



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:40 PM UTC

PDB ID : 1OK6 / pdb_00001ok6
Title : Orthorhombic crystal form of an Archaeal fructose 1,6-bisphosphate aldolase
Authors : Lorentzen, E.; Zwart, P.; Stark, A.; Hensel, R.; Siebers, B.; Pohl, E.
Deposited on : 2003-07-18
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	:	9.0.010 (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

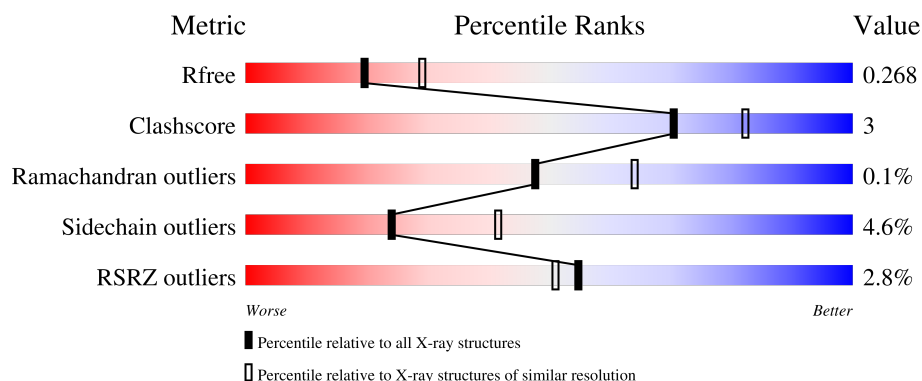
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	263	3% 86% 10% .
1	B	263	2% 86% 9% ..
1	C	263	4% 84% 10% ..
1	D	263	3% 85% 9% ..
1	E	263	87% 8% ..

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Mol	Chain	Length	Quality of chain
1	F	263	2% 84% 9%
1	G	263	2% 86% 8%
1	H	263	5% 84% 11%
1	I	263	3% 83% 11%
1	J	263	2% 89% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20126 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 FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1937	1246	329	357	5			
1	B	252	Total	C	N	O	S	0	0	0
			1927	1241	327	354	5			
1	C	252	Total	C	N	O	S	0	0	0
			1916	1237	322	352	5			
1	D	252	Total	C	N	O	S	0	0	0
			1913	1234	324	350	5			
1	E	252	Total	C	N	O	S	0	0	0
			1931	1244	328	354	5			
1	F	252	Total	C	N	O	S	0	0	0
			1921	1239	325	352	5			
1	G	252	Total	C	N	O	S	0	0	0
			1914	1235	324	350	5			
1	H	252	Total	C	N	O	S	0	0	0
			1921	1238	324	354	5			
1	I	252	Total	C	N	O	S	0	0	0
			1911	1231	325	350	5			
1	J	252	Total	C	N	O	S	0	0	0
			1913	1234	324	350	5			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

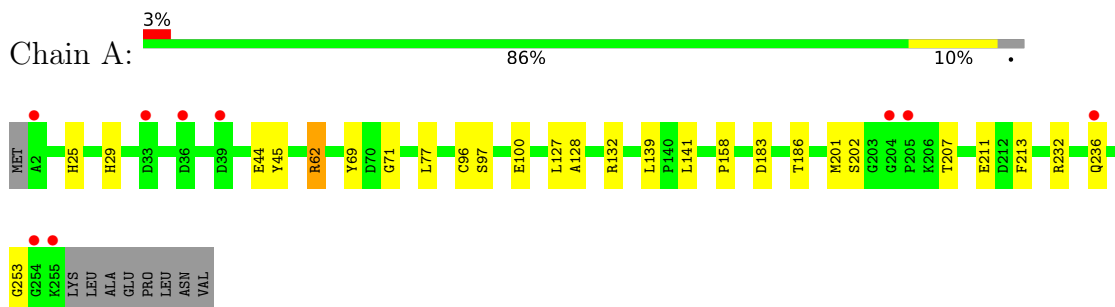
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	80	Total	O	0	0
			80	80		
3	C	89	Total	O	0	0
			89	89		
3	D	91	Total	O	0	0
			91	91		
3	E	84	Total	O	0	0
			84	84		
3	F	100	Total	O	0	0
			100	100		
3	G	84	Total	O	0	0
			84	84		
3	H	89	Total	O	0	0
			89	89		
3	I	101	Total	O	0	0
			101	101		
3	J	86	Total	O	0	0
			86	86		

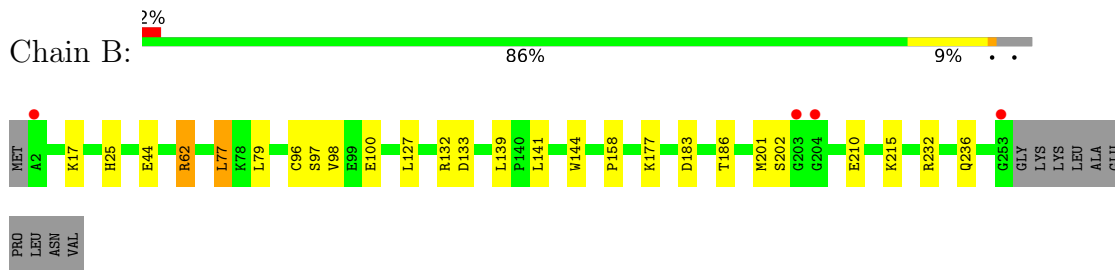
3 Residue-property plots

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.

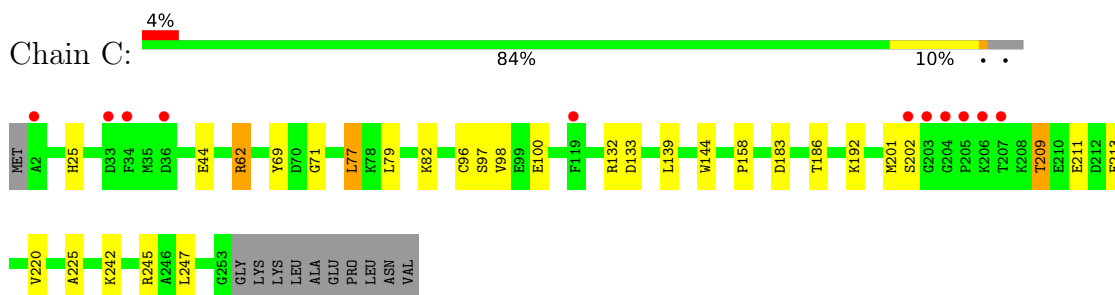
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



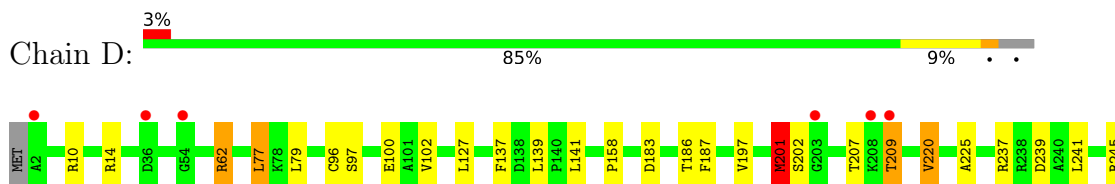
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

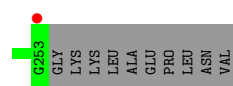


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

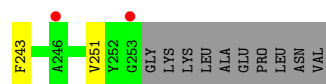
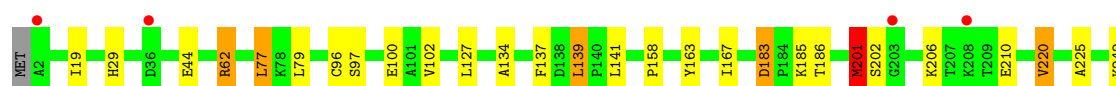
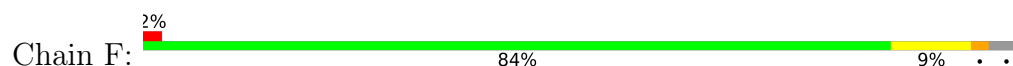




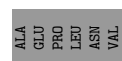
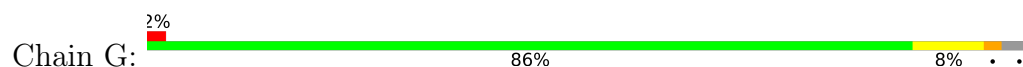
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



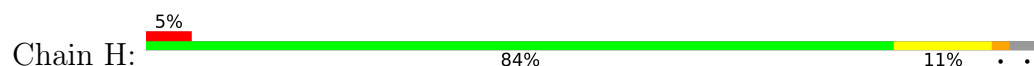
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



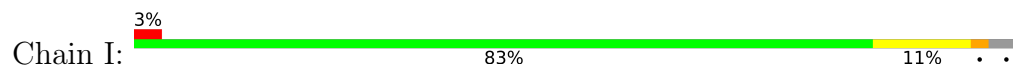
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

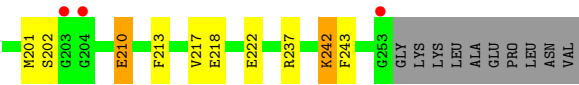


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

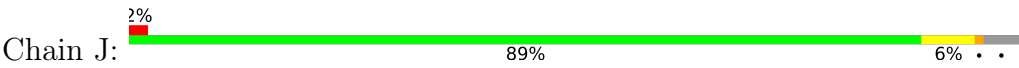


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I





● Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.90Å 176.50Å 185.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.00-2.40) 94.1 (20.00-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.263 0.243 , 0.268	Depositor DCC
R_{free} test set	2725 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.796	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20126	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.24 % 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 1.5671e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.78	0/1980	1.01	3/2685 (0.1%)
1	B	0.67	0/1970	0.95	3/2672 (0.1%)
1	C	0.71	0/1959	0.96	4/2658 (0.2%)
1	D	0.77	1/1956 (0.1%)	0.97	1/2655 (0.0%)
1	E	0.68	0/1974	0.93	1/2676 (0.0%)
1	F	0.80	1/1964 (0.1%)	0.98	0/2664
1	G	0.70	1/1957 (0.1%)	0.93	0/2656
1	H	0.73	3/1964 (0.2%)	0.98	3/2665 (0.1%)
1	I	0.76	0/1954	1.00	4/2654 (0.2%)
1	J	0.70	1/1956 (0.1%)	0.91	1/2655 (0.0%)
All	All	0.73	7/19634 (0.0%)	0.96	20/26640 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	201	MET	SD-CE	6.93	1.96	1.79
1	G	201	MET	SD-CE	5.68	1.93	1.79
1	H	15	ARG	CD-NE	-5.67	1.38	1.46
1	H	245	ARG	C-O	5.60	1.31	1.24
1	D	201	MET	SD-CE	5.58	1.93	1.79
1	H	201	MET	SD-CE	5.47	1.93	1.79
1	J	201	MET	SD-CE	5.15	1.92	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ARG	NE-CZ-NH2	9.36	127.62	119.20
1	A	132	ARG	NE-CZ-NH2	9.00	127.30	119.20
1	B	132	ARG	NE-CZ-NH2	8.98	127.28	119.20
1	I	132	ARG	NE-CZ-NH2	8.72	127.05	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ARG	NE-CZ-NH1	-8.38	113.11	121.50
1	H	15	ARG	NE-CZ-NH2	-8.36	111.67	119.20
1	A	132	ARG	NE-CZ-NH1	-8.32	113.18	121.50
1	C	132	ARG	NE-CZ-NH1	-8.30	113.20	121.50
1	I	132	ARG	NE-CZ-NH1	-8.13	113.37	121.50
1	I	132	ARG	CD-NE-CZ	6.67	133.75	124.40
1	C	132	ARG	CD-NE-CZ	6.57	133.60	124.40
1	A	132	ARG	CD-NE-CZ	6.44	133.41	124.40
1	H	15	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	B	132	ARG	CD-NE-CZ	6.34	133.28	124.40
1	I	197	VAL	N-CA-C	5.92	113.74	107.76
1	D	197	VAL	N-CA-C	5.41	113.22	107.76
1	H	15	ARG	CG-CD-NE	5.20	123.45	112.00
1	J	197	VAL	N-CA-C	5.17	112.98	107.76
1	E	197	VAL	N-CA-C	5.10	112.91	107.76
1	C	144	TRP	N-CA-C	-5.01	101.59	109.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1937	0	1925	12	0
1	B	1927	0	1920	14	0
1	C	1916	0	1907	13	0
1	D	1913	0	1901	16	0
1	E	1931	0	1931	12	0
1	F	1921	0	1916	15	0
1	G	1914	0	1903	11	0
1	H	1921	0	1909	13	0
1	I	1911	0	1890	17	0
1	J	1913	0	1901	8	0
2	A	6	0	8	0	0
3	A	112	0	0	4	0
3	B	80	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	89	0	0	4	0
3	D	91	0	0	4	0
3	E	84	0	0	1	0
3	F	100	0	0	3	0
3	G	84	0	0	2	0
3	H	89	0	0	1	0
3	I	101	0	0	2	0
3	J	86	0	0	2	0
All	All	20126	0	19111	130	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 3.

All (130) 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)
3:G:2070:HOH:O	1:H:62:ARG:HD2	1.48	1.12
1:F:62:ARG:HD2	3:F:2028:HOH:O	1.59	1.01
1:D:62:ARG:HD2	3:D:2026:HOH:O	1.61	0.99
1:H:96:CYS:SG	1:H:97:SER:N	2.34	0.96
1:B:96:CYS:SG	1:B:97:SER:N	2.33	0.94
1:I:96:CYS:SG	1:I:97:SER:N	2.32	0.93
1:D:96:CYS:SG	1:D:97:SER:N	2.38	0.92
1:E:96:CYS:SG	1:E:97:SER:N	2.37	0.91
1:F:96:CYS:SG	1:F:97:SER:N	2.38	0.89
1:J:96:CYS:SG	1:J:97:SER:N	2.41	0.88
1:C:96:CYS:SG	1:C:97:SER:N	2.39	0.87
1:A:96:CYS:SG	1:A:97:SER:N	2.38	0.87
3:A:2088:HOH:O	1:E:62:ARG:HD2	1.73	0.86
1:G:96:CYS:SG	1:G:97:SER:N	2.45	0.82
1:G:25:HIS:HB3	3:G:2008:HOH:O	1.86	0.75
3:F:2074:HOH:O	1:G:62:ARG:HD2	1.87	0.73
1:A:62:ARG:HD2	3:B:2066:HOH:O	1.89	0.71
1:F:62:ARG:NH2	1:F:100:GLU:OE2	2.23	0.71
1:D:14:ARG:HD3	3:D:2011:HOH:O	1.91	0.71
1:I:62:ARG:NH2	1:I:100:GLU:OE2	2.25	0.69
1:B:62:ARG:NH2	1:B:100:GLU:OE2	2.26	0.69
1:E:62:ARG:NH2	1:E:100:GLU:OE2	2.26	0.68
1:A:62:ARG:NH2	1:A:100:GLU:OE2	2.27	0.67
1:D:62:ARG:NH2	1:D:100:GLU:OE2	2.27	0.66
1:H:62:ARG:NH2	1:H:100:GLU:OE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HD2	3:C:2070:HOH:O	1.94	0.66
1:G:62:ARG:NH2	1:G:100:GLU:OE2	2.29	0.66
1:C:62:ARG:NH2	1:C:100:GLU:OE2	2.28	0.65
1:J:62:ARG:NH2	1:J:100:GLU:OE2	2.29	0.65
1:A:29:HIS:NE2	3:A:2022:HOH:O	2.30	0.63
1:C:213:PHE:HE2	1:C:247:LEU:HD11	1.65	0.62
1:I:25:HIS:HB3	3:I:2020:HOH:O	2.01	0.60
1:C:158:PRO:HB3	1:C:186:THR:HB	1.85	0.59
1:I:158:PRO:HB3	1:I:186:THR:HB	1.85	0.58
1:A:158:PRO:HB3	1:A:186:THR:HB	1.86	0.58
1:B:96:CYS:HG	1:B:97:SER:N	2.03	0.56
1:G:158:PRO:HB3	1:G:186:THR:HB	1.87	0.56
1:B:158:PRO:HB3	1:B:186:THR:HB	1.87	0.56
1:J:158:PRO:HB3	1:J:186:THR:HB	1.87	0.56
1:H:232:ARG:HG2	1:H:236:GLN:OE1	2.05	0.56
1:D:158:PRO:HB3	1:D:186:THR:HB	1.88	0.55
1:B:96:CYS:HG	1:B:97:SER:H	1.49	0.55
1:E:158:PRO:HB3	1:E:186:THR:HB	1.89	0.54
1:H:158:PRO:HB3	1:H:186:THR:HB	1.89	0.54
1:F:158:PRO:HB3	1:F:186:THR:HB	1.89	0.54
1:B:25:HIS:HB2	3:B:2017:HOH:O	2.08	0.53
1:C:25:HIS:H	1:C:25:HIS:CD2	2.27	0.53
1:D:245:ARG:NH2	3:D:2089:HOH:O	2.43	0.52
1:B:127:LEU:HD11	1:B:141:LEU:HD21	1.92	0.51
1:F:183:ASP:OD2	1:F:185:LYS:HB2	2.10	0.51
1:I:210:GLU:HB3	1:I:243:PHE:CE1	2.45	0.51
1:A:45:TYR:HB2	3:A:2032:HOH:O	2.11	0.51
1:I:242:LYS:HG2	3:I:2099:HOH:O	2.11	0.50
1:A:25:HIS:HB3	3:A:2026:HOH:O	2.11	0.50
1:A:232:ARG:HG2	1:A:236:GLN:OE1	2.12	0.50
1:I:213:PHE:O	1:I:217:VAL:HG23	2.12	0.50
1:F:201:MET:HB2	1:F:220:VAL:HG21	1.93	0.50
1:D:127:LEU:HD11	1:D:141:LEU:HD21	1.94	0.49
1:I:218:GLU:O	1:I:222:GLU:HG3	2.11	0.49
1:H:82:LYS:NZ	3:H:2032:HOH:O	2.14	0.49
1:H:213:PHE:O	1:H:216:GLN:HB2	2.13	0.49
1:F:210:GLU:HG2	1:F:243:PHE:CE1	2.48	0.49
1:G:241:LEU:HD21	1:G:245:ARG:NH2	2.28	0.48
1:F:29:HIS:NE2	3:F:2021:HOH:O	2.35	0.48
1:J:148:ARG:NH1	3:J:2061:HOH:O	2.40	0.48
1:D:241:LEU:HD21	1:D:245:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:LEU:HD11	1:H:141:LEU:HD21	1.95	0.47
1:F:220:VAL:HG13	1:F:225:ALA:HB3	1.97	0.47
1:G:77:LEU:HD12	1:G:79:LEU:HD23	1.97	0.47
1:F:127:LEU:HD11	1:F:141:LEU:HD21	1.96	0.47
1:D:237:ARG:HB3	1:D:239:ASP:OD1	2.14	0.47
1:C:211:GLU:HB2	3:C:2082:HOH:O	2.15	0.47
1:A:127:LEU:HD11	1:A:141:LEU:HD21	1.98	0.46
1:B:17:LYS:NZ	3:B:2012:HOH:O	2.45	0.46
1:B:232:ARG:HG2	1:B:236:GLN:OE1	2.15	0.46
1:D:62:ARG:O	1:D:62:ARG:HG2	2.12	0.45
1:J:77:LEU:HD12	1:J:79:LEU:HD23	1.98	0.45
1:J:127:LEU:HD11	1:J:141:LEU:HD21	1.99	0.45
1:E:163:TYR:CD2	1:E:167:ILE:HD11	2.52	0.45
1:H:19:ILE:HD11	1:H:251:VAL:HB	1.98	0.45
1:J:62:ARG:O	1:J:62:ARG:HG2	2.16	0.45
1:D:220:VAL:HG13	1:D:225:ALA:HB3	1.98	0.45
1:J:25:HIS:HB3	3:J:2015:HOH:O	2.17	0.44
1:I:77:LEU:HD12	1:I:79:LEU:HD23	1.98	0.44
1:C:77:LEU:HD12	1:C:79:LEU:HD23	1.98	0.44
1:I:144:TRP:HE1	1:I:177:LYS:NZ	2.14	0.44
1:G:127:LEU:HD11	1:G:141:LEU:HD21	2.00	0.44
1:B:77:LEU:HD12	1:B:79:LEU:HD23	1.99	0.43
1:E:77:LEU:HD12	1:E:79:LEU:HD23	1.99	0.43
1:C:98:VAL:HB	1:C:133:ASP:HB3	2.00	0.43
1:D:187:PHE:CE2	1:D:220:VAL:HG22	2.54	0.43
1:G:98:VAL:HB	1:G:133:ASP:HB3	2.01	0.43
1:D:102:VAL:HG21	1:D:137:PHE:HB3	2.01	0.43
1:F:102:VAL:HG21	1:F:137:PHE:HB3	2.01	0.43
1:E:62:ARG:O	1:E:62:ARG:HG2	2.16	0.43
1:E:89:GLU:HG3	1:E:118:GLY:HA3	2.00	0.42
1:E:98:VAL:HB	1:E:133:ASP:HB3	2.01	0.42
1:G:102:VAL:HG21	1:G:137:PHE:HB3	2.01	0.42
1:E:127:LEU:HD11	1:E:141:LEU:HD21	2.00	0.42
1:D:77:LEU:HD12	1:D:79:LEU:HD23	2.01	0.42
1:G:220:VAL:HG13	1:G:225:ALA:HB3	2.00	0.42
1:I:210:GLU:OE2	1:I:237:ARG:HD3	2.20	0.42
1:I:127:LEU:HD11	1:I:141:LEU:HD21	2.02	0.42
1:B:98:VAL:HB	1:B:133:ASP:HB3	2.01	0.42
1:E:25:HIS:HB3	3:E:2017:HOH:O	2.18	0.42
1:F:77:LEU:HD12	1:F:79:LEU:HD23	2.02	0.42
1:A:69:TYR:CZ	1:A:71:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TRP:HE1	1:B:177:LYS:NZ	2.18	0.42
1:C:82:LYS:NZ	3:C:2031:HOH:O	2.36	0.41
1:C:220:VAL:HG13	1:C:225:ALA:HB3	2.02	0.41
1:F:19:ILE:HD11	1:F:251:VAL:HB	2.02	0.41
1:I:163:TYR:CD2	1:I:167:ILE:HD11	2.55	0.41
1:A:128:ALA:HB2	1:E:95:ASN:HA	2.03	0.41
1:D:10:ARG:HD2	3:D:2006:HOH:O	2.20	0.41
1:B:144:TRP:NE1	1:B:177:LYS:NZ	2.68	0.41
1:C:213:PHE:CE2	1:C:247:LEU:HD11	2.50	0.41
1:D:201:MET:HB2	1:D:220:VAL:HG21	2.02	0.41
1:I:144:TRP:NE1	1:I:177:LYS:NZ	2.67	0.41
1:F:134:ALA:HB1	1:F:139:LEU:O	2.20	0.41
1:A:207:THR:OG1	1:A:213:PHE:HB2	2.21	0.41
1:H:163:TYR:CD2	1:H:167:ILE:HD11	2.56	0.41
1:I:102:VAL:HG21	1:I:137:PHE:HB3	2.03	0.41
1:C:69:TYR:CZ	1:C:71:GLY:HA2	2.56	0.41
1:C:209:THR:HB	3:C:2082:HOH:O	2.21	0.40
1:H:25:HIS:CE1	1:H:33:ASP:HB2	2.56	0.40
1:I:134:ALA:HB1	1:I:139:LEU:O	2.21	0.40
1:F:163:TYR:CD2	1:F:167:ILE:HD11	2.56	0.40
1:H:98:VAL:HB	1:H:133:ASP:HB3	2.03	0.40
1:H:77:LEU:HD12	1:H:79:LEU:HD23	2.04	0.40
1:I:57:GLY:HA2	1:I:73:VAL:HG12	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	252/263 (96%)	244 (97%)	7 (3%)	1 (0%)	30 43
1	B	250/263 (95%)	245 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	250/263 (95%)	244 (98%)	6 (2%)	0	100	100
1	D	250/263 (95%)	243 (97%)	6 (2%)	1 (0%)	30	43
1	E	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
1	F	250/263 (95%)	244 (98%)	6 (2%)	0	100	100
1	G	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
1	H	250/263 (95%)	244 (98%)	6 (2%)	0	100	100
1	I	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
1	J	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
All	All	2502/2630 (95%)	2444 (98%)	56 (2%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	GLY
1	D	209	THR

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	193/206 (94%)	185 (96%)	8 (4%)	27	46
1	B	193/206 (94%)	184 (95%)	9 (5%)	23	41
1	C	191/206 (93%)	180 (94%)	11 (6%)	18	32
1	D	190/206 (92%)	181 (95%)	9 (5%)	23	41
1	E	194/206 (94%)	188 (97%)	6 (3%)	35	57
1	F	192/206 (93%)	182 (95%)	10 (5%)	21	36
1	G	190/206 (92%)	181 (95%)	9 (5%)	23	41
1	H	192/206 (93%)	182 (95%)	10 (5%)	21	36
1	I	189/206 (92%)	180 (95%)	9 (5%)	23	40
1	J	190/206 (92%)	183 (96%)	7 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1914/2060 (93%)	1826 (95%)	88 (5%)	24	41

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	62	ARG
1	A	77	LEU
1	A	139	LEU
1	A	183	ASP
1	A	201	MET
1	A	202	SER
1	A	211	GLU
1	B	44	GLU
1	B	62	ARG
1	B	77	LEU
1	B	139	LEU
1	B	183	ASP
1	B	201	MET
1	B	202	SER
1	B	210	GLU
1	B	215	LYS
1	C	44	GLU
1	C	62	ARG
1	C	77	LEU
1	C	139	LEU
1	C	183	ASP
1	C	192	LYS
1	C	201	MET
1	C	202	SER
1	C	209	THR
1	C	242	LYS
1	C	245	ARG
1	D	62	ARG
1	D	77	LEU
1	D	139	LEU
1	D	183	ASP
1	D	201	MET
1	D	202	SER
1	D	207	THR
1	D	209	THR
1	D	220	VAL

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Mol	Chain	Res	Type
1	E	62	ARG
1	E	77	LEU
1	E	139	LEU
1	E	185	LYS
1	E	201	MET
1	E	202	SER
1	F	44	GLU
1	F	62	ARG
1	F	77	LEU
1	F	139	LEU
1	F	183	ASP
1	F	201	MET
1	F	202	SER
1	F	206	LYS
1	F	220	VAL
1	F	242	LYS
1	G	62	ARG
1	G	77	LEU
1	G	139	LEU
1	G	183	ASP
1	G	201	MET
1	G	202	SER
1	G	206	LYS
1	G	220	VAL
1	G	242	LYS
1	H	15	ARG
1	H	44	GLU
1	H	62	ARG
1	H	77	LEU
1	H	139	LEU
1	H	183	ASP
1	H	201	MET
1	H	202	SER
1	H	206	LYS
1	H	242	LYS
1	I	44	GLU
1	I	62	ARG
1	I	77	LEU
1	I	139	LEU
1	I	183	ASP
1	I	201	MET
1	I	202	SER

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Mol	Chain	Res	Type
1	I	210	GLU
1	I	242	LYS
1	J	62	ARG
1	J	77	LEU
1	J	139	LEU
1	J	183	ASP
1	J	201	MET
1	J	202	SER
1	J	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	GLN
1	C	25	HIS
1	C	29	HIS
1	D	29	HIS
1	E	25	HIS
1	E	29	HIS
1	F	216	GLN
1	G	29	HIS
1	H	25	HIS
1	H	29	HIS
1	I	25	HIS
1	I	29	HIS
1	J	25	HIS
1	J	29	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	A	264	-	5,5,5	0.37	0	5,5,5	0.36	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	GOL	A	264	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	264	GOL	O2-C2-C3-O3
2	A	264	GOL	C1-C2-C3-O3
2	A	264	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	254/263 (96%)	0.24	9 (3%) 47 43	6, 17, 35, 45	0
1	B	252/263 (95%)	-0.03	4 (1%) 70 66	6, 17, 35, 45	0
1	C	252/263 (95%)	0.19	11 (4%) 39 34	6, 17, 35, 46	0
1	D	252/263 (95%)	0.12	7 (2%) 55 51	6, 16, 34, 45	0
1	E	252/263 (95%)	-0.15	1 (0%) 88 86	6, 17, 35, 45	0
1	F	252/263 (95%)	0.19	6 (2%) 59 55	6, 16, 35, 45	0
1	G	252/263 (95%)	-0.03	5 (1%) 65 60	6, 17, 35, 46	0
1	H	252/263 (95%)	0.21	13 (5%) 33 29	6, 17, 35, 47	0
1	I	252/263 (95%)	0.11	9 (3%) 46 42	6, 17, 34, 45	0
1	J	252/263 (95%)	-0.15	6 (2%) 59 55	6, 17, 35, 45	0
All	All	2522/2630 (95%)	0.07	71 (2%) 55 51	6, 17, 35, 47	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	253	GLY	3.9
1	A	254	GLY	3.8
1	H	182	GLY	3.7
1	J	36	ASP	3.4
1	F	2	ALA	3.3
1	C	204	GLY	3.2
1	H	205	PRO	3.2
1	I	253	GLY	3.2
1	H	2	ALA	3.2
1	A	204	GLY	3.1
1	D	253	GLY	3.1
1	C	205	PRO	2.9
1	C	203	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	204	GLY	2.9
1	H	203	GLY	2.9
1	A	2	ALA	2.8
1	A	33	ASP	2.8
1	J	32	ALA	2.8
1	B	204	GLY	2.8
1	C	207	THR	2.8
1	F	253	GLY	2.7
1	J	253	GLY	2.7
1	C	33	ASP	2.6
1	H	245	ARG	2.6
1	I	156	THR	2.6
1	D	208	LYS	2.6
1	G	253	GLY	2.6
1	C	119	PHE	2.6
1	H	248	ALA	2.5
1	J	33	ASP	2.5
1	D	2	ALA	2.5
1	D	209	THR	2.5
1	D	36	ASP	2.5
1	J	208	LYS	2.5
1	C	202	SER	2.4
1	A	255	LYS	2.4
1	C	206	LYS	2.4
1	H	207	THR	2.4
1	G	208	LYS	2.4
1	F	203	GLY	2.4
1	I	33	ASP	2.4
1	H	219	GLY	2.3
1	C	34	PHE	2.3
1	H	215	LYS	2.3
1	G	2	ALA	2.3
1	A	236	GLN	2.3
1	E	204	GLY	2.3
1	I	203	GLY	2.3
1	H	250	LEU	2.3
1	I	53	ALA	2.2
1	A	36	ASP	2.2
1	F	246	ALA	2.2
1	A	39	ASP	2.2
1	B	203	GLY	2.2
1	C	2	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	54	GLY	2.1
1	I	87	ASN	2.1
1	D	203	GLY	2.1
1	I	204	GLY	2.1
1	C	36	ASP	2.1
1	F	208	LYS	2.1
1	G	36	ASP	2.1
1	G	53	ALA	2.1
1	F	36	ASP	2.1
1	I	183	ASP	2.1
1	A	205	PRO	2.1
1	H	183	ASP	2.0
1	H	35	MET	2.0
1	I	187	PHE	2.0
1	B	2	ALA	2.0
1	B	253	GLY	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	GOL	A	264	6/6	0.45	0.28	75,77,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.