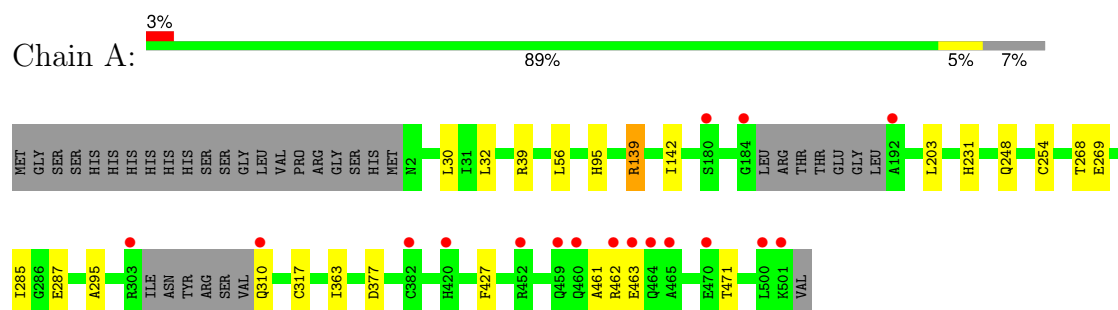
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	134	Total O 134 134	0	0
6	B	112	Total O 112 112	0	0
6	C	111	Total O 111 111	0	0
6	D	94	Total O 94 94	0	0

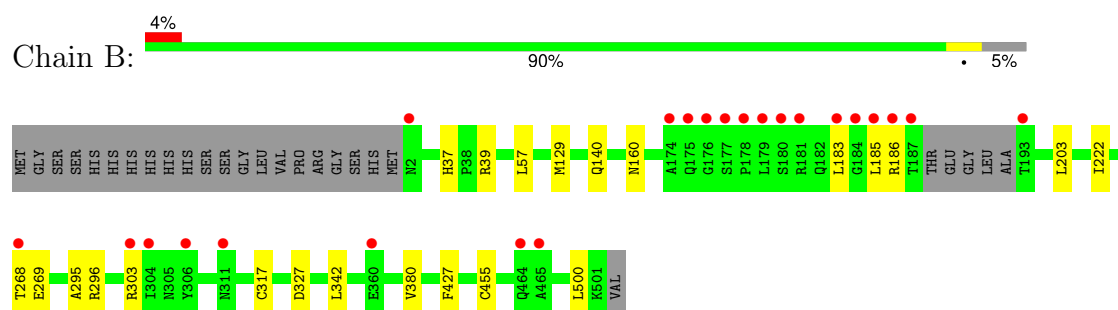
3 Residue-property plots [i](#)

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

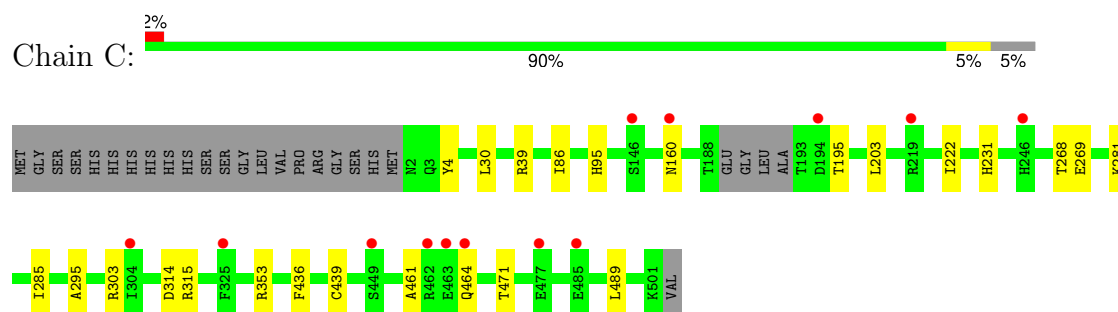
• Molecule 1: Halogenase PltM



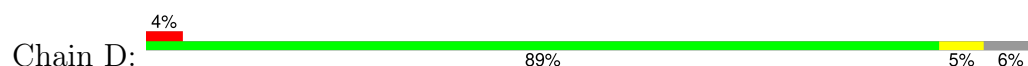
• Molecule 1: Halogenase PltM

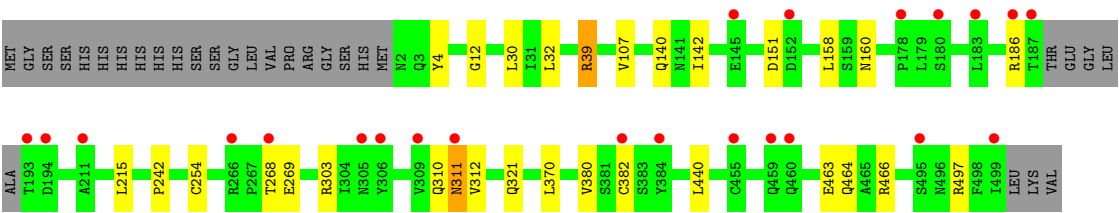


• Molecule 1: Halogenase PltM



• Molecule 1: Halogenase PltM





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.72Å 156.34Å 216.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.40 45.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (45.00-2.40) 96.3 (45.00-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.209 , 0.256 0.213 , 0.257	Depositor DCC
R_{free} test set	4092 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16117	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HG, EMC, CA

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	0.56	0/3941	0.82	0/5348
1	B	0.57	0/4024	0.84	0/5462
1	C	0.57	0/4021	0.81	0/5459
1	D	0.57	0/4003	0.83	1/5435 (0.0%)
All	All	0.57	0/15989	0.82	1/21704 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	ASN	N-CA-C	-5.18	105.03	112.13

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	3844	0	3773	10	0
1	B	3925	0	3855	7	0
1	C	3922	0	3857	10	0
1	D	3904	0	3829	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	0	0	0
3	B	8	0	0	0	0
3	C	4	0	0	0	0
3	D	6	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	D	6	0	8	0	0
5	A	3	0	0	0	0
5	B	6	0	0	0	0
5	C	9	0	0	0	0
5	D	6	0	0	1	0
6	A	134	0	0	0	0
6	B	112	0	0	0	0
6	C	111	0	0	0	0
6	D	94	0	0	0	0
All	All	16117	0	15338	35	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 1.

All (35) 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:C:203:LEU:HD22	1:C:295:ALA:HB2	1.87	0.56
1:C:195:THR:O	1:C:303:ARG:HB3	2.06	0.55
1:B:327:ASP:HB3	1:B:380:VAL:HG21	1.88	0.55
1:A:203:LEU:HD22	1:A:295:ALA:HB2	1.90	0.53
1:C:4:TYR:CE2	1:C:30:LEU:HD22	2.45	0.52
1:A:30:LEU:HD11	1:A:139:ARG:HD3	1.92	0.51
1:A:203:LEU:CD2	1:A:295:ALA:HB2	2.41	0.51
1:D:370:LEU:HG	5:D:610:EMC:C1	2.41	0.50
1:A:231:HIS:CG	1:A:285:ILE:HD12	2.46	0.50
1:D:142:ILE:HD11	1:D:158:LEU:HD13	1.94	0.48
1:D:242:PRO:HA	1:D:254[B]:CYS:SG	2.55	0.47
1:C:231:HIS:CG	1:C:285:ILE:HD12	2.51	0.45
1:D:311:ASN:HB3	1:D:312:VAL:HG13	1.98	0.45
1:A:268:THR:HG23	1:A:269:GLU:HG3	1.97	0.45
1:A:461:ALA:HB1	1:A:471:THR:HG21	1.98	0.45
1:D:32:LEU:HD22	1:D:142:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HG	1:B:342:LEU:CD1	2.47	0.44
1:A:56:LEU:HD22	1:A:427:PHE:CE1	2.53	0.43
1:D:268:THR:HG23	1:D:269:GLU:HG3	2.01	0.43
1:C:461:ALA:CB	1:C:471:THR:HG21	2.48	0.43
1:A:95:HIS:CD2	1:A:285:ILE:HD11	2.54	0.42
1:C:314:ASP:C	1:C:315:ARG:HG2	2.44	0.42
1:B:37:HIS:HA	1:B:39:ARG:HG2	2.00	0.42
1:B:342:LEU:HD23	1:B:427:PHE:HZ	1.85	0.42
1:D:107:VAL:HG12	1:D:497:ARG:HB3	2.01	0.42
1:D:12:GLY:HA2	1:D:39:ARG:NH2	2.35	0.42
1:C:268:THR:HG23	1:C:269:GLU:HG3	2.01	0.41
1:C:461:ALA:HB2	1:C:471:THR:HG21	2.02	0.41
1:B:268:THR:HG23	1:B:269:GLU:HG3	2.03	0.41
1:C:95:HIS:CD2	1:C:285:ILE:HD11	2.56	0.41
1:A:203:LEU:HD21	1:B:129:MET:HG2	2.02	0.40
1:D:4:TYR:CE2	1:D:30:LEU:HD22	2.56	0.40
1:B:203:LEU:HD22	1:B:295:ALA:HB2	2.03	0.40
1:A:32:LEU:HB3	1:A:142:ILE:HD11	2.03	0.40
1:C:436:PHE:HB3	1:C:439:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/522 (92%)	471 (98%)	10 (2%)	0	100	100
1	B	493/522 (94%)	483 (98%)	10 (2%)	0	100	100
1	C	493/522 (94%)	485 (98%)	8 (2%)	0	100	100
1	D	491/522 (94%)	483 (98%)	8 (2%)	0	100	100
All	All	1958/2088 (94%)	1922 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/440 (93%)	398 (97%)	11 (3%)	39	62
1	B	419/440 (95%)	407 (97%)	12 (3%)	37	60
1	C	418/440 (95%)	410 (98%)	8 (2%)	50	71
1	D	416/440 (94%)	401 (96%)	15 (4%)	31	52
All	All	1662/1760 (94%)	1616 (97%)	46 (3%)	39	60

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	139	ARG
1	A	248	GLN
1	A	254	CYS
1	A	287	GLU
1	A	310	GLN
1	A	317	CYS
1	A	363	ILE
1	A	377	ASP
1	A	462	ARG
1	A	463	GLU
1	B	140	GLN
1	B	160	ASN
1	B	183	LEU
1	B	185	LEU
1	B	186	ARG
1	B	222	ILE
1	B	296	ARG
1	B	303	ARG
1	B	317	CYS
1	B	455[A]	CYS
1	B	455[B]	CYS

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Mol	Chain	Res	Type
1	B	500	LEU
1	C	39	ARG
1	C	86	ILE
1	C	160	ASN
1	C	222	ILE
1	C	281	LYS
1	C	353	ARG
1	C	464	GLN
1	C	489	LEU
1	D	39	ARG
1	D	140	GLN
1	D	151	ASP
1	D	160	ASN
1	D	186	ARG
1	D	215	LEU
1	D	303	ARG
1	D	310	GLN
1	D	321	GLN
1	D	380	VAL
1	D	382	CYS
1	D	440	LEU
1	D	463	GLU
1	D	464	GLN
1	D	466	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	368	HIS
1	A	412	GLN
1	A	416	HIS
1	B	98	ASN
1	B	262	ASN
1	B	311	ASN
1	B	361	GLN
1	B	378	GLN
1	B	405	ASN
1	C	140	GLN
1	C	141	ASN
1	C	182	GLN
1	C	259	GLN

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Mol	Chain	Res	Type
1	C	294	ASN
1	C	311	ASN
1	C	378	GLN
1	C	426	GLN
1	D	98	ASN
1	D	305	ASN
1	D	310	GLN
1	D	368	HIS
1	D	378	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 29 are 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	GOL	A	609	-	5,5,5	0.41	0	5,5,5	0.44	0
5	EMC	C	608	1	1,2,2	0.50	0	-		
5	EMC	D	610	1	1,2,2	0.08	0	-		
4	GOL	D	608	-	5,5,5	0.44	0	5,5,5	0.25	0
5	EMC	B	611	1	1,2,2	0.44	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EMC	C	606	1	1,2,2	0.41	0	-		
5	EMC	B	612	1	1,2,2	0.45	0	-		
5	EMC	D	609	1	1,2,2	0.17	0	-		
5	EMC	C	607	1	1,2,2	0.46	0	-		
4	GOL	B	610	-	5,5,5	0.23	0	5,5,5	0.33	0
5	EMC	A	610	1	1,2,2	0.42	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
4	GOL	A	609	-	-	0/4/4/4	-
4	GOL	B	610	-	-	2/4/4/4	-
4	GOL	D	608	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	610	GOL	C1-C2-C3-O3
4	D	608	GOL	O1-C1-C2-C3
4	D	608	GOL	C1-C2-C3-O3
4	D	608	GOL	O1-C1-C2-O2
4	D	608	GOL	O2-C2-C3-O3
4	B	610	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	610	EMC	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/522 (93%)	0.11	17 (3%) 47 43	11, 24, 46, 86	0
1	B	495/522 (94%)	0.18	23 (4%) 37 33	11, 24, 56, 93	2 (0%)
1	C	496/522 (95%)	0.21	13 (2%) 57 53	9, 26, 46, 81	1 (0%)
1	D	493/522 (94%)	0.27	23 (4%) 36 32	11, 26, 53, 82	2 (0%)
All	All	1971/2088 (94%)	0.19	76 (3%) 43 39	9, 25, 50, 93	5 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ALA	6.1
1	B	180	SER	4.8
1	D	187	THR	4.4
1	B	185	LEU	4.3
1	A	184	GLY	4.3
1	B	184	GLY	4.0
1	B	193	THR	3.7
1	B	187	THR	3.6
1	A	464	GLN	3.4
1	A	420	HIS	3.3
1	A	465	ALA	3.3
1	B	304	ILE	3.3
1	D	459	GLN	3.2
1	A	460	GLN	3.0
1	D	384	TYR	3.0
1	D	186	ARG	3.0
1	A	501	LYS	3.0
1	B	306	TYR	2.9
1	D	460	GLN	2.9
1	B	178	PRO	2.9
1	A	310	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	304	ILE	2.8
1	D	178	PRO	2.8
1	A	463	GLU	2.8
1	A	303	ARG	2.7
1	D	152	ASP	2.7
1	B	465	ALA	2.6
1	C	464	GLN	2.6
1	B	186	ARG	2.6
1	C	463	GLU	2.6
1	D	311	ASN	2.6
1	D	183	LEU	2.5
1	B	2	ASN	2.5
1	A	462	ARG	2.5
1	A	452	ARG	2.5
1	D	180	SER	2.5
1	D	382	CYS	2.4
1	B	176	GLY	2.4
1	D	455[A]	CYS	2.4
1	B	183	LEU	2.4
1	B	303	ARG	2.4
1	A	382	CYS	2.4
1	A	180	SER	2.3
1	D	306	TYR	2.3
1	D	193	THR	2.3
1	C	160	ASN	2.3
1	D	268	THR	2.3
1	A	459	GLN	2.3
1	D	495	SER	2.3
1	C	325	PHE	2.3
1	B	181	ARG	2.3
1	B	179	LEU	2.2
1	D	499	ILE	2.2
1	A	470	GLU	2.2
1	A	500	LEU	2.2
1	B	177	SER	2.2
1	D	266	ARG	2.2
1	C	462	ARG	2.2
1	C	485	GLU	2.1
1	C	146	SER	2.1
1	C	219	ARG	2.1
1	C	246	HIS	2.1
1	B	175	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	464	GLN	2.1
1	D	194	ASP	2.1
1	B	174	ALA	2.1
1	D	309	VAL	2.0
1	D	211	ALA	2.0
1	B	311	ASN	2.0
1	D	305	ASN	2.0
1	B	360	GLU	2.0
1	B	268	THR	2.0
1	C	449	SER	2.0
1	C	477	GLU	2.0
1	D	145	GLU	2.0
1	C	194	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	609	6/6	0.70	0.16	25,27,28,28	0
3	HG	A	608	1/1	0.78	0.22	104,104,104,104	0
4	GOL	D	608	6/6	0.78	0.16	27,28,29,30	0
3	HG	B	609	1/1	0.88	0.14	42,42,42,42	1
4	GOL	B	610	6/6	0.90	0.11	36,37,37,37	0
3	HG	A	604	1/1	0.92	0.21	77,77,77,77	1
3	HG	D	607	1/1	0.93	0.07	53,53,53,53	1
3	HG	B	608	1/1	0.93	0.18	72,72,72,72	1
3	HG	C	605	1/1	0.94	0.13	64,64,64,64	1
3	HG	B	605	1/1	0.95	0.05	36,36,36,36	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HG	D	604	1/1	0.95	0.09	41,41,41,41	1
3	HG	B	607	1/1	0.95	0.06	50,50,50,50	1
3	HG	A	607	1/1	0.95	0.05	29,29,29,29	1
2	CA	B	601	1/1	0.95	0.04	25,25,25,25	0
3	HG	C	604	1/1	0.95	0.06	42,42,42,42	1
2	CA	D	601	1/1	0.96	0.06	26,26,26,26	0
3	HG	D	606	1/1	0.96	0.09	39,39,39,39	1
2	CA	C	601	1/1	0.96	0.03	23,23,23,23	0
3	HG	D	605	1/1	0.97	0.07	39,39,39,39	1
2	CA	A	601	1/1	0.97	0.04	24,24,24,24	0
3	HG	C	603	1/1	0.98	0.03	23,23,23,23	1
3	HG	D	603	1/1	0.98	0.04	24,24,24,24	1
3	HG	B	606	1/1	0.98	0.09	42,42,42,42	1
3	HG	A	606	1/1	0.99	0.04	20,20,20,20	1
3	HG	B	603	1/1	0.99	0.02	22,22,22,22	1
3	HG	B	604	1/1	0.99	0.02	32,32,32,32	1
3	HG	D	602	1/1	0.99	0.06	18,18,18,18	1
3	HG	A	603	1/1	0.99	0.04	31,31,31,31	1
3	HG	C	602	1/1	0.99	0.02	33,33,33,33	1
5	EMC	A	610	3/3	0.99	0.14	25,25,25,25	3
5	EMC	B	612	3/3	0.99	0.12	15,15,15,16	3
5	EMC	C	606	3/3	0.99	0.16	10,10,11,11	3
3	HG	B	602	1/1	1.00	0.06	19,19,19,19	1
5	EMC	B	611	3/3	1.00	0.15	10,10,11,11	3
3	HG	A	605	1/1	1.00	0.06	10,10,10,10	1
3	HG	A	602	1/1	1.00	0.06	18,18,18,18	1
5	EMC	C	607	3/3	1.00	0.13	18,18,19,19	3
5	EMC	C	608	3/3	1.00	0.14	13,13,13,13	3
5	EMC	D	609	3/3	1.00	0.10	12,12,13,13	3
5	EMC	D	610	3/3	1.00	0.13	18,18,20,20	3

6.5 Other polymers ⓘ

There are no such residues in this entry.