



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:45 AM UTC

PDB ID : 6XUP / pdb_00006xup
Title : Archaeoglobus fulgidus Argonaute protein with DNA oligoduplex 5'-pATCGTGGCCACGAT
Authors : Grazulis, S.; Zaremba, M.
Deposited on : 2020-01-20
Resolution : 1.90 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

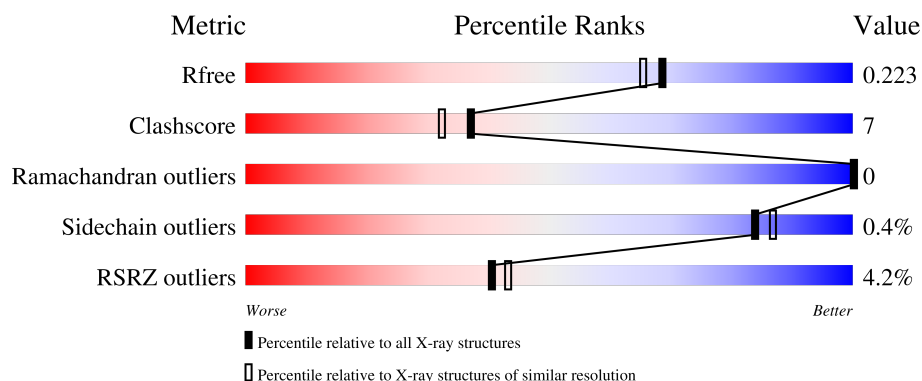
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	441	3% 80% 11% 9%
1	B	441	5% 77% 14% 9%
2	P	14	14% 29% 57%
2	Q	14	29% 21% 50%
2	R	14	50% 50%

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Mol	Chain	Length	Quality of chain
2	S	14	

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
5	BME	A	504	-	-	X	-
6	GOL	A	513	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7669 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 Piwi protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	7	0
			3315	2139	551	615	10			
1	B	401	Total	C	N	O	S	0	6	0
			3304	2134	548	612	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A101DYYI0
A	-12	GLY	-	expression tag	UNP A0A101DYYI0
A	-11	SER	-	expression tag	UNP A0A101DYYI0
A	-10	SER	-	expression tag	UNP A0A101DYYI0
A	-9	HIS	-	expression tag	UNP A0A101DYYI0
A	-8	HIS	-	expression tag	UNP A0A101DYYI0
A	-7	HIS	-	expression tag	UNP A0A101DYYI0
A	-6	HIS	-	expression tag	UNP A0A101DYYI0
A	-5	HIS	-	expression tag	UNP A0A101DYYI0
A	-4	HIS	-	expression tag	UNP A0A101DYYI0
A	-3	SER	-	expression tag	UNP A0A101DYYI0
A	-2	GLN	-	expression tag	UNP A0A101DYYI0
A	-1	ASP	-	expression tag	UNP A0A101DYYI0
A	0	PRO	-	expression tag	UNP A0A101DYYI0
B	-13	MET	-	initiating methionine	UNP A0A101DYYI0
B	-12	GLY	-	expression tag	UNP A0A101DYYI0
B	-11	SER	-	expression tag	UNP A0A101DYYI0
B	-10	SER	-	expression tag	UNP A0A101DYYI0
B	-9	HIS	-	expression tag	UNP A0A101DYYI0
B	-8	HIS	-	expression tag	UNP A0A101DYYI0
B	-7	HIS	-	expression tag	UNP A0A101DYYI0
B	-6	HIS	-	expression tag	UNP A0A101DYYI0
B	-5	HIS	-	expression tag	UNP A0A101DYYI0
B	-4	HIS	-	expression tag	UNP A0A101DYYI0
B	-3	SER	-	expression tag	UNP A0A101DYYI0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP A0A101DYI0
B	-1	ASP	-	expression tag	UNP A0A101DYI0
B	0	PRO	-	expression tag	UNP A0A101DYI0

- Molecule 2 is a DNA chain called 5'-D(*AP*TP*CP*GP*TP*GP*GP*CP*CP*AP*CP*GP*AP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	7	Total 147	C 69	N 27	O 44	P 7	0	0	0
2	S	5	Total 103	C 49	N 20	O 29	P 5	0	0	0
2	P	6	Total 125	C 59	N 22	O 38	P 6	0	0	0
2	Q	7	Total 141	C 67	N 26	O 41	P 7	0	0	0

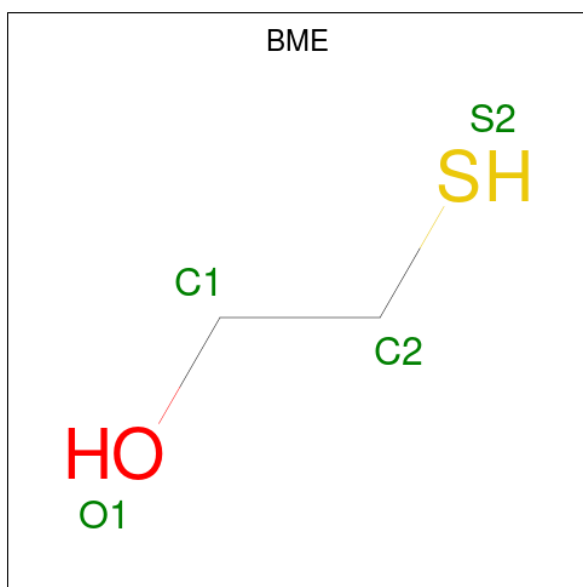
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

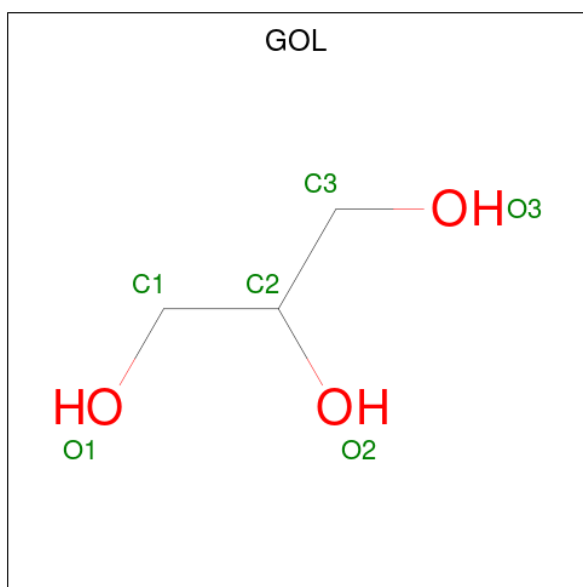
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



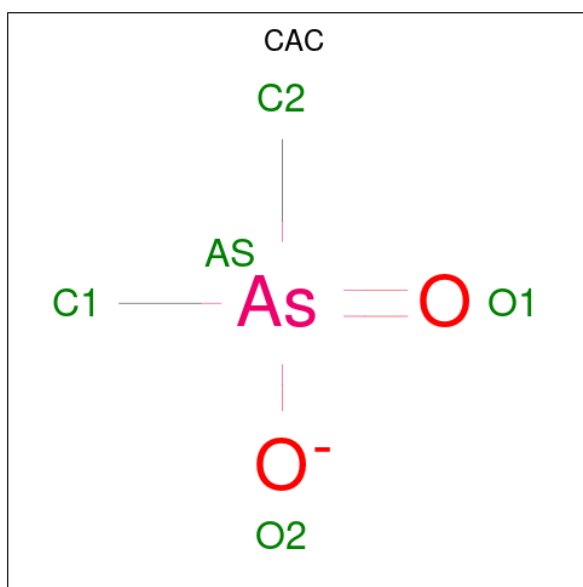
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		
7	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	K	0	0
			1	1		

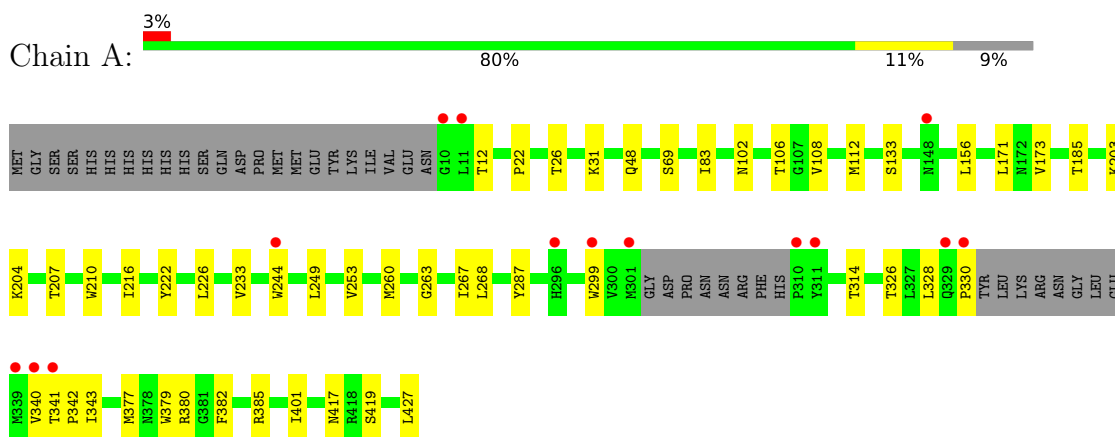
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	263	Total	O	0	0
			263	263		
9	R	7	Total	O	0	0
			7	7		
9	S	4	Total	O	0	0
			4	4		
9	B	167	Total	O	0	0
			167	167		
9	P	5	Total	O	0	0
			5	5		
9	Q	3	Total	O	0	0
			3	3		

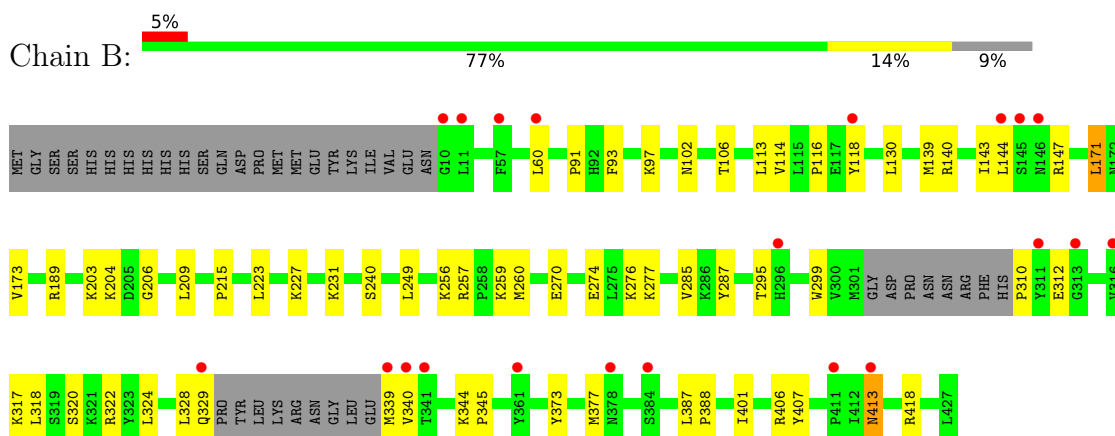
3 Residue-property plots [i](#)

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: Piwi protein



- Molecule 1: Piwi protein

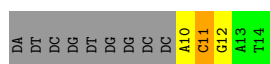


- Molecule 2: 5'-D(*AP*TP*CP*GP*TP*GP*GP*CP*CP*AP*CP*GP*AP*TP)-3'



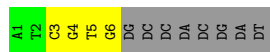
- Molecule 2: 5'-D(*AP*TP*CP*GP*TP*GP*GP*CP*CP*AP*CP*GP*AP*TP)-3'

Chain S:  14% 14% 7% 64%



- Molecule 2: 5'-D(*AP*TP*CP*GP*TP*GP*GP*CP*CP*AP*CP*GP*AP*TP)-3'

Chain P:  14% 29% 57%



- Molecule 2: 5'-D(*AP*TP*CP*GP*TP*GP*GP*CP*CP*AP*CP*GP*AP*TP)-3'

Chain Q:  29% 21% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.80Å 60.87Å 101.72Å 76.56° 75.59° 79.39°	Depositor
Resolution (Å)	40.72 – 1.90 40.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.6 (40.72-1.90) 91.6 (40.72-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.181 , 0.224 0.179 , 0.223	Depositor DCC
R_{free} test set	8400 reflections (9.19%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7669	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: K, BME, CAC, MG, CL, GOL

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	0.48	0/3396	0.63	1/4609 (0.0%)
1	B	0.35	0/3385	0.53	1/4593 (0.0%)
2	P	0.53	0/139	0.64	0/211
2	Q	0.41	0/157	0.61	0/239
2	R	0.48	0/164	0.59	0/250
2	S	0.43	0/115	0.73	1/175 (0.6%)
All	All	0.42	0/7356	0.59	3/10077 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	PRO	N-CA-CB	6.66	110.33	103.00
1	A	330	PRO	N-CA-CB	6.61	110.28	103.00
2	S	11	DC	C4'-C3'-O3'	5.26	117.89	110.00

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	3315	0	3317	36	0
1	B	3304	0	3306	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	125	0	69	10	0
2	Q	141	0	79	7	0
2	R	147	0	80	0	0
2	S	103	0	57	6	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	24	0	36	7	0
5	B	4	0	6	0	0
6	A	30	0	40	7	0
6	B	12	0	15	2	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	1	0	0	0	0
9	A	263	0	0	2	0
9	B	167	0	0	1	0
9	P	5	0	0	0	0
9	Q	3	0	0	0	0
9	R	7	0	0	0	0
9	S	4	0	0	0	0
All	All	7669	0	7005	101	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 7.

All (101) 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)
2:S:10:DA:H2''	2:S:11:DC:O5'	1.41	1.19
2:S:10:DA:H2'	2:S:11:DC:H5''	1.18	1.12
2:S:10:DA:C2'	2:S:11:DC:H5''	1.82	1.07
2:P:5:DT:H2''	2:P:6:DG:C5'	1.88	1.04
2:S:10:DA:C2'	2:S:11:DC:C5'	2.38	1.02
2:P:6:DG:N2	2:Q:10:DA:C2	2.32	0.97
1:A:207[A]:THR:HA	5:A:504:BME:H21	1.47	0.94
2:S:10:DA:H2''	2:S:11:DC:C5'	1.99	0.89
2:P:6:DG:C2	2:Q:10:DA:C2	2.60	0.89
1:A:207[B]:THR:HA	5:A:504:BME:H21	1.53	0.88
2:P:5:DT:H2''	2:P:6:DG:H5'	1.51	0.88
2:P:5:DT:H2''	2:P:6:DG:H5''	1.57	0.86
2:Q:10:DA:H1'	2:Q:11:DC:H5'	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASN:HD21	6:A:513:GOL:C3	2.00	0.74
2:P:5:DT:C2'	2:P:6:DG:H5''	2.17	0.74
1:B:317:LYS:HZ1	1:B:320:SER:HA	1.54	0.71
1:B:413:ASN:N	1:B:413:ASN:OD1	2.23	0.69
1:A:207[A]:THR:HG21	9:A:716:HOH:O	1.92	0.68
1:B:206:GLY:HA3	1:B:377:MET:HG3	1.75	0.67
1:B:339:MET:HG3	1:B:340:VAL:HG12	1.76	0.67
1:B:317:LYS:NZ	1:B:320:SER:HA	2.10	0.66
1:B:60:LEU:HD21	1:B:144:LEU:HG	1.79	0.64
1:B:203:LYS:HG3	1:B:209:LEU:HD11	1.81	0.63
1:B:227:LYS:HG3	1:B:231:LYS:HE2	1.80	0.63
1:B:140:ARG:NH1	1:B:143:ILE:HD11	2.14	0.62
1:B:274:GLU:HA	1:B:277:LYS:HE3	1.82	0.62
1:A:48:GLN:HG2	1:A:108:VAL:HG12	1.81	0.61
1:A:419:SER:CB	6:A:513:GOL:H2	2.31	0.60
1:A:133:SER:O	6:A:513:GOL:H12	2.01	0.60
1:B:189:ARG:HD2	1:B:256:LYS:HG2	1.84	0.59
1:A:171:LEU:HG	1:A:377:MET:HE3	1.84	0.59
1:B:140:ARG:HD3	1:B:143:ILE:HD12	1.84	0.58
1:B:171:LEU:HD11	1:B:373:TYR:O	2.02	0.58
1:A:299:TRP:HB3	1:A:340:VAL:HG13	1.85	0.58
1:B:102:ASN:O	1:B:106:THR:HG23	2.03	0.58
2:P:6:DG:C2	2:Q:10:DA:N1	2.70	0.58
1:A:173:VAL:HG21	1:A:204:LYS:HG3	1.87	0.57
1:B:312:GLU:HG2	1:B:328:LEU:HD13	1.87	0.57
1:B:171:LEU:HD13	1:B:373:TYR:HB3	1.86	0.57
1:B:118:TYR:HB2	1:B:140:ARG:NH2	2.20	0.56
1:B:401:ILE:HD12	6:B:503:GOL:H11	1.87	0.56
2:S:11:DC:H2''	2:S:12:DG:C8	2.40	0.56
1:B:324:LEU:HD11	1:B:345:PRO:HB2	1.89	0.54
2:P:6:DG:N2	2:Q:10:DA:N3	2.55	0.53
1:A:222:TYR:HD2	1:A:260:MET:HE3	1.75	0.52
1:A:328:LEU:HD23	1:A:343:ILE:HD13	1.92	0.52
1:A:401:ILE:HG23	5:A:509:BME:H22	1.92	0.52
1:B:140:ARG:CZ	1:B:143:ILE:HD11	2.40	0.51
1:B:227:LYS:CG	1:B:231:LYS:HE2	2.41	0.51
1:B:60:LEU:HD21	1:B:144:LEU:CD2	2.40	0.51
1:A:419:SER:OG	6:A:513:GOL:H2	2.11	0.50
1:B:204:LYS:NZ	9:B:604:HOH:O	2.32	0.50
1:A:380:ARG:HG2	1:A:427:LEU:HD22	1.94	0.50
1:A:203:LYS:HG3	1:A:244:TRP:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:TRP:CZ3	5:A:504:BME:H22	2.47	0.49
1:A:379:TRP:CH2	5:A:504:BME:H22	2.48	0.49
1:B:240:SER:OG	1:B:418:ARG:NH2	2.40	0.49
1:B:189:ARG:HH11	1:B:189:ARG:HG2	1.78	0.49
1:B:270:GLU:O	1:B:274:GLU:HG3	2.13	0.48
2:P:3:DC:H2''	2:P:4:DG:O5'	2.13	0.48
1:A:385:ARG:O	1:A:385:ARG:HG3	2.15	0.47
1:A:417:ASN:HD21	6:A:513:GOL:H32	1.78	0.47
1:B:257:ARG:O	1:B:259:LYS:HD2	2.15	0.47
5:A:509:BME:H21	9:A:653:HOH:O	2.15	0.47
1:B:60:LEU:HD21	1:B:144:LEU:CG	2.45	0.47
1:B:91:PRO:HB3	1:B:116:PRO:HG2	1.97	0.47
1:A:112:MET:CE	1:A:156:LEU:HD21	2.45	0.46
1:A:226:LEU:HD21	1:A:268:LEU:HD21	1.96	0.46
1:B:173:VAL:HG21	1:B:204:LYS:HG3	1.98	0.46
1:B:299:TRP:HB3	1:B:340:VAL:HG23	1.97	0.46
1:B:329:GLN:CD	1:B:344:LYS:HE3	2.41	0.46
1:A:12:THR:HG22	1:A:22:PRO:HA	1.97	0.45
1:A:69:SER:OG	1:A:83:ILE:HD12	2.16	0.45
1:A:203:LYS:HG3	1:A:244:TRP:CZ2	2.52	0.45
1:B:276:LYS:HD3	1:B:285:VAL:HG12	1.99	0.45
1:B:171:LEU:HD12	1:B:377:MET:HG2	1.99	0.45
1:B:223:LEU:HD11	1:B:260:MET:HE2	1.99	0.45
1:B:93:PHE:CE2	1:B:97:LYS:HD2	2.52	0.45
1:A:314:THR:HB	1:A:326:THR:OG1	2.17	0.44
1:A:419:SER:HB3	6:A:513:GOL:H2	1.97	0.44
1:A:102:ASN:O	1:A:106:THR:HG23	2.18	0.44
2:P:6:DG:N1	2:Q:10:DA:N1	2.65	0.44
1:B:329:GLN:NE2	1:B:344:LYS:HB3	2.33	0.44
1:A:249:LEU:O	1:A:287:TYR:HA	2.17	0.43
1:B:113:LEU:HD12	1:B:130:LEU:HD11	2.00	0.43
1:A:210:TRP:HD1	1:A:233:VAL:HG23	1.84	0.43
1:B:249:LEU:O	1:B:287:TYR:HA	2.19	0.43
1:B:215:PRO:HA	6:B:503:GOL:H31	2.00	0.43
1:A:263:GLY:O	1:A:267:ILE:HG12	2.19	0.42
1:A:341:THR:HA	1:A:342:PRO:HD3	1.91	0.42
1:A:377:MET:CG	5:A:504:BME:H11	2.49	0.42
1:B:406:ARG:HD3	1:B:407:TYR:CZ	2.55	0.42
1:A:216:ILE:HB	6:A:511:GOL:H11	2.02	0.42
1:B:318:LEU:HD12	1:B:322:ARG:HG2	2.02	0.41
1:B:387:LEU:HD12	1:B:388:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG22	1:B:139:MET:HE3	2.03	0.41
1:A:185:THR:O	1:A:253:VAL:HA	2.21	0.41
1:B:147:ARG:HD2	2:Q:13:DA:H61	1.86	0.41
1:B:223:LEU:HD11	1:B:260:MET:CE	2.50	0.40
1:B:295:THR:OG1	1:B:345:PRO:HG2	2.21	0.40
1:A:26:THR:HG23	1:A:382:PHE:HB3	2.02	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	403/441 (91%)	390 (97%)	13 (3%)	0	100	100
1	B	401/441 (91%)	385 (96%)	16 (4%)	0	100	100
All	All	804/882 (91%)	775 (96%)	29 (4%)	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	377/407 (93%)	376 (100%)	1 (0%)	86	88
1	B	375/407 (92%)	373 (100%)	2 (0%)	81	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	752/814 (92%)	749 (100%)	3 (0%)	84	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	B	171	LEU
1	B	413	ASN

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	47	ASN
1	A	278	GLN
1	B	148	ASN
1	B	392	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 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	BME	A	508	-	3,3,3	0.50	0	2,2,2	0.78	0
6	GOL	A	512	-	5,5,5	0.46	0	5,5,5	1.40	1 (20%)
7	CAC	A	515	-	2,4,4	2.62	2 (100%)	4,6,6	1.66	1 (25%)
6	GOL	A	510	-	5,5,5	1.00	0	5,5,5	0.94	0
6	GOL	B	504	-	5,5,5	1.76	3 (60%)	5,5,5	0.74	0
7	CAC	B	505	-	2,4,4	2.64	2 (100%)	4,6,6	1.61	1 (25%)
5	BME	B	502	-	3,3,3	0.32	0	2,2,2	0.26	0
5	BME	A	507	-	3,3,3	0.32	0	2,2,2	0.25	0
5	BME	A	506	-	3,3,3	0.35	0	2,2,2	0.28	0
5	BME	A	505	-	3,3,3	0.38	0	2,2,2	0.46	0
6	GOL	A	511	-	5,5,5	0.34	0	5,5,5	0.62	0
6	GOL	B	503	-	5,5,5	1.00	0	5,5,5	1.20	1 (20%)
6	GOL	A	514	-	5,5,5	1.22	0	5,5,5	0.92	0
5	BME	A	504	-	3,3,3	0.45	0	2,2,2	0.47	0
5	BME	A	509	-	3,3,3	0.26	0	2,2,2	0.66	0
6	GOL	A	513	-	5,5,5	0.26	0	5,5,5	0.32	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	BME	A	508	-	-	1/1/1/1	-
6	GOL	A	512	-	-	2/4/4/4	-
6	GOL	A	510	-	-	0/4/4/4	-
6	GOL	B	504	-	-	2/4/4/4	-
5	BME	B	502	-	-	1/1/1/1	-
5	BME	A	507	-	-	1/1/1/1	-
5	BME	A	506	-	-	1/1/1/1	-
5	BME	A	505	-	-	0/1/1/1	-
6	GOL	A	511	-	-	2/4/4/4	-
6	GOL	B	503	-	-	2/4/4/4	-
6	GOL	A	514	-	-	0/4/4/4	-
5	BME	A	504	-	-	1/1/1/1	-
5	BME	A	509	-	-	1/1/1/1	-
6	GOL	A	513	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	515	CAC	AS-C1	2.91	1.97	1.90
7	B	505	CAC	AS-C1	2.64	1.96	1.90
7	B	505	CAC	AS-C2	2.64	1.96	1.90
6	B	504	GOL	O2-C2	-2.46	1.36	1.43
7	A	515	CAC	AS-C2	2.30	1.95	1.90
6	B	504	GOL	C1-C2	2.26	1.60	1.51
6	B	504	GOL	C3-C2	2.05	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	515	CAC	O1-AS-C1	-2.76	108.06	111.50
7	B	505	CAC	O1-AS-C2	-2.38	108.55	111.50
6	B	503	GOL	C3-C2-C1	-2.29	103.38	111.80
6	A	512	GOL	C3-C2-C1	-2.29	103.41	111.80

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	509	BME	O1-C1-C2-S2
5	B	502	BME	O1-C1-C2-S2
6	A	512	GOL	O1-C1-C2-C3
6	B	503	GOL	O2-C2-C3-O3
6	B	504	GOL	C1-C2-C3-O3
6	A	511	GOL	O1-C1-C2-C3
6	B	503	GOL	C1-C2-C3-O3
6	A	512	GOL	O1-C1-C2-O2
6	B	504	GOL	O2-C2-C3-O3
5	A	504	BME	O1-C1-C2-S2
5	A	506	BME	O1-C1-C2-S2
5	A	508	BME	O1-C1-C2-S2
6	A	511	GOL	O1-C1-C2-O2
5	A	507	BME	O1-C1-C2-S2

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	511	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	503	GOL	2	0
5	A	504	BME	5	0
5	A	509	BME	2	0
6	A	513	GOL	6	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 ⓘ

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	402/441 (91%)	0.05	14 (3%)	47	50	15, 38, 63, 95	7 (1%)
1	B	401/441 (90%)	0.39	21 (5%)	33	35	17, 47, 75, 107	6 (1%)
2	P	6/14 (42%)	0.18	0	100	100	51, 61, 88, 100	0
2	Q	7/14 (50%)	0.82	0	100	100	67, 90, 122, 123	0
2	R	7/14 (50%)	0.58	0	100	100	38, 55, 111, 120	0
2	S	5/14 (35%)	0.25	0	100	100	46, 55, 95, 106	0
All	All	828/938 (88%)	0.23	35 (4%)	40	43	15, 43, 75, 123	13 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361[A]	TYR	5.8
1	B	340	VAL	3.7
1	A	11	LEU	3.4
1	B	341	THR	3.2
1	A	330	PRO	3.2
1	B	339	MET	3.1
1	A	10	GLY	3.1
1	A	311	TYR	3.0
1	A	310	PRO	3.0
1	A	296[A]	HIS	2.7
1	A	340	VAL	2.7
1	A	244	TRP	2.7
1	B	311	TYR	2.5
1	B	144	LEU	2.5
1	B	10	GLY	2.4
1	B	378	ASN	2.4
1	B	329	GLN	2.4
1	B	296[A]	HIS	2.4
1	A	339	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	146	ASN	2.3
1	B	11	LEU	2.2
1	B	313	GLY	2.2
1	A	301	MET	2.2
1	B	60	LEU	2.2
1	A	329	GLN	2.1
1	B	413	ASN	2.1
1	A	299	TRP	2.1
1	B	384	SER	2.1
1	B	57	PHE	2.1
1	B	118	TYR	2.1
1	B	145	SER	2.0
1	B	316	VAL	2.0
1	A	341	THR	2.0
1	A	148[A]	ASN	2.0
1	B	411	PRO	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(Å ²)	Q<0.9
5	BME	A	505	4/4	0.77	0.16	53,59,68,86	0
5	BME	A	506	4/4	0.77	0.17	70,70,72,82	0
5	BME	A	508	4/4	0.79	0.17	54,57,57,87	0
7	CAC	A	515	5/5	0.79	0.16	62,82,100,159	0
6	GOL	A	513	6/6	0.82	0.14	51,54,57,60	0
6	GOL	A	512	6/6	0.82	0.15	56,57,64,65	0
6	GOL	B	504	6/6	0.83	0.20	47,53,68,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	511	6/6	0.83	0.11	48,60,63,70	0
7	CAC	B	505	5/5	0.83	0.12	51,63,106,174	0
6	GOL	A	514	6/6	0.85	0.12	55,75,82,85	0
6	GOL	A	510	6/6	0.86	0.13	58,61,67,70	0
8	K	A	516	1/1	0.88	0.26	77,77,77,77	0
6	GOL	B	503	6/6	0.89	0.11	53,59,64,71	0
5	BME	A	504	4/4	0.91	0.20	33,40,54,55	0
5	BME	A	507	4/4	0.92	0.14	56,64,67,86	0
5	BME	A	509	4/4	0.92	0.09	35,41,51,67	0
5	BME	B	502	4/4	0.93	0.09	50,59,61,83	0
4	CL	A	503	1/1	0.95	0.08	48,48,48,48	0
3	MG	A	502	1/1	0.95	0.12	59,59,59,59	0
3	MG	B	501	1/1	0.98	0.05	39,39,39,39	0
3	MG	A	501	1/1	0.99	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.