



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:39 AM UTC

PDB ID : 2QNE / pdb_00002qne
Title : Crystal structure of putative methyltransferase (ZP_00558420.1) from *Desulfitobacterium hafniense* Y51 at 2.30 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-07-18
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

<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	:	9.0.010 (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

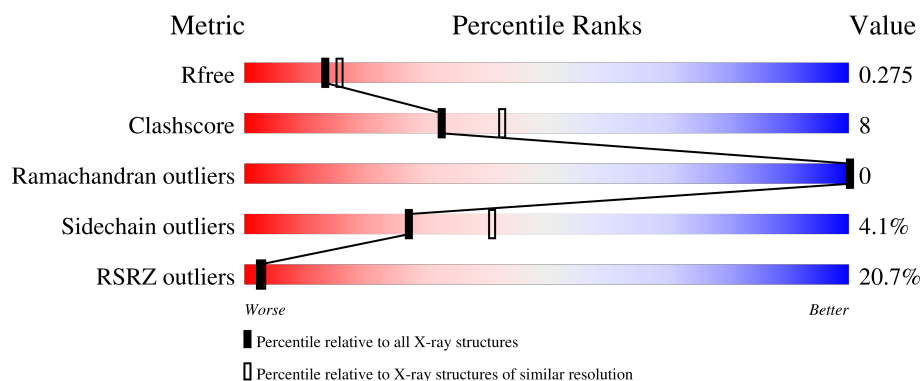
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	495	5% 82% 13% • •
1	B	495	33% 75% 19% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7406 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 Putative methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	Se	0	2	0
			3625	2302	600	701	2	20			
1	B	475	Total	C	N	O	S	Se	0	3	0
			3596	2279	598	697	2	20			

There are 38 discrepancies between the modelled and reference sequences:

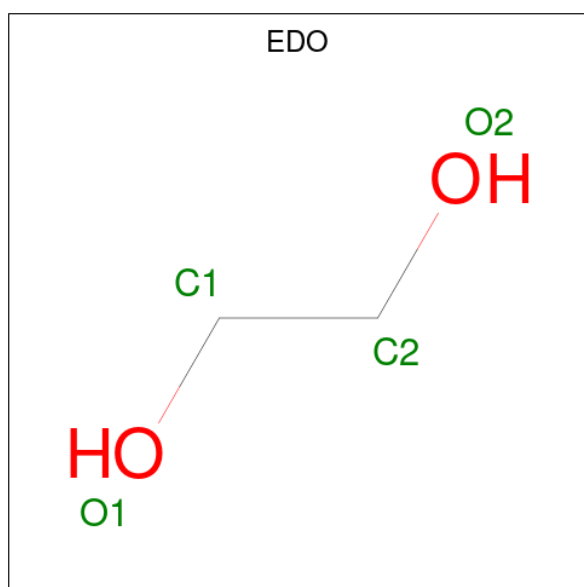
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	expression tag	UNP Q24SP7
A	-17	GLY	-	expression tag	UNP Q24SP7
A	-16	SER	-	expression tag	UNP Q24SP7
A	-15	ASP	-	expression tag	UNP Q24SP7
A	-14	LYS	-	expression tag	UNP Q24SP7
A	-13	ILE	-	expression tag	UNP Q24SP7
A	-12	HIS	-	expression tag	UNP Q24SP7
A	-11	HIS	-	expression tag	UNP Q24SP7
A	-10	HIS	-	expression tag	UNP Q24SP7
A	-9	HIS	-	expression tag	UNP Q24SP7
A	-8	HIS	-	expression tag	UNP Q24SP7
A	-7	HIS	-	expression tag	UNP Q24SP7
A	-6	GLU	-	expression tag	UNP Q24SP7
A	-5	ASN	-	expression tag	UNP Q24SP7
A	-4	LEU	-	expression tag	UNP Q24SP7
A	-3	TYR	-	expression tag	UNP Q24SP7
A	-2	PHE	-	expression tag	UNP Q24SP7
A	-1	GLN	-	expression tag	UNP Q24SP7
A	0	GLY	-	expression tag	UNP Q24SP7
B	-18	MSE	-	expression tag	UNP Q24SP7
B	-17	GLY	-	expression tag	UNP Q24SP7
B	-16	SER	-	expression tag	UNP Q24SP7
B	-15	ASP	-	expression tag	UNP Q24SP7
B	-14	LYS	-	expression tag	UNP Q24SP7
B	-13	ILE	-	expression tag	UNP Q24SP7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP Q24SP7
B	-11	HIS	-	expression tag	UNP Q24SP7
B	-10	HIS	-	expression tag	UNP Q24SP7
B	-9	HIS	-	expression tag	UNP Q24SP7
B	-8	HIS	-	expression tag	UNP Q24SP7
B	-7	HIS	-	expression tag	UNP Q24SP7
B	-6	GLU	-	expression tag	UNP Q24SP7
B	-5	ASN	-	expression tag	UNP Q24SP7
B	-4	LEU	-	expression tag	UNP Q24SP7
B	-3	TYR	-	expression tag	UNP Q24SP7
B	-2	PHE	-	expression tag	UNP Q24SP7
B	-1	GLN	-	expression tag	UNP Q24SP7
B	0	GLY	-	expression tag	UNP Q24SP7

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

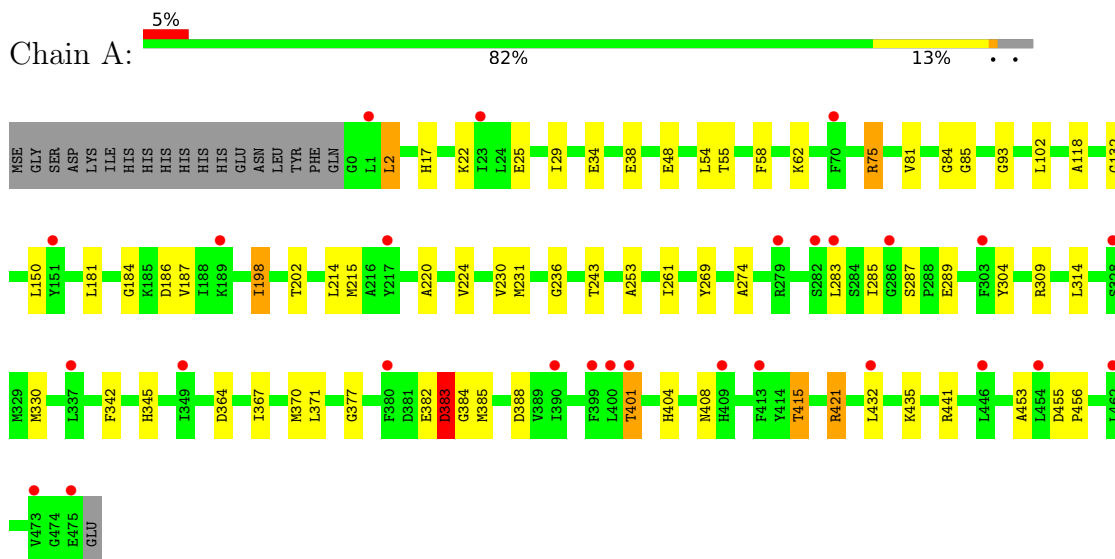
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	120	Total O 120 120	0	0
3	B	25	Total O 25 25	0	0

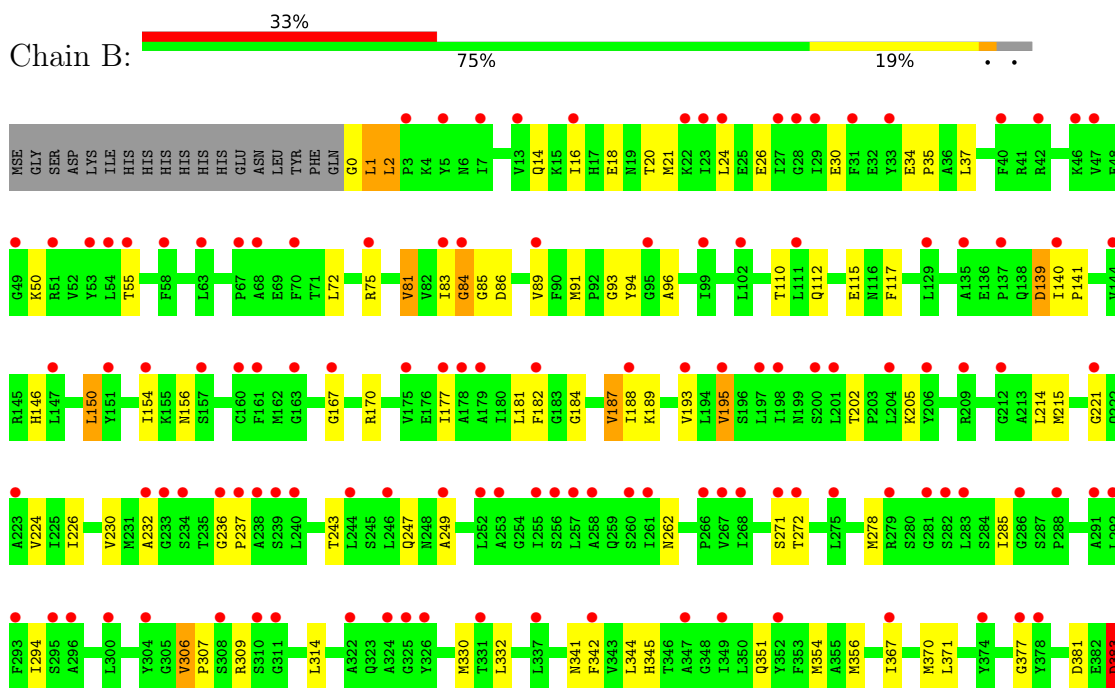
3 Residue-property plots [i](#)

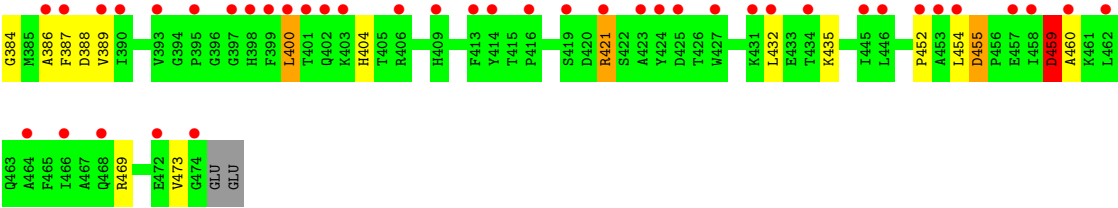
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative methyltransferase



- Molecule 1: Putative methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.86Å 123.86Å 122.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 2.30 29.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.75-2.30) 99.6 (29.75-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.158 , 0.204 0.258 , 0.275	Depositor DCC
R_{free} test set	1933 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7406	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: EDO

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	1.01	3/3676 (0.1%)	1.05	10/4939 (0.2%)
1	B	0.93	6/3648 (0.2%)	1.15	8/4908 (0.2%)
All	All	0.97	9/7324 (0.1%)	1.10	18/9847 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	LEU	C-O	14.22	1.42	1.24
1	B	112	GLN	CD-NE2	12.38	1.59	1.33
1	B	459	ASP	CG-OD2	10.49	1.45	1.25
1	B	459	ASP	CG-OD1	6.12	1.36	1.25
1	A	198	ILE	CA-CB	5.96	1.61	1.53
1	A	342	PHE	CA-C	5.34	1.58	1.52
1	A	118	ALA	CA-CB	5.26	1.61	1.53
1	B	460	ALA	C-O	5.21	1.30	1.24
1	B	170	ARG	C-O	5.19	1.30	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	GLN	OE1-CD-NE2	-36.54	86.06	122.60
1	B	112	GLN	CG-CD-NE2	22.09	149.54	116.40
1	B	383	ASP	N-CA-C	10.61	124.73	111.69
1	A	383	ASP	N-CA-C	8.81	123.76	112.92
1	B	86	ASP	N-CA-C	-7.50	104.10	113.18
1	B	167	GLY	N-CA-C	6.99	118.59	111.95
1	A	220	ALA	CA-C-N	-5.86	109.92	121.41
1	A	220	ALA	C-N-CA	-5.86	109.92	121.41
1	A	441	ARG	N-CA-C	5.69	117.16	111.07
1	A	84	GLY	CA-C-N	-5.63	110.37	121.41
1	A	84	GLY	C-N-CA	-5.63	110.37	121.41
1	A	220	ALA	O-C-N	-5.56	116.18	122.68
1	A	75	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	B	84	GLY	N-CA-C	5.44	126.08	113.18
1	A	415	THR	CB-CA-C	5.43	116.05	109.85
1	B	455	ASP	CA-C-N	5.40	126.59	119.84
1	B	455	ASP	C-N-CA	5.40	126.59	119.84
1	A	75	ARG	CB-CA-C	-5.34	102.26	110.81

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLY	Peptide
1	B	383	ASP	Peptide
1	B	459	ASP	Sidechain
1	B	55	THR	Mainchain
1	B	83	ILE	Peptide
1	B	85	GLY	Peptide

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	3625	0	3544	49	0
1	B	3596	0	3466	76	0
2	A	28	0	42	3	0
2	B	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	120	0	0	2	0
3	B	25	0	0	1	0
All	All	7406	0	7070	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (113) 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:454:LEU:HD23	1:B:459:ASP:HB3	1.49	0.93
1:A:330[A]:MSE:HE3	1:B:371:LEU:HD23	1.59	0.82
1:A:370:MSE:HE2	1:B:330[A]:MSE:SE	2.30	0.81
1:A:330[B]:MSE:SE	1:B:370:MSE:HE2	2.32	0.80
1:B:454:LEU:CD2	1:B:459:ASP:HB3	2.14	0.77
1:B:84:GLY:HA2	1:B:341:ASN:ND2	2.03	0.73
1:A:330[A]:MSE:HE3	1:B:371:LEU:CD2	2.19	0.72
1:A:421:ARG:HD2	3:B:497:HOH:O	1.88	0.72
3:A:568:HOH:O	1:B:421:ARG:HD2	1.89	0.72
1:B:75:ARG:NH1	1:B:154:ILE:O	2.22	0.71
1:A:214:LEU:HD23	1:A:214:LEU:C	2.17	0.69
1:A:385:MSE:HE1	1:B:16:ILE:HD13	1.75	0.69
1:B:214:LEU:C	1:B:214:LEU:HD23	2.20	0.67
1:A:330[A]:MSE:CE	1:B:371:LEU:HD23	2.27	0.65
1:B:0:GLY:O	1:B:1:LEU:HD22	1.98	0.63
1:B:35:PRO:CB	1:B:215:MSE:HE1	2.29	0.63
1:B:146:HIS:O	1:B:150:LEU:HD22	1.98	0.63
1:A:383:ASP:N	1:A:384:GLY:HA3	2.13	0.63
1:B:232:ALA:HA	1:B:243:THR:HG21	1.82	0.62
1:B:81:VAL:HG13	1:B:89:VAL:HG11	1.82	0.62
1:A:330[B]:MSE:HE1	1:B:370:MSE:CE	2.29	0.62
1:B:224:VAL:HG23	1:B:226:ILE:HD11	1.81	0.62
1:A:184:GLY:O	1:A:187:VAL:HG12	2.02	0.60
1:B:14:GLN:O	1:B:18:GLU:HG2	2.02	0.59
1:B:20:THR:HG22	1:B:21:MSE:HE2	1.86	0.58
1:B:84:GLY:HA2	1:B:341:ASN:CG	2.28	0.58
1:B:383:ASP:O	1:B:404:HIS:NE2	2.31	0.58
1:A:75:ARG:HD3	3:A:583:HOH:O	2.04	0.58
1:A:93:GLY:HA2	1:A:345:HIS:HA	1.85	0.58
1:A:371:LEU:HD23	1:B:330[B]:MSE:HE3	1.85	0.58
1:B:306:VAL:HG22	1:B:307:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:CD2	1:B:177:ILE:HD13	2.35	0.57
1:A:214:LEU:HD23	1:A:214:LEU:O	2.05	0.57
1:B:81:VAL:CG1	1:B:89:VAL:HG11	2.35	0.57
1:B:93:GLY:HA2	1:B:345:HIS:HA	1.88	0.56
1:B:454:LEU:O	1:B:455:ASP:C	2.48	0.56
1:B:224:VAL:HG23	1:B:226:ILE:CD1	2.36	0.56
1:A:2:LEU:HD13	1:A:377:GLY:HA3	1.88	0.55
1:B:35:PRO:HB3	1:B:215:MSE:HE1	1.89	0.55
1:A:330[B]:MSE:CE	1:B:370:MSE:CE	2.85	0.55
1:A:17:HIS:HD2	1:A:304:TYR:OH	1.90	0.54
1:B:224:VAL:CG2	1:B:226:ILE:HD11	2.38	0.53
1:B:94:TYR:HB2	1:B:344:LEU:HD11	1.91	0.52
1:A:75:ARG:HG2	1:A:181:LEU:HD11	1.91	0.52
1:A:230:VAL:CG1	1:A:243:THR:HG23	2.40	0.51
1:B:237:PRO:O	1:B:243:THR:HG23	2.10	0.51
1:B:110:THR:HB	1:B:139:ASP:OD2	2.10	0.51
1:B:214:LEU:HD23	1:B:214:LEU:O	2.10	0.51
1:B:184:GLY:O	1:B:187:VAL:CG1	2.60	0.50
1:B:72:LEU:HD13	1:B:195:VAL:HG22	1.93	0.50
1:A:198:ILE:HD13	1:A:224:VAL:HB	1.93	0.50
1:B:34:GLU:HB3	1:B:35:PRO:HD3	1.93	0.50
1:A:231:MSE:HG2	1:A:283:LEU:HD13	1.93	0.50
1:A:75:ARG:NH2	1:A:453:ALA:O	2.45	0.49
1:A:309:ARG:HH22	2:A:478:EDO:H21	1.77	0.49
1:A:22:LYS:HG2	1:B:387:PHE:CE1	2.47	0.48
1:B:72:LEU:CD1	1:B:195:VAL:HG22	2.43	0.48
1:B:351:GLN:O	1:B:354:MSE:HB2	2.13	0.48
1:B:2:LEU:HD13	1:B:377:GLY:HA3	1.95	0.48
1:A:330[A]:MSE:SE	1:B:370:MSE:HE2	2.64	0.48
1:A:102:LEU:CD1	1:A:435:LYS:HG3	2.44	0.48
1:B:140:ILE:HG23	1:B:141:PRO:HD2	1.94	0.48
1:B:75:ARG:NH2	1:B:452:PRO:HB2	2.29	0.47
1:A:102:LEU:HD11	1:A:435:LYS:HG2	1.95	0.47
1:B:91:MSE:HE1	1:B:342:PHE:CZ	2.49	0.47
1:B:294:ILE:HG12	2:B:479:EDO:H21	1.96	0.47
1:B:226:ILE:HD12	1:B:226:ILE:N	2.29	0.47
1:B:214:LEU:C	1:B:214:LEU:CD2	2.87	0.46
1:B:182:PHE:CD1	1:B:193:VAL:HG21	2.49	0.46
1:A:214:LEU:C	1:A:214:LEU:CD2	2.87	0.46
1:A:230:VAL:CG1	1:A:236:GLY:HA3	2.46	0.46
1:A:102:LEU:CD1	1:A:435:LYS:CG	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLY:HA2	2:A:477:EDO:H22	1.98	0.46
1:B:30:GLU:HB2	1:B:205:LYS:HG2	1.97	0.46
1:B:332:LEU:HD23	1:B:367:ILE:HG13	1.98	0.45
1:A:274:ALA:HB3	1:A:283:LEU:HD11	1.99	0.45
1:B:262:ASN:OD1	1:B:262:ASN:C	2.59	0.45
1:B:381:ASP:O	1:B:384:GLY:HA3	2.17	0.45
1:B:96:ALA:HB3	1:B:356:MSE:HG2	2.00	0.44
1:A:382:GLU:C	1:A:384:GLY:HA3	2.42	0.44
1:B:202:THR:HG21	1:B:230:VAL:HG22	1.99	0.44
1:B:37:LEU:HD11	1:B:50:LYS:HA	1.98	0.44
1:A:364:ASP:HA	1:A:367:ILE:HG12	2.00	0.44
1:B:72:LEU:HD13	1:B:195:VAL:CG2	2.48	0.44
1:B:187:VAL:HG13	1:B:188:ILE:HG23	2.00	0.44
1:B:2:LEU:HD13	1:B:377:GLY:CA	2.48	0.43
1:A:285:ILE:HD12	1:A:314:LEU:HB3	1.99	0.43
1:B:189:LYS:HA	1:B:221:GLY:HA3	1.99	0.43
1:A:401:THR:O	1:A:401:THR:HG23	2.18	0.43
1:B:232:ALA:CA	1:B:243:THR:HG21	2.48	0.43
1:A:287:SER:HB2	1:A:289:GLU:OE1	2.19	0.43
1:B:230:VAL:CG1	1:B:236:GLY:HA3	2.49	0.43
1:A:370:MSE:CE	1:B:330[A]:MSE:HE1	2.49	0.43
1:A:455:ASP:HA	1:A:456:PRO:HD3	1.91	0.43
1:B:115:GLU:HG3	1:B:156:ASN:ND2	2.35	0.42
1:A:202:THR:HG21	1:A:230:VAL:HG22	2.00	0.42
2:A:479:EDO:H12	1:B:400:LEU:HD12	2.02	0.42
1:B:35:PRO:HB2	1:B:215:MSE:HE1	2.02	0.42
1:B:469:ARG:HH12	1:B:473:VAL:HG23	1.85	0.42
1:B:306:VAL:HG22	1:B:307:PRO:CD	2.47	0.41
1:A:54:LEU:HD22	1:A:58:PHE:CE2	2.55	0.41
1:A:29:ILE:HD12	1:A:253:ALA:CB	2.50	0.41
1:A:269:TYR:CD1	1:A:269:TYR:C	2.98	0.41
1:B:386:ALA:HB1	1:B:389:VAL:CG1	2.50	0.41
1:A:34:GLU:O	1:A:38[B]:GLU:HG3	2.21	0.41
1:B:24:LEU:HD21	1:B:249:ALA:O	2.20	0.41
1:B:285:ILE:HD12	1:B:314:LEU:HD22	2.03	0.41
1:A:215:MSE:HG2	1:A:261:ILE:CD1	2.51	0.41
1:A:25:GLU:HG2	1:A:55:THR:HA	2.03	0.40
1:B:247:GLN:NE2	1:B:271:SER:OG	2.54	0.40
1:A:102:LEU:HD12	1:A:435:LYS:HG3	2.04	0.40
1:A:383:ASP:O	1:A:404:HIS:NE2	2.53	0.40
1:B:117:PHE:CE1	1:B:356:MSE:HE3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/495 (96%)	463 (97%)	13 (3%)	0	100	100
1	B	476/495 (96%)	459 (96%)	17 (4%)	0	100	100
All	All	952/990 (96%)	922 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	372/385 (97%)	359 (96%)	13 (4%)	32	48
1	B	364/385 (94%)	347 (95%)	17 (5%)	23	35
All	All	736/770 (96%)	706 (96%)	30 (4%)	27	41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	48	GLU
1	A	62	LYS
1	A	81	VAL
1	A	150	LEU

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Mol	Chain	Res	Type
1	A	186	ASP
1	A	383	ASP
1	A	388	ASP
1	A	401	THR
1	A	408	ASN
1	A	415	THR
1	A	421	ARG
1	A	432	LEU
1	B	1	LEU
1	B	2	LEU
1	B	26	GLU
1	B	81	VAL
1	B	139	ASP
1	B	150	LEU
1	B	187	VAL
1	B	195	VAL
1	B	272	THR
1	B	278	MSE
1	B	306	VAL
1	B	309	ARG
1	B	388	ASP
1	B	400	LEU
1	B	421	ARG
1	B	432	LEU
1	B	435	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	148	GLN
1	A	156	ASN
1	A	247	GLN
1	B	17	HIS
1	B	45	GLN
1	B	79	ASN
1	B	138	GLN
1	B	156	ASN
1	B	247	GLN
1	B	248	ASN
1	B	341	ASN
1	B	443	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](#)

10 ligands are 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	$\# Z > 2$
2	EDO	A	478	-	3,3,3	1.05	0	2,2,2	0.18	0
2	EDO	A	481	-	3,3,3	0.95	0	2,2,2	0.68	0
2	EDO	A	480	-	3,3,3	0.28	0	2,2,2	0.82	0
2	EDO	A	482	-	3,3,3	0.55	0	2,2,2	0.12	0
2	EDO	A	483	-	3,3,3	0.50	0	2,2,2	0.40	0
2	EDO	B	477	-	3,3,3	0.56	0	2,2,2	0.14	0
2	EDO	B	479	-	3,3,3	0.47	0	2,2,2	0.41	0
2	EDO	B	478	-	3,3,3	0.64	0	2,2,2	0.35	0
2	EDO	A	479	-	3,3,3	0.51	0	2,2,2	0.24	0
2	EDO	A	477	-	3,3,3	0.79	0	2,2,2	0.91	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
2	EDO	A	478	-	-	1/1/1/1	-
2	EDO	A	481	-	-	1/1/1/1	-
2	EDO	A	480	-	-	1/1/1/1	-
2	EDO	A	482	-	-	1/1/1/1	-
2	EDO	A	483	-	-	1/1/1/1	-
2	EDO	B	477	-	-	0/1/1/1	-
2	EDO	B	479	-	-	0/1/1/1	-
2	EDO	B	478	-	-	1/1/1/1	-
2	EDO	A	479	-	-	1/1/1/1	-
2	EDO	A	477	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	483	EDO	O1-C1-C2-O2
2	A	478	EDO	O1-C1-C2-O2
2	A	481	EDO	O1-C1-C2-O2
2	B	478	EDO	O1-C1-C2-O2
2	A	482	EDO	O1-C1-C2-O2
2	A	479	EDO	O1-C1-C2-O2
2	A	480	EDO	O1-C1-C2-O2
2	A	477	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	478	EDO	1	0
2	B	479	EDO	1	0
2	A	479	EDO	1	0
2	A	477	EDO	1	0

5.7 Other polymers [i](#)

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	457/495 (92%)	0.89	27 (5%)	28 30	26, 57, 69, 91	1 (0%)
1	B	456/495 (92%)	1.69	162 (35%)	1 1	24, 57, 68, 89	2 (0%)
All	All	913/990 (92%)	1.29	189 (20%)	2 3	24, 57, 68, 91	3 (0%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	ILE	4.7
1	B	233	GLY	4.4
1	B	464	ALA	4.3
1	B	195	VAL	4.2
1	B	63	LEU	4.0
1	B	279	ARG	4.0
1	B	178	ALA	3.9
1	B	390	ILE	3.9
1	B	255	ILE	3.7
1	B	95	GLY	3.7
1	B	400	LEU	3.7
1	B	386	ALA	3.6
1	B	31	PHE	3.6
1	B	427	TRP	3.6
1	B	293	PHE	3.6
1	B	387	PHE	3.6
1	B	240	LEU	3.5
1	B	238	ALA	3.5
1	B	261	ILE	3.5
1	B	275	LEU	3.5
1	B	292	LEU	3.5
1	B	137	PRO	3.4
1	B	16	ILE	3.4
1	B	249	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	423	ALA	3.3
1	B	236	GLY	3.3
1	B	40	PHE	3.3
1	B	102	LEU	3.2
1	B	188	ILE	3.2
1	B	175	VAL	3.2
1	B	401	THR	3.2
1	B	434	THR	3.2
1	B	212	GLY	3.2
1	B	326	TYR	3.1
1	B	452	PRO	3.1
1	B	154	ILE	3.1
1	B	260	SER	3.1
1	B	288	PRO	3.1
1	B	425	ASP	3.1
1	B	13	VAL	3.1
1	B	89	VAL	3.0
1	B	389	VAL	3.0
1	B	446	LEU	3.0
1	B	58	PHE	3.0
1	B	253	ALA	3.0
1	B	54	LEU	3.0
1	B	5	TYR	3.0
1	B	454	LEU	3.0
1	B	416	PRO	3.0
1	B	258	ALA	2.9
1	B	397	GLY	2.9
1	B	395	PRO	2.9
1	A	337	LEU	2.9
1	B	337	LEU	2.9
1	B	421	ARG	2.9
1	A	23	ILE	2.9
1	B	99	ILE	2.9
1	B	424	TYR	2.9
1	B	399	PHE	2.9
1	B	378	TYR	2.8
1	B	160	CYS	2.8
1	B	322	ALA	2.8
1	B	198	ILE	2.8
1	B	84	GLY	2.8
1	B	310	SER	2.8
1	B	177	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	234	SER	2.8
1	B	398	HIS	2.7
1	A	286	GLY	2.7
1	A	400	LEU	2.7
1	B	147	LEU	2.7
1	B	462	LEU	2.7
1	B	135	ALA	2.7
1	B	161	PHE	2.7
1	B	271	SER	2.7
1	B	460	ALA	2.7
1	B	221	GLY	2.7
1	B	458	ILE	2.7
1	B	244	LEU	2.7
1	A	473	VAL	2.7
1	B	239	SER	2.7
1	B	409	HIS	2.6
1	B	431	LYS	2.6
1	B	163	GLY	2.6
1	B	377	GLY	2.6
1	B	347	ALA	2.6
1	B	413	PHE	2.6
1	B	445	ILE	2.6
1	A	409	HIS	2.6
1	B	432	LEU	2.6
1	A	390	ILE	2.6
1	B	7	ILE	2.6
1	A	189	LYS	2.5
1	B	151	TYR	2.5
1	B	51[A]	ARG	2.5
1	B	204	LEU	2.5
1	B	29	ILE	2.5
1	B	304	TYR	2.5
1	B	266	PRO	2.5
1	B	325	GLY	2.5
1	B	272	THR	2.5
1	B	268	ILE	2.5
1	A	217	TYR	2.5
1	B	252	LEU	2.5
1	B	257	LEU	2.5
1	B	28	GLY	2.5
1	B	457	GLU	2.4
1	B	352	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	223	ALA	2.4
1	B	291	ALA	2.4
1	B	331	THR	2.4
1	B	200	SER	2.4
1	B	182	PHE	2.4
1	B	367	ILE	2.4
1	B	201	LEU	2.4
1	B	33	TYR	2.4
1	B	206	TYR	2.4
1	B	453	ALA	2.4
1	A	70	PHE	2.4
1	A	380	PHE	2.4
1	B	111	LEU	2.4
1	A	151	TYR	2.3
1	B	179	ALA	2.3
1	B	83	ILE	2.3
1	B	140	ILE	2.3
1	B	193	VAL	2.3
1	B	374	TYR	2.3
1	B	49	GLY	2.3
1	B	296	ALA	2.3
1	A	328	SER	2.3
1	B	157	SER	2.3
1	B	419	SER	2.3
1	B	42	ARG	2.3
1	B	246	LEU	2.3
1	A	279	ARG	2.3
1	B	402	GLN	2.3
1	A	349	ILE	2.3
1	B	237	PRO	2.3
1	B	53	TYR	2.3
1	B	129	LEU	2.2
1	B	300	LEU	2.2
1	B	67	PRO	2.2
1	B	403	LYS	2.2
1	A	283	LEU	2.2
1	B	295	SER	2.2
1	A	399	PHE	2.2
1	B	311	GLY	2.2
1	B	468	GLN	2.2
1	B	324	ALA	2.2
1	A	462	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	47	VAL	2.2
1	B	342	PHE	2.2
1	B	474	GLY	2.2
1	B	256	SER	2.2
1	A	432	LEU	2.1
1	A	446	LEU	2.1
1	A	413	PHE	2.1
1	B	167	GLY	2.1
1	B	209	ARG	2.1
1	A	454	LEU	2.1
1	B	24	LEU	2.1
1	B	46	LYS	2.1
1	A	475	GLU	2.1
1	B	267	VAL	2.1
1	B	393	VAL	2.1
1	B	70	PHE	2.1
1	A	401	THR	2.1
1	B	75	ARG	2.1
1	B	3	PRO	2.1
1	A	303	PHE	2.1
1	A	1	LEU	2.1
1	B	197	LEU	2.1
1	B	283	LEU	2.1
1	B	27	ILE	2.1
1	B	144	VAL	2.1
1	B	281	GLY	2.1
1	B	286	GLY	2.1
1	A	282	SER	2.0
1	B	55	THR	2.0
1	B	68	ALA	2.0
1	B	232	ALA	2.0
1	B	23	ILE	2.0
1	B	414	TYR	2.0
1	B	282	SER	2.0
1	B	308	SER	2.0
1	B	472	GLU	2.0
1	B	349	ILE	2.0
1	B	406	ARG	2.0
1	B	22	LYS	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
2	EDO	B	478	4/4	0.61	0.17	76,77,79,84	0
2	EDO	B	479	4/4	0.69	0.27	63,65,65,68	0
2	EDO	A	482	4/4	0.78	0.17	70,72,73,82	0
2	EDO	B	477	4/4	0.78	0.16	65,65,73,81	0
2	EDO	A	480	4/4	0.80	0.15	72,76,77,81	0
2	EDO	A	483	4/4	0.83	0.15	55,71,74,75	0
2	EDO	A	477	4/4	0.83	0.26	56,58,63,68	0
2	EDO	A	478	4/4	0.84	0.15	38,46,48,57	0
2	EDO	A	479	4/4	0.89	0.16	60,69,71,72	0
2	EDO	A	481	4/4	0.92	0.23	44,53,59,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.