



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 06:16 pm GMT

PDB ID : 8PHA
Title : O(S)-methyltransferase from *Pleurotus sapidus*
Authors : Korf, L.; Essen, L.-O.
Deposited on : 2023-06-19
Resolution : 2.02 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

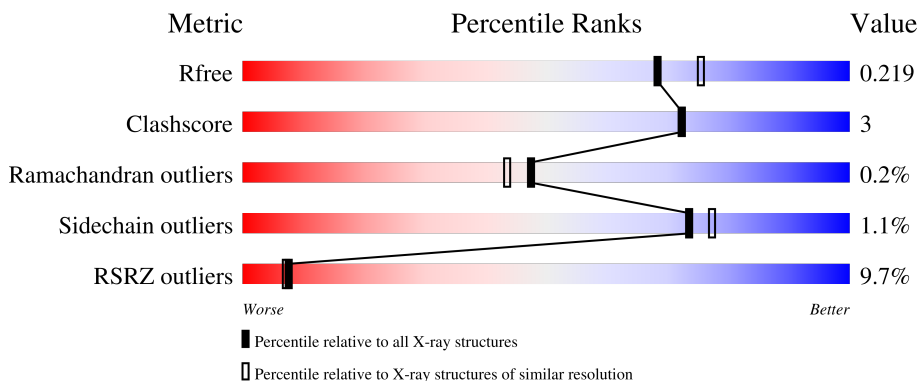
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	479	 4% 86% 8% 6%
1	B	479	 5% 87% 7% 6%
1	C	479	 12% 86% 9% .
1	D	479	 15% 86% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15629 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 O-methyltransferase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	Total 3538	C 2258	N 591	O 670	S 19	0	7	0
1	B	450	Total 3555	C 2266	N 594	O 677	S 18	0	8	0
1	C	458	Total 3623	C 2305	N 611	O 688	S 19	0	8	0
1	D	460	Total 3626	C 2307	N 613	O 687	S 19	0	7	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP A0A067NAT9
A	-14	ASN	-	expression tag	UNP A0A067NAT9
A	-13	HIS	-	expression tag	UNP A0A067NAT9
A	-12	LYS	-	expression tag	UNP A0A067NAT9
A	-11	VAL	-	expression tag	UNP A0A067NAT9
A	-10	HIS	-	expression tag	UNP A0A067NAT9
A	-9	HIS	-	expression tag	UNP A0A067NAT9
A	-8	HIS	-	expression tag	UNP A0A067NAT9
A	-7	HIS	-	expression tag	UNP A0A067NAT9
A	-6	HIS	-	expression tag	UNP A0A067NAT9
A	-5	HIS	-	expression tag	UNP A0A067NAT9
A	-4	ILE	-	expression tag	UNP A0A067NAT9
A	-3	GLU	-	expression tag	UNP A0A067NAT9
A	-2	GLY	-	expression tag	UNP A0A067NAT9
A	-1	ARG	-	expression tag	UNP A0A067NAT9
A	0	HIS	-	expression tag	UNP A0A067NAT9
A	35	GLU	GLY	conflict	UNP A0A067NAT9
A	45	GLU	LYS	conflict	UNP A0A067NAT9
A	46	PRO	ALA	conflict	UNP A0A067NAT9
A	64	ILE	VAL	conflict	UNP A0A067NAT9
A	104	VAL	ILE	conflict	UNP A0A067NAT9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	378	LYS	GLU	conflict	UNP A0A067NAT9
A	456	HIS	-	expression tag	UNP A0A067NAT9
A	457	HIS	-	expression tag	UNP A0A067NAT9
A	458	HIS	-	expression tag	UNP A0A067NAT9
A	459	HIS	-	expression tag	UNP A0A067NAT9
A	460	HIS	-	expression tag	UNP A0A067NAT9
A	461	HIS	-	expression tag	UNP A0A067NAT9
A	462	SER	-	expression tag	UNP A0A067NAT9
A	463	ARG	-	expression tag	UNP A0A067NAT9
B	-15	MET	-	initiating methionine	UNP A0A067NAT9
B	-14	ASN	-	expression tag	UNP A0A067NAT9
B	-13	HIS	-	expression tag	UNP A0A067NAT9
B	-12	LYS	-	expression tag	UNP A0A067NAT9
B	-11	VAL	-	expression tag	UNP A0A067NAT9
B	-10	HIS	-	expression tag	UNP A0A067NAT9
B	-9	HIS	-	expression tag	UNP A0A067NAT9
B	-8	HIS	-	expression tag	UNP A0A067NAT9
B	-7	HIS	-	expression tag	UNP A0A067NAT9
B	-6	HIS	-	expression tag	UNP A0A067NAT9
B	-5	HIS	-	expression tag	UNP A0A067NAT9
B	-4	ILE	-	expression tag	UNP A0A067NAT9
B	-3	GLU	-	expression tag	UNP A0A067NAT9
B	-2	GLY	-	expression tag	UNP A0A067NAT9
B	-1	ARG	-	expression tag	UNP A0A067NAT9
B	0	HIS	-	expression tag	UNP A0A067NAT9
B	35	GLU	GLY	conflict	UNP A0A067NAT9
B	45	GLU	LYS	conflict	UNP A0A067NAT9
B	46	PRO	ALA	conflict	UNP A0A067NAT9
B	64	ILE	VAL	conflict	UNP A0A067NAT9
B	104	VAL	ILE	conflict	UNP A0A067NAT9
B	378	LYS	GLU	conflict	UNP A0A067NAT9
B	456	HIS	-	expression tag	UNP A0A067NAT9
B	457	HIS	-	expression tag	UNP A0A067NAT9
B	458	HIS	-	expression tag	UNP A0A067NAT9
B	459	HIS	-	expression tag	UNP A0A067NAT9
B	460	HIS	-	expression tag	UNP A0A067NAT9
B	461	HIS	-	expression tag	UNP A0A067NAT9
B	462	SER	-	expression tag	UNP A0A067NAT9
B	463	ARG	-	expression tag	UNP A0A067NAT9
C	-15	MET	-	initiating methionine	UNP A0A067NAT9
C	-14	ASN	-	expression tag	UNP A0A067NAT9
C	-13	HIS	-	expression tag	UNP A0A067NAT9

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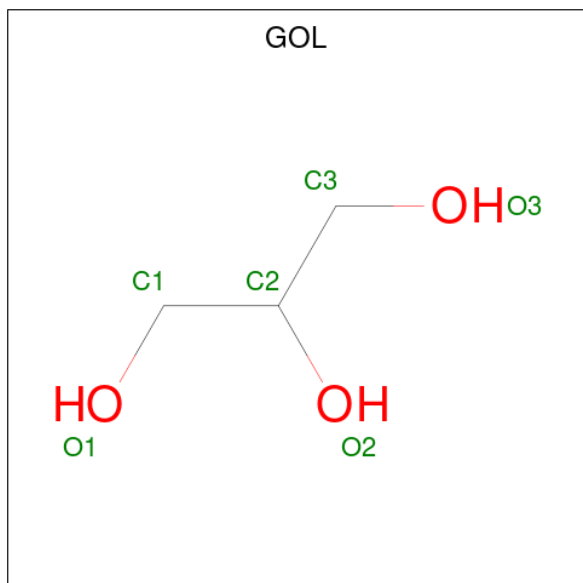
Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	LYS	-	expression tag	UNP A0A067NAT9
C	-11	VAL	-	expression tag	UNP A0A067NAT9
C	-10	HIS	-	expression tag	UNP A0A067NAT9
C	-9	HIS	-	expression tag	UNP A0A067NAT9
C	-8	HIS	-	expression tag	UNP A0A067NAT9
C	-7	HIS	-	expression tag	UNP A0A067NAT9
C	-6	HIS	-	expression tag	UNP A0A067NAT9
C	-5	HIS	-	expression tag	UNP A0A067NAT9
C	-4	ILE	-	expression tag	UNP A0A067NAT9
C	-3	GLU	-	expression tag	UNP A0A067NAT9
C	-2	GLY	-	expression tag	UNP A0A067NAT9
C	-1	ARG	-	expression tag	UNP A0A067NAT9
C	0	HIS	-	expression tag	UNP A0A067NAT9
C	35	GLU	GLY	conflict	UNP A0A067NAT9
C	45	GLU	LYS	conflict	UNP A0A067NAT9
C	46	PRO	ALA	conflict	UNP A0A067NAT9
C	64	ILE	VAL	conflict	UNP A0A067NAT9
C	104	VAL	ILE	conflict	UNP A0A067NAT9
C	378	LYS	GLU	conflict	UNP A0A067NAT9
C	456	HIS	-	expression tag	UNP A0A067NAT9
C	457	HIS	-	expression tag	UNP A0A067NAT9
C	458	HIS	-	expression tag	UNP A0A067NAT9
C	459	HIS	-	expression tag	UNP A0A067NAT9
C	460	HIS	-	expression tag	UNP A0A067NAT9
C	461	HIS	-	expression tag	UNP A0A067NAT9
C	462	SER	-	expression tag	UNP A0A067NAT9
C	463	ARG	-	expression tag	UNP A0A067NAT9
D	-15	MET	-	initiating methionine	UNP A0A067NAT9
D	-14	ASN	-	expression tag	UNP A0A067NAT9
D	-13	HIS	-	expression tag	UNP A0A067NAT9
D	-12	LYS	-	expression tag	UNP A0A067NAT9
D	-11	VAL	-	expression tag	UNP A0A067NAT9
D	-10	HIS	-	expression tag	UNP A0A067NAT9
D	-9	HIS	-	expression tag	UNP A0A067NAT9
D	-8	HIS	-	expression tag	UNP A0A067NAT9
D	-7	HIS	-	expression tag	UNP A0A067NAT9
D	-6	HIS	-	expression tag	UNP A0A067NAT9
D	-5	HIS	-	expression tag	UNP A0A067NAT9
D	-4	ILE	-	expression tag	UNP A0A067NAT9
D	-3	GLU	-	expression tag	UNP A0A067NAT9
D	-2	GLY	-	expression tag	UNP A0A067NAT9
D	-1	ARG	-	expression tag	UNP A0A067NAT9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A0A067NAT9
D	35	GLU	GLY	conflict	UNP A0A067NAT9
D	45	GLU	LYS	conflict	UNP A0A067NAT9
D	46	PRO	ALA	conflict	UNP A0A067NAT9
D	64	ILE	VAL	conflict	UNP A0A067NAT9
D	104	VAL	ILE	conflict	UNP A0A067NAT9
D	378	LYS	GLU	conflict	UNP A0A067NAT9
D	456	HIS	-	expression tag	UNP A0A067NAT9
D	457	HIS	-	expression tag	UNP A0A067NAT9
D	458	HIS	-	expression tag	UNP A0A067NAT9
D	459	HIS	-	expression tag	UNP A0A067NAT9
D	460	HIS	-	expression tag	UNP A0A067NAT9
D	461	HIS	-	expression tag	UNP A0A067NAT9
D	462	SER	-	expression tag	UNP A0A067NAT9
D	463	ARG	-	expression tag	UNP A0A067NAT9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



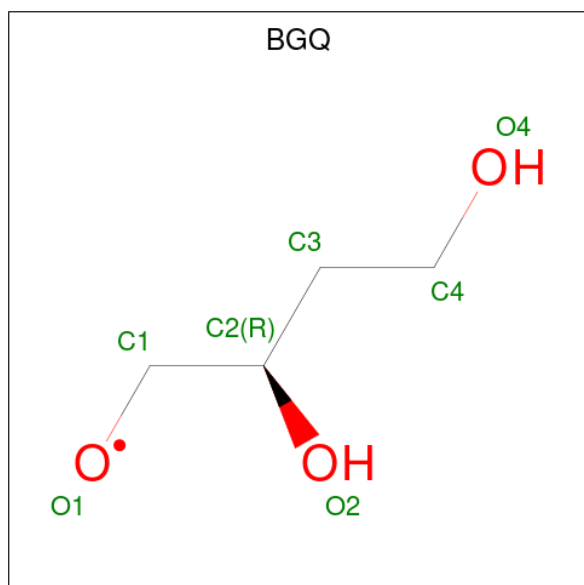
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

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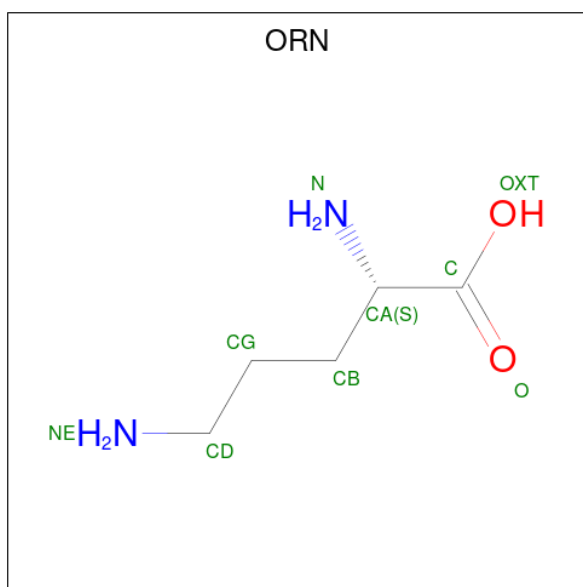
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-HYDROXY BUTANE-1,4-DIOL (three-letter code: BGQ) (formula: C₄H₉O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	2	2		
4	B	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Na	0	0
			2	2		
5	D	2	Total	Na	0	0
			2	2		

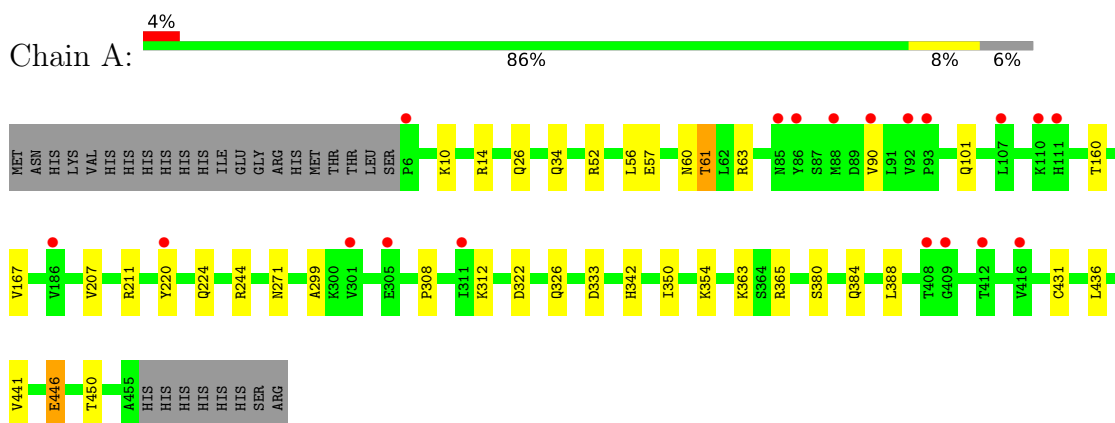
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	331	Total	O	0	0
			331	331		
6	B	340	Total	O	0	0
			340	340		
6	C	275	Total	O	0	0
			275	275		
6	D	269	Total	O	0	0
			269	269		

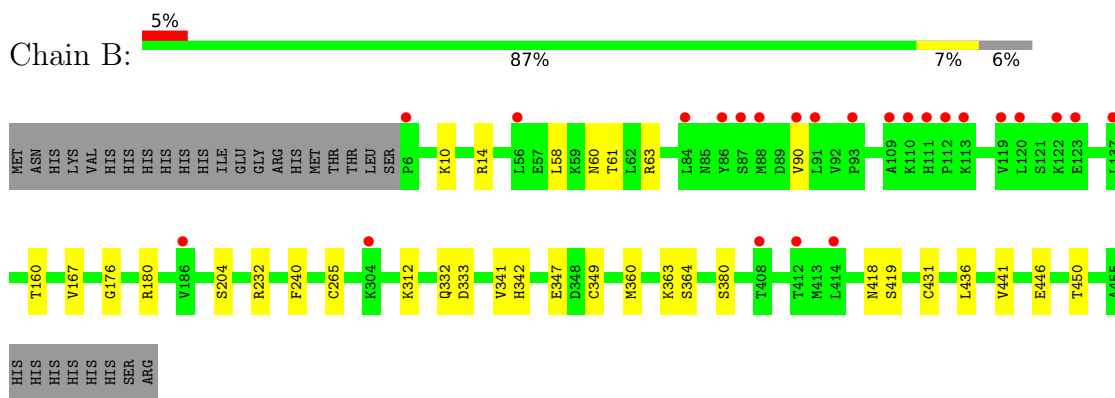
3 Residue-property plots [i](#)

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.

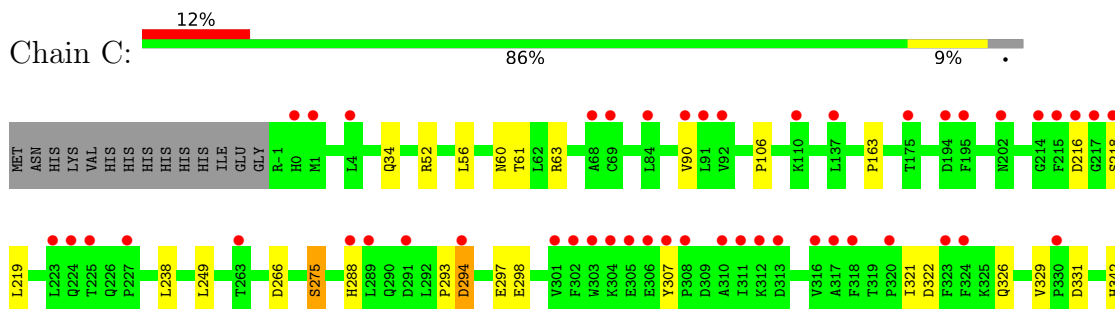
- Molecule 1: O-methyltransferase domain-containing protein

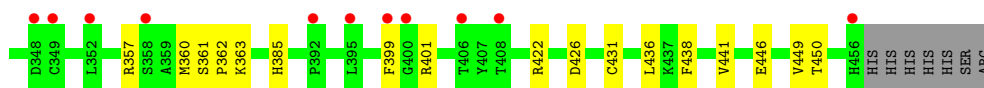


- Molecule 1: O-methyltransferase domain-containing protein

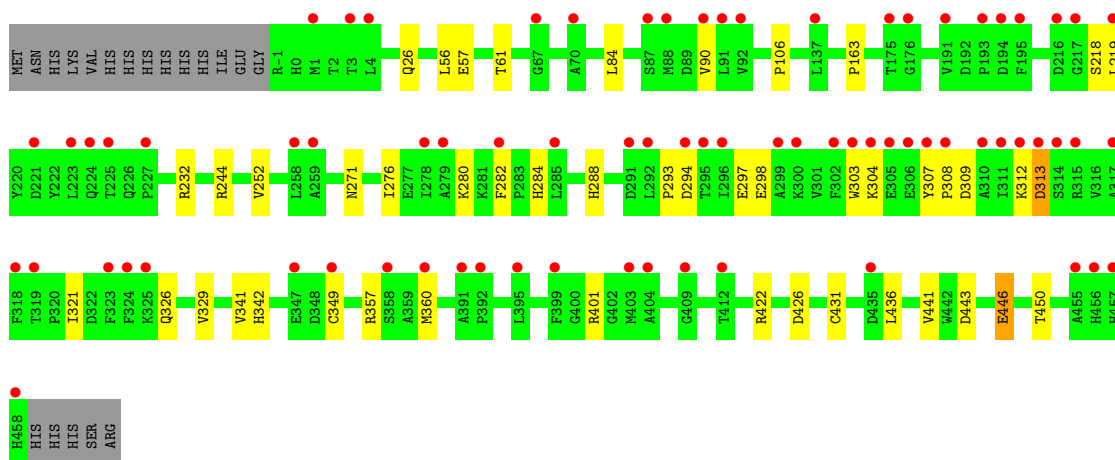
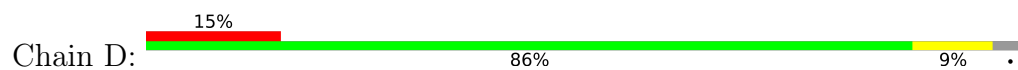


- Molecule 1: O-methyltransferase domain-containing protein





- Molecule 1: O-methyltransferase domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.36Å 109.12Å 192.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.02 48.23 – 2.02	Depositor EDS
% Data completeness (in resolution range)	88.5 (48.23-2.02) 98.8 (48.23-2.02)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.01Å)	Xtrriage
Refinement program	PHENIX dev_4788	Depositor
R, R_{free}	0.171 , 0.212 0.181 , 0.219	Depositor DCC
R_{free} test set	6643 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtrriage
Anisotropy	0.375	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15629	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1655e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ORN, BGQ, GOL, NA

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	0.35	0/3641	0.54	0/4959
1	B	0.34	0/3655	0.53	0/4977
1	C	0.33	0/3715	0.54	0/5059
1	D	0.33	0/3718	0.55	0/5063
All	All	0.34	0/14729	0.54	0/20058

There are no bond length outliers.

There are no bond angle outliers.

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	3538	0	3539	27	0
1	B	3555	0	3550	19	0
1	C	3623	0	3610	27	0
1	D	3626	0	3609	30	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	D	12	0	16	0	0
3	A	7	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	9	1	0
4	A	9	0	11	1	0
4	B	9	0	11	1	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	331	0	0	3	1
6	B	340	0	0	1	1
6	C	275	0	0	0	0
6	D	269	0	0	2	0
All	All	15629	0	14396	99	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (99) 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:380:SER:HB3	4:B:503:ORN:H	1.33	0.91
1:A:380:SER:HB3	4:A:503:ORN:H	1.38	0.89
1:A:60[B]:ASN:OD1	1:A:63:ARG:NH2	2.10	0.84
1:C:322:ASP:H	1:C:326:GLN:HE21	1.31	0.79
1:D:56:LEU:HD11	1:D:252:VAL:HG22	1.69	0.74
1:A:322:ASP:H	1:A:326:GLN:HE21	1.35	0.74
1:A:60[A]:ASN:ND2	6:A:604:HOH:O	2.25	0.69
1:B:60[A]:ASN:OD1	1:B:63:ARG:NH2	2.27	0.68
1:C:441:VAL:HG22	1:C:450[A]:THR:HG22	1.76	0.67
1:D:443:ASP:OD1	6:D:601:HOH:O	2.14	0.65
1:A:101:GLN:NE2	6:A:609:HOH:O	2.32	0.63
1:A:90:VAL:HG22	1:C:90:VAL:HG23	1.79	0.62
1:A:365:ARG:NH2	6:A:602:HOH:O	2.24	0.62
1:B:160:THR:HB	1:B:167:VAL:HG11	1.81	0.62
1:C:288:HIS:HD1	1:C:329:VAL:HG21	1.64	0.61
1:D:357:ARG:HD2	1:D:360:MET:HE2	1.83	0.61
1:A:26:GLN:HB3	1:A:61[A]:THR:HG21	1.85	0.59
1:C:357:ARG:HD2	1:C:360:MET:HE2	1.86	0.58
1:D:321:ILE:HG13	1:D:326:GLN:HG3	1.85	0.57
1:C:106:PRO:HG3	1:C:163:PRO:HD3	1.86	0.56
1:A:26:GLN:CG	1:A:61[B]:THR:HG21	2.36	0.55
1:C:321:ILE:HG13	1:C:326:GLN:HG3	1.88	0.55
1:C:294:ASP:O	1:C:298:GLU:HG2	2.07	0.54
1:C:34:GLN:HE21	1:C:52:ARG:HH11	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HB	1:A:167:VAL:HG11	1.89	0.54
1:C:288:HIS:HE1	1:C:329:VAL:HG11	1.72	0.54
1:C:431:CYS:HB3	1:C:436:LEU:HB2	1.91	0.53
1:B:90:VAL:HG22	1:D:90:VAL:HG23	1.90	0.52
1:A:431:CYS:HB3	1:A:436:LEU:HB2	1.91	0.52
3:A:502:BGQ:H11C	1:C:401:ARG:HH11	1.74	0.52
1:C:63:ARG:HG2	1:C:399:PHE:CD1	2.45	0.52
1:A:57:GLU:O	1:A:61[A]:THR:OG1	2.27	0.52
1:B:431:CYS:HB3	1:B:436:LEU:HB2	1.90	0.51
1:C:34:GLN:NE2	1:C:52:ARG:HH11	2.10	0.50
1:C:288:HIS:ND1	1:C:329:VAL:HG21	2.27	0.50
1:D:431:CYS:HB3	1:D:436:LEU:HB2	1.92	0.50
1:C:288:HIS:CE1	1:C:329:VAL:HG11	2.47	0.49
1:C:361:SER:HB2	1:C:362:PRO:HD2	1.94	0.49
1:A:333:ASP:OD1	1:A:363:LYS:HE2	2.12	0.49
1:C:218[A]:SER:OG	1:C:219:LEU:N	2.44	0.49
1:C:331:ASP:O	1:C:363:LYS:NZ	2.45	0.49
1:A:441:VAL:HG22	1:A:450:THR:HG22	1.95	0.49
1:B:240:PHE:HE1	1:D:84[A]:LEU:HD21	1.77	0.49
1:D:276:ILE:HG12	1:D:280:LYS:NZ	2.29	0.48
1:A:26:GLN:HG2	1:A:61[B]:THR:HG21	1.94	0.48
1:C:322:ASP:N	1:C:326:GLN:HE21	2.06	0.48
1:C:385:HIS:CD2	1:C:438:PHE:HE2	2.31	0.47
1:B:58:LEU:O	1:B:61[A]:THR:HG22	2.14	0.47
1:D:304:LYS:O	1:D:308:PRO:HG3	2.15	0.47
1:A:57:GLU:O	1:A:61[B]:THR:HG23	2.15	0.47
1:B:441:VAL:HG22	1:B:450:THR:HG22	1.96	0.47
1:D:288:HIS:ND1	1:D:329:VAL:HG11	2.30	0.46
1:D:57[B]:GLU:O	1:D:61:THR:HG23	2.16	0.46
1:A:350:ILE:HG22	1:A:354:LYS:HE2	1.97	0.46
1:C:266:ASP:OD2	1:C:275:SER:OG	2.34	0.46
1:C:293:PRO:O	1:C:297:GLU:HG2	2.16	0.46
1:D:56:LEU:HD11	1:D:252:VAL:CG2	2.42	0.46
1:D:276:ILE:HA	1:D:303:TRP:CH2	2.51	0.46
1:C:249:LEU:HD13	1:C:449:VAL:HG21	1.98	0.45
1:B:333:ASP:OD1	1:B:363:LYS:HE2	2.17	0.45
1:D:282:PHE:HB3	1:D:284:HIS:CE1	2.52	0.45
1:D:309:ASP:O	1:D:313:ASP:HB2	2.17	0.45
1:B:160:THR:HB	1:B:167:VAL:CG1	2.46	0.45
1:D:341:VAL:HG13	1:D:349:CYS:SG	2.56	0.45
1:A:34:GLN:OE1	1:A:52:ARG:NH1	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:ARG:HB3	1:D:426:ASP:HB2	1.99	0.45
1:A:322:ASP:N	1:A:326:GLN:HE21	2.10	0.44
1:A:160:THR:HB	1:A:167:VAL:CG1	2.47	0.44
1:B:232:ARG:NH2	6:B:622:HOH:O	2.44	0.44
1:D:232:ARG:NH2	6:D:611:HOH:O	2.44	0.44
1:D:441:VAL:HG22	1:D:450:THR:HG22	2.00	0.44
1:A:10:LYS:O	1:A:14:ARG:HG3	2.18	0.43
1:B:312:LYS:HE2	1:B:312:LYS:HB3	1.87	0.43
1:B:176:GLY:O	1:B:180:ARG:HG3	2.18	0.43
1:C:294:ASP:OD1	1:C:294:ASP:N	2.52	0.43
1:D:276:ILE:HG12	1:D:280:LYS:HZ3	1.83	0.43
1:D:106:PRO:HG3	1:D:163:PRO:HD3	2.01	0.43
1:D:57[A]:GLU:O	1:D:61:THR:HG23	2.17	0.43
1:D:271:ASN:OD1	1:D:298:GLU:HG3	2.19	0.43
1:D:293:PRO:O	1:D:297:GLU:HG2	2.19	0.43
1:D:308:PRO:O	1:D:312:LYS:HG2	2.19	0.43
1:A:244:ARG:HB3	1:A:446:GLU:HG2	2.01	0.42
1:A:220:TYR:O	1:A:224:GLN:HG3	2.20	0.42
1:B:265:CYS:HB2	1:B:332:GLN:HG3	2.01	0.42
3:B:502:BGQ:H12C	1:D:401:ARG:HH11	1.85	0.42
1:A:308:PRO:O	1:A:312:LYS:HG2	2.20	0.41
1:B:204:SER:HB3	1:B:418:ASN:HB2	2.02	0.41
1:C:60:ASN:ND2	1:C:63:ARG:HH21	2.18	0.41
1:C:422:ARG:HB3	1:C:426:ASP:HB2	2.01	0.41
1:A:207:VAL:O	1:A:211:ARG:HG2	2.21	0.41
1:A:384:GLN:HB2	1:A:388:LEU:HD12	2.03	0.41
1:D:244:ARG:HB3	1:D:446:GLU:HG2	2.02	0.41
1:B:240:PHE:CE1	1:D:84[A]:LEU:HD21	2.55	0.41
1:B:10:LYS:O	1:B:14:ARG:HG3	2.21	0.41
1:A:271:ASN:HA	1:A:299:ALA:HB2	2.02	0.41
1:D:26[B]:GLN:CG	1:D:61:THR:HG21	2.51	0.41
1:D:218:SER:OG	1:D:219:LEU:N	2.52	0.40
1:B:360:MET:HB3	1:B:364:SER:HB2	2.04	0.40
1:B:341:VAL:HG13	1:B:349:CYS:SG	2.61	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:688:HOH:O	6:B:606:HOH:O[1_455]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/479 (95%)	451 (99%)	3 (1%)	1 (0%)	47	43
1	B	456/479 (95%)	453 (99%)	2 (0%)	1 (0%)	47	43
1	C	464/479 (97%)	459 (99%)	4 (1%)	1 (0%)	47	43
1	D	465/479 (97%)	455 (98%)	9 (2%)	1 (0%)	47	43
All	All	1840/1916 (96%)	1818 (99%)	18 (1%)	4 (0%)	47	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	GLU
1	B	446	GLU
1	D	446	GLU
1	C	446	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/418 (94%)	391 (99%)	4 (1%)	76	80
1	B	398/418 (95%)	394 (99%)	4 (1%)	76	80
1	C	404/418 (97%)	395 (98%)	9 (2%)	52	53
1	D	403/418 (96%)	399 (99%)	4 (1%)	76	80
All	All	1600/1672 (96%)	1579 (99%)	21 (1%)	73	72

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	61[A]	THR
1	A	61[B]	THR
1	A	342	HIS
1	B	342	HIS
1	B	347[A]	GLU
1	B	347[B]	GLU
1	B	419	SER
1	C	56	LEU
1	C	61[A]	THR
1	C	61[B]	THR
1	C	216	ASP
1	C	238	LEU
1	C	275	SER
1	C	294	ASP
1	C	307	TYR
1	C	342	HIS
1	D	294	ASP
1	D	307	TYR
1	D	313	ASP
1	D	342	HIS

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	111	HIS
1	A	154	ASN
1	A	273	ASN
1	A	326	GLN
1	B	111	HIS
1	B	273	ASN
1	C	34	GLN
1	C	60	ASN
1	C	326	GLN
1	D	355	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z > 2$
3	BGQ	A	502	-	6,6,6	0.54	0	4,6,6	0.38	0
2	GOL	C	502	-	5,5,5	0.27	0	5,5,5	0.71	0
2	GOL	D	501	-	5,5,5	0.32	0	5,5,5	0.91	0
2	GOL	A	501	-	5,5,5	0.48	0	5,5,5	0.38	0
4	ORN	B	503	-	7,8,8	0.68	0	8,9,9	1.26	1 (12%)
2	GOL	C	501	-	5,5,5	0.29	0	5,5,5	0.36	0
4	ORN	A	503	-	7,8,8	0.82	0	8,9,9	1.12	1 (12%)
3	BGQ	B	502	-	6,6,6	0.53	0	4,6,6	0.39	0
2	GOL	B	501	-	5,5,5	0.32	0	5,5,5	0.41	0
2	GOL	D	502	-	5,5,5	0.34	0	5,5,5	0.84	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
3	BGQ	A	502	-	-	2/5/5/5	-
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	D	501	-	-	1/4/4/4	-
2	GOL	A	501	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ORN	B	503	-	-	5/8/8/8	-
2	GOL	C	501	-	-	0/4/4/4	-
4	ORN	A	503	-	-	5/8/8/8	-
3	BGQ	B	502	-	-	2/5/5/5	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	D	502	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	ORN	OXT-C-CA	2.32	121.29	113.38
4	A	503	ORN	CG-CB-CA	-2.15	106.42	113.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	BGQ	O1-C1-C2-C3
4	A	503	ORN	N-CA-CB-CG
4	A	503	ORN	C-CA-CB-CG
4	A	503	ORN	O-C-CA-N
4	B	503	ORN	N-CA-CB-CG
4	B	503	ORN	OXT-C-CA-N
4	A	503	ORN	OXT-C-CA-N
3	A	502	BGQ	O1-C1-C2-C3
2	C	502	GOL	O1-C1-C2-C3
3	A	502	BGQ	O1-C1-C2-O2
3	B	502	BGQ	O1-C1-C2-O2
2	C	502	GOL	O1-C1-C2-O2
4	B	503	ORN	O-C-CA-N
4	B	503	ORN	C-CA-CB-CG
2	D	501	GOL	O1-C1-C2-O2
2	B	501	GOL	C1-C2-C3-O3
4	A	503	ORN	CA-CB-CG-CD
4	B	503	ORN	CA-CB-CG-CD
2	B	501	GOL	O2-C2-C3-O3
2	A	501	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	BGQ	1	0
4	B	503	ORN	1	0
4	A	503	ORN	1	0
3	B	502	BGQ	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	A	450/479 (93%)	0.20	19 (4%) 36 35	19, 31, 52, 108	1 (0%)
1	B	450/479 (93%)	0.26	24 (5%) 26 26	20, 32, 53, 99	0
1	C	458/479 (95%)	0.79	59 (12%) 3 3	19, 37, 80, 126	0
1	D	460/479 (96%)	0.82	74 (16%) 1 1	18, 36, 85, 135	0
All	All	1818/1916 (94%)	0.52	176 (9%) 7 7	18, 34, 68, 135	1 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	307	TYR	7.3
1	D	219	LEU	7.1
1	C	305	GLU	6.2
1	C	289	LEU	5.4
1	D	90	VAL	5.2
1	D	457	HIS	5.0
1	D	458	HIS	4.9
1	D	324	PHE	4.8
1	C	302	PHE	4.8
1	C	318	PHE	4.8
1	D	323	PHE	4.7
1	D	310	ALA	4.7
1	C	217	GLY	4.6
1	B	113	LYS	4.5
1	D	304	LYS	4.5
1	D	456	HIS	4.4
1	C	324	PHE	4.3
1	D	216	ASP	4.2
1	D	303	TRP	4.2
1	C	216	ASP	4.1
1	C	311	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	227	PRO	4.0
1	D	4	LEU	3.9
1	D	299	ALA	3.8
1	C	90	VAL	3.8
1	C	323	PHE	3.8
1	C	4	LEU	3.7
1	A	111	HIS	3.6
1	C	194	ASP	3.6
1	C	223	LEU	3.6
1	D	311	ILE	3.6
1	C	316	VAL	3.5
1	D	282	PHE	3.5
1	C	294	ASP	3.5
1	C	218[A]	SER	3.5
1	C	320	PRO	3.5
1	C	224	GLN	3.3
1	A	186	VAL	3.3
1	D	455	ALA	3.3
1	D	223	LEU	3.3
1	C	307	TYR	3.3
1	A	107	LEU	3.3
1	D	221	ASP	3.2
1	D	295	THR	3.2
1	C	1	MET	3.2
1	B	137	LEU	3.1
1	D	313	ASP	3.1
1	B	90	VAL	3.1
1	D	305	GLU	3.1
1	B	304	LYS	3.1
1	C	215	PHE	3.1
1	D	259	ALA	3.1
1	C	263	THR	3.1
1	C	92	VAL	3.1
1	D	315	ARG	3.0
1	D	302	PHE	3.0
1	C	301	VAL	3.0
1	B	86	TYR	3.0
1	C	317	ALA	3.0
1	A	409	GLY	2.9
1	D	225	THR	2.9
1	A	6	PRO	2.9
1	C	456	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	3	THR	2.9
1	A	85	ASN	2.9
1	C	0	HIS	2.9
1	D	70	ALA	2.9
1	B	414	LEU	2.8
1	C	91	LEU	2.8
1	D	395	LEU	2.8
1	C	304	LYS	2.8
1	C	395	LEU	2.8
1	A	86	TYR	2.8
1	D	306	GLU	2.7
1	C	137	LEU	2.7
1	A	110	LYS	2.7
1	D	217	GLY	2.7
1	B	91	LEU	2.7
1	D	137	LEU	2.7
1	D	292	LEU	2.7
1	C	399	PHE	2.7
1	B	408	THR	2.7
1	B	110	LYS	2.7
1	C	400	GLY	2.7
1	D	391	ALA	2.7
1	D	175	THR	2.6
1	B	412	THR	2.6
1	D	392	PRO	2.6
1	A	88	MET	2.6
1	D	314	SER	2.6
1	D	296	ILE	2.6
1	D	294	ASP	2.6
1	A	412	THR	2.6
1	D	227	PRO	2.6
1	D	224	GLN	2.6
1	D	87	SER	2.5
1	C	313	ASP	2.5
1	C	392	PRO	2.5
1	C	202	ASN	2.5
1	D	291	ASP	2.5
1	B	112	PRO	2.5
1	D	91	LEU	2.5
1	D	349	CYS	2.5
1	B	120	LEU	2.5
1	A	408	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	109	ALA	2.5
1	D	318	PHE	2.5
1	C	69	CYS	2.4
1	C	349	CYS	2.4
1	C	408	THR	2.4
1	D	404	ALA	2.4
1	D	319	THR	2.4
1	D	279	ALA	2.4
1	C	406	THR	2.4
1	D	285	LEU	2.4
1	A	93	PRO	2.4
1	C	288	HIS	2.4
1	C	214	GLY	2.4
1	A	92	VAL	2.3
1	C	225	THR	2.3
1	C	291	ASP	2.3
1	C	358	SER	2.3
1	A	220	TYR	2.3
1	A	90	VAL	2.3
1	B	123	GLU	2.3
1	C	308	PRO	2.3
1	D	399	PHE	2.3
1	A	416	VAL	2.3
1	D	317	ALA	2.3
1	B	6	PRO	2.3
1	C	330	PRO	2.3
1	C	312	LYS	2.2
1	D	325	LYS	2.2
1	D	258	LEU	2.2
1	D	412	THR	2.2
1	C	110	LYS	2.2
1	B	84	LEU	2.2
1	D	176	GLY	2.2
1	D	308	PRO	2.2
1	D	88	MET	2.2
1	C	84	LEU	2.2
1	B	119	VAL	2.2
1	C	175	THR	2.2
1	C	348	ASP	2.2
1	B	87	SER	2.2
1	C	303	TRP	2.1
1	A	305	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	92	VAL	2.1
1	B	88	MET	2.1
1	D	312	LYS	2.1
1	A	301	VAL	2.1
1	D	67	GLY	2.1
1	D	358	SER	2.1
1	A	311	ILE	2.1
1	C	352	LEU	2.1
1	C	310	ALA	2.1
1	D	300	LYS	2.1
1	D	347	GLU	2.1
1	D	360	MET	2.1
1	C	195	PHE	2.1
1	D	435	ASP	2.1
1	B	122	LYS	2.1
1	D	278	ILE	2.1
1	D	1	MET	2.1
1	D	194	ASP	2.0
1	D	403	MET	2.0
1	C	68	ALA	2.0
1	D	191	VAL	2.0
1	D	195	PHE	2.0
1	D	193	PRO	2.0
1	B	56	LEU	2.0
1	D	409	GLY	2.0
1	B	93	PRO	2.0
1	B	111	HIS	2.0
1	C	306	GLU	2.0
1	B	186	VAL	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 monosaccharides 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(Å ²)	Q<0.9
3	BGQ	A	502	7/7	0.71	0.39	38,41,54,55	0
2	GOL	D	502	6/6	0.82	0.22	33,37,40,40	6
2	GOL	C	502	6/6	0.84	0.19	36,40,47,48	6
3	BGQ	B	502	7/7	0.84	0.42	27,41,49,53	7
5	NA	C	503	1/1	0.86	0.21	47,47,47,47	0
2	GOL	D	501	6/6	0.89	0.14	30,36,39,49	0
4	ORN	A	503	9/9	0.90	0.26	19,36,48,49	0
5	NA	D	504	1/1	0.90	0.12	59,59,59,59	0
4	ORN	B	503	9/9	0.91	0.21	29,39,52,56	0
2	GOL	A	501	6/6	0.93	0.12	28,33,35,37	0
5	NA	D	503	1/1	0.94	0.34	47,47,47,47	0
5	NA	C	504	1/1	0.94	0.12	53,53,53,53	0
2	GOL	C	501	6/6	0.95	0.14	34,37,41,47	0
2	GOL	B	501	6/6	0.95	0.09	27,39,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.