



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:42 am BST

PDB ID : 1OK6
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

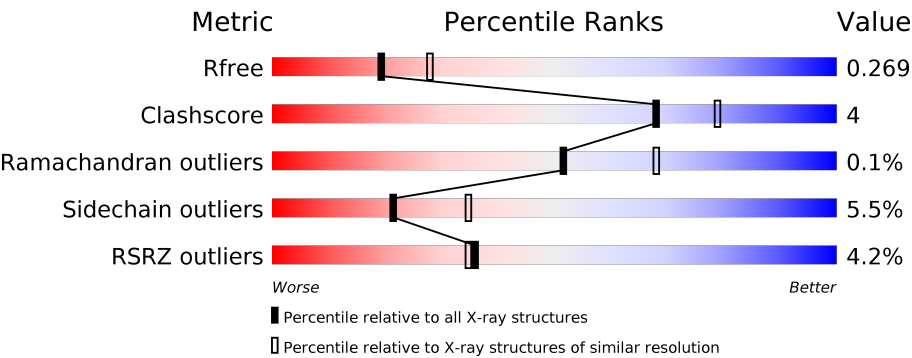
1 Overall quality at a glance i

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>84%11% . .</div></div>
1	B	263	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>85%9% . .</div></div>
1	C	263	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>83%11% . .</div></div>
1	D	263	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>83%10% . .</div></div>
1	E	263	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>85%9% . .</div></div>
1	F	263	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>82%11% . . .</div></div>

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Mol	Chain	Length	Quality of chain
1	G	263	<div><div></div><div>3%</div><div>84%</div><div>10%</div><div></div><div></div></div>
1	H	263	<div><div></div><div>8%</div><div>83%</div><div>10%</div><div></div><div></div></div>
1	I	263	<div><div></div><div>3%</div><div>82%</div><div>10%</div><div></div><div></div></div>
1	J	263	<div><div></div><div>5%</div><div>87%</div><div>7%</div><div></div><div></div></div>

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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

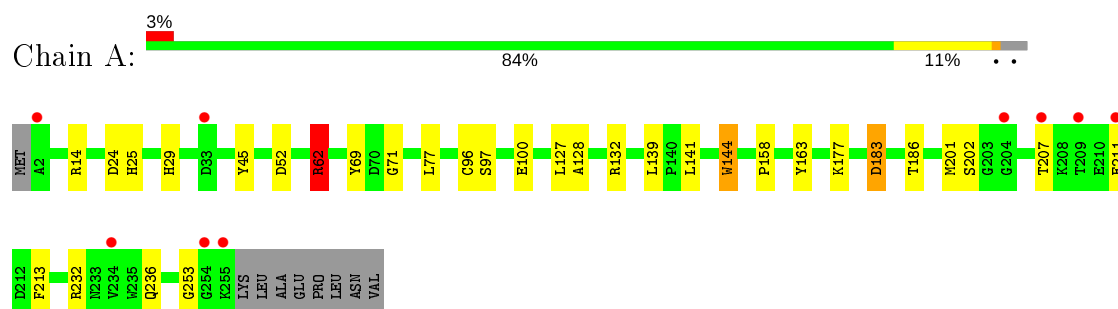
- Molecule 3 is water.

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		

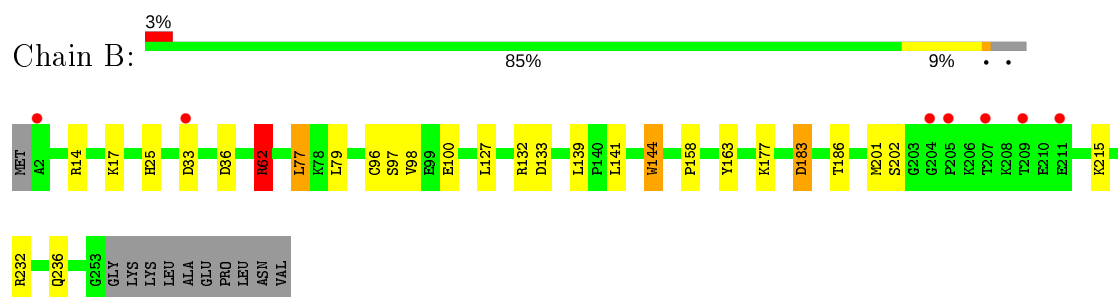
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

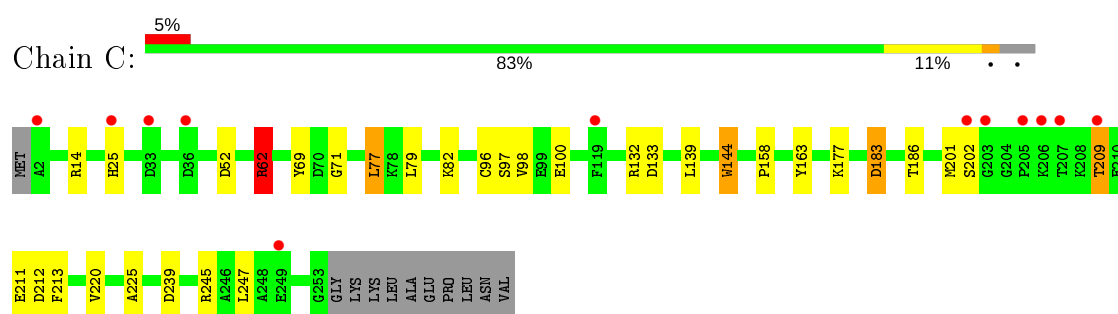
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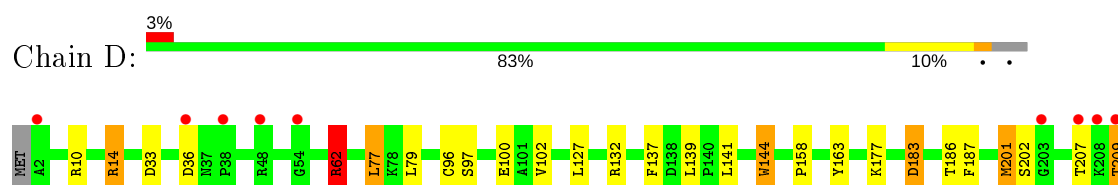
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

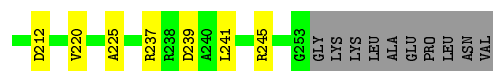


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

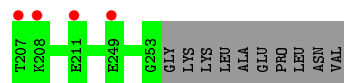
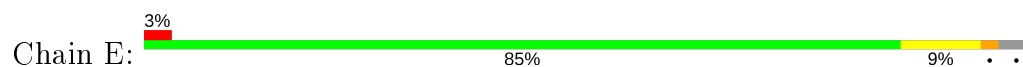


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

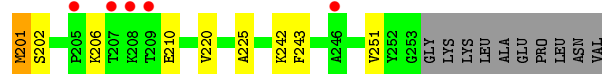
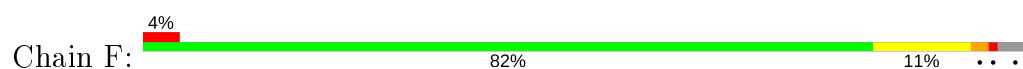




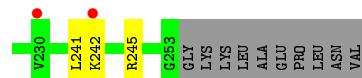
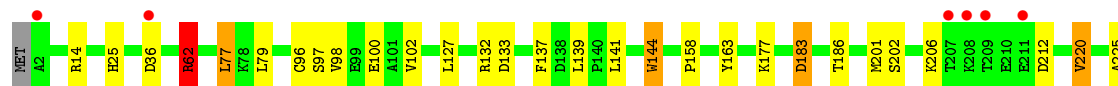
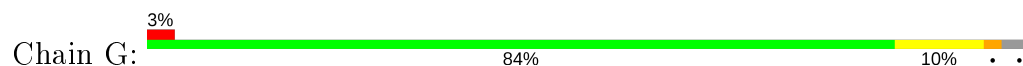
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



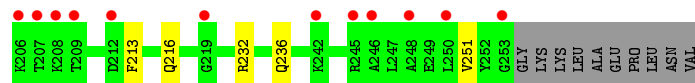
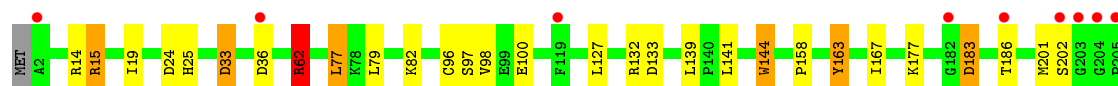
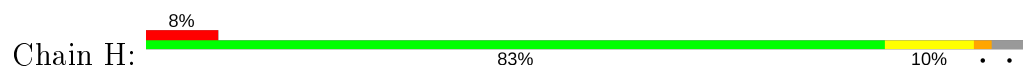
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



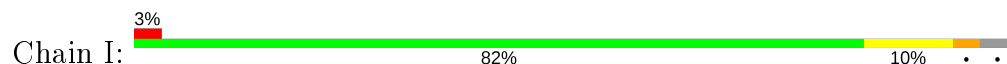
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

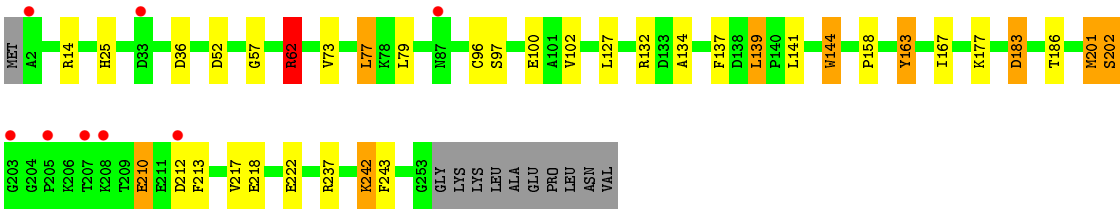


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

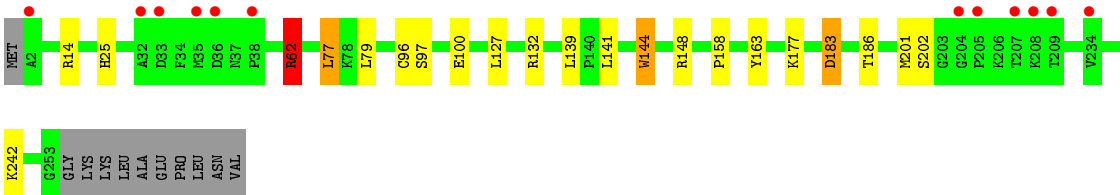
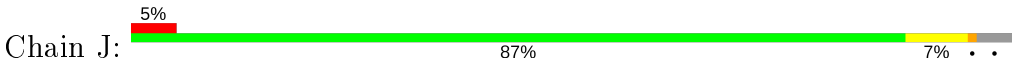


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I





● 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	89.90 Å 176.50 Å 185.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.00-2.40) 94.3 (19.98-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.41 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.263 0.244 , 0.269	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)	0.39 , 49.1	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	0.64	0/1980	0.89	7/2685 (0.3%)
1	B	0.57	0/1970	0.87	7/2672 (0.3%)
1	C	0.60	0/1959	0.88	8/2658 (0.3%)
1	D	0.63	0/1956	0.84	8/2655 (0.3%)
1	E	0.56	0/1974	0.81	7/2676 (0.3%)
1	F	0.65	0/1964	0.83	9/2664 (0.3%)
1	G	0.58	0/1957	0.82	7/2656 (0.3%)
1	H	0.60	0/1964	0.94	11/2665 (0.4%)
1	I	0.62	0/1954	0.89	8/2654 (0.3%)
1	J	0.57	0/1956	0.79	5/2655 (0.2%)
All	All	0.60	0/19634	0.86	77/26640 (0.3%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	15	ARG	NE-CZ-NH2	-17.25	111.67	120.30
1	H	15	ARG	NE-CZ-NH1	15.23	127.91	120.30
1	C	132	ARG	NE-CZ-NH2	14.64	127.62	120.30
1	B	132	ARG	NE-CZ-NH1	-14.37	113.11	120.30
1	A	132	ARG	NE-CZ-NH1	-14.24	113.18	120.30
1	C	132	ARG	NE-CZ-NH1	-14.19	113.20	120.30
1	A	132	ARG	NE-CZ-NH2	14.01	127.30	120.30
1	B	132	ARG	NE-CZ-NH2	13.96	127.28	120.30
1	I	132	ARG	NE-CZ-NH1	-13.86	113.37	120.30
1	I	132	ARG	NE-CZ-NH2	13.50	127.05	120.30
1	E	132	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	J	132	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	D	132	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	F	132	ARG	NE-CZ-NH1	9.59	125.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	132	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	D	132	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	E	132	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	H	132	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	F	132	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	J	132	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	D	62	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	G	132	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	E	62	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	H	132	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	62	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	J	62	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	62	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	F	62	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	I	62	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	H	62	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	I	132	ARG	CD-NE-CZ	7.25	133.75	123.60
1	C	132	ARG	CD-NE-CZ	7.14	133.60	123.60
1	A	132	ARG	CD-NE-CZ	7.01	133.41	123.60
1	B	132	ARG	CD-NE-CZ	6.91	133.28	123.60
1	G	62	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	H	183	ASP	CB-CG-OD2	6.67	124.31	118.30
1	B	183	ASP	CB-CG-OD2	6.39	124.05	118.30
1	E	183	ASP	CB-CG-OD2	6.12	123.81	118.30
1	G	212	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	62	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	33	ASP	CB-CG-OD2	5.96	123.66	118.30
1	F	183	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	212	ASP	CB-CG-OD2	5.79	123.52	118.30
1	A	183	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	183	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	52	ASP	CB-CG-OD2	5.67	123.41	118.30
1	I	183	ASP	CB-CG-OD2	5.64	123.37	118.30
1	C	183	ASP	CB-CG-OD2	5.59	123.33	118.30
1	I	212	ASP	CB-CG-OD2	5.59	123.33	118.30
1	J	183	ASP	CB-CG-OD2	5.58	123.33	118.30
1	H	15	ARG	CG-CD-NE	5.55	123.45	111.80
1	F	24	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	24	ASP	CB-CG-OD2	5.49	123.25	118.30
1	G	183	ASP	CB-CG-OD2	5.44	123.20	118.30
1	H	33	ASP	CB-CG-OD2	5.43	123.19	118.30
1	G	36	ASP	CB-CG-OD2	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	ASP	CB-CG-OD2	5.39	123.15	118.30
1	G	132	ARG	CD-NE-CZ	5.33	131.07	123.60
1	F	70	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	36	ASP	CB-CG-OD2	5.30	123.08	118.30
1	I	36	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	52	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	36	ASP	CB-CG-OD2	5.26	123.03	118.30
1	D	33	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	24	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	132	ARG	CD-NE-CZ	5.18	130.85	123.60
1	D	132	ARG	CD-NE-CZ	5.18	130.85	123.60
1	F	174	ASP	CB-CG-OD2	5.14	122.93	118.30
1	J	132	ARG	CD-NE-CZ	5.14	130.80	123.60
1	F	132	ARG	CD-NE-CZ	5.13	130.78	123.60
1	E	36	ASP	CB-CG-OD2	5.11	122.90	118.30
1	H	132	ARG	CD-NE-CZ	5.08	130.72	123.60
1	A	24	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	36	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	36	ASP	CB-CG-OD2	5.05	122.84	118.30
1	I	52	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	239	ASP	CB-CG-OD2	5.03	122.83	118.30

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	14	0
1	B	1927	0	1920	14	0
1	C	1916	0	1907	14	0
1	D	1913	0	1901	17	0
1	E	1931	0	1931	13	0
1	F	1921	0	1916	16	0
1	G	1914	0	1903	12	0
1	H	1921	0	1909	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1911	0	1890	22	0
1	J	1913	0	1901	9	0
2	A	6	0	8	0	0
3	A	112	0	0	4	0
3	B	80	0	0	3	0
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	2	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	144	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 4.

All (144) 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:A:96:CYS:SG	1:A:97:SER:N	2.38	0.95
1:I:96:CYS:SG	1:I:97:SER:N	2.32	0.94
1:C:96:CYS:SG	1:C:97:SER:N	2.39	0.94
1:B:96:CYS:SG	1:B:97:SER:N	2.33	0.94
1:E:96:CYS:SG	1:E:97:SER:N	2.37	0.93
1:J:96:CYS:SG	1:J:97:SER:N	2.41	0.93
1:D:96:CYS:SG	1:D:97:SER:N	2.38	0.92
1:F:96:CYS:SG	1:F:97:SER:N	2.38	0.91
1:G:96:CYS:SG	1:G:97:SER:N	2.45	0.88
3:A:2088:HOH:O	1:E:62:ARG:HD2	1.73	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:TRP:HE1	1:J:177:LYS:HZ3	1.39	0.69
1:B:62:ARG:NH2	1:B:100:GLU:OE2	2.26	0.69
1:D:144:TRP:HE1	1:D:177:LYS:HZ3	1.39	0.69
1:E:62:ARG:NH2	1:E:100:GLU:OE2	2.26	0.68
1:I:96:CYS:HG	1:I:97:SER:H	1.39	0.67
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
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:I:96:CYS:HG	1:I:97:SER:N	1.94	0.63
1:C:213:PHE:HE2	1:C:247:LEU:HD11	1.65	0.62
1:F:144:TRP:HE1	1:F:177:LYS:HZ3	1.47	0.61
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:I:144:TRP:HE1	1:I:177:LYS:HZ3	1.52	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:C:144:TRP:HE1	1:C:177:LYS:HZ3	1.56	0.52
1:D:245:ARG:NH2	3:D:2089:HOH:O	2.43	0.52
1:A:29:HIS:NE2	3:A:2022:HOH:O	2.30	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:B:144:TRP:HE1	1:B:177:LYS:HZ3	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:213:PHE:O	1:H:216:GLN:HB2	2.13	0.49
1:G:144:TRP:HE1	1:G:177:LYS:HZ3	1.60	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:B:17:LYS:NZ	3:B:2012:HOH:O	2.45	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
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: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:I:201:MET:HE2	1:I:202:SER:O	2.17	0.45
1:J:77:LEU:HD12	1:J:79:LEU:HD23	1.98	0.45
1:A:144:TRP:HE1	1:A:177:LYS:HZ3	1.63	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:F:62:ARG:HG2	1:F:62:ARG:O	2.17	0.45
1:H:19:ILE:HD11	1:H:251:VAL:HB	1.98	0.45
1:J:62:ARG:HG2	1:J:62:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LYS:NZ	3:H:2032:HOH:O	2.14	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:A:62:ARG:HG2	1:A:62:ARG:O	2.19	0.43
1:E:62:ARG:HG2	1:E:62:ARG:O	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:H:144:TRP:HE1	1:H:177:LYS:HZ3	1.66	0.42
1:A:69:TYR:CZ	1:A:71:GLY:HA2	2.55	0.42
1:I:62:ARG:HG2	1:I:62:ARG:O	2.19	0.42
1:B:144:TRP:HE1	1:B:177:LYS:NZ	2.18	0.42
1:C:220:VAL:HG13	1:C:225:ALA:HB3	2.02	0.41
1:C:82:LYS:NZ	3:C:2031:HOH:O	2.36	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: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:E:144:TRP:HE1	1:E:177:LYS:HZ3	1.68	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:I:144:TRP:NE1	1:I:177:LYS:NZ	2.67	0.40
1:H:77:LEU:HD12	1:H:79:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	34	48
1	B	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
1	C	250/263 (95%)	244 (98%)	6 (2%)	0	100	100
1	D	250/263 (95%)	243 (97%)	6 (2%)	1 (0%)	34	48
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%)	51	68

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/206 (94%)	183 (95%)	10 (5%)	23	38
1	B	193/206 (94%)	183 (95%)	10 (5%)	23	38
1	C	191/206 (93%)	180 (94%)	11 (6%)	20	32
1	D	190/206 (92%)	179 (94%)	11 (6%)	20	32
1	E	194/206 (94%)	184 (95%)	10 (5%)	23	38
1	F	192/206 (93%)	181 (94%)	11 (6%)	20	33
1	G	190/206 (92%)	178 (94%)	12 (6%)	18	28
1	H	192/206 (93%)	182 (95%)	10 (5%)	23	38
1	I	189/206 (92%)	178 (94%)	11 (6%)	20	32
1	J	190/206 (92%)	180 (95%)	10 (5%)	22	37
All	All	1914/2060 (93%)	1808 (94%)	106 (6%)	21	35

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	62	ARG
1	A	77	LEU
1	A	139	LEU
1	A	144	TRP
1	A	163	TYR
1	A	183	ASP
1	A	201	MET
1	A	202	SER
1	A	211	GLU
1	B	14	ARG
1	B	62	ARG
1	B	77	LEU
1	B	139	LEU
1	B	144	TRP
1	B	163	TYR

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Mol	Chain	Res	Type
1	B	183	ASP
1	B	201	MET
1	B	202	SER
1	B	215	LYS
1	C	14	ARG
1	C	62	ARG
1	C	77	LEU
1	C	139	LEU
1	C	144	TRP
1	C	163	TYR
1	C	183	ASP
1	C	201	MET
1	C	202	SER
1	C	209	THR
1	C	245	ARG
1	D	14	ARG
1	D	62	ARG
1	D	77	LEU
1	D	139	LEU
1	D	144	TRP
1	D	163	TYR
1	D	183	ASP
1	D	201	MET
1	D	202	SER
1	D	207	THR
1	D	209	THR
1	E	14	ARG
1	E	62	ARG
1	E	77	LEU
1	E	139	LEU
1	E	144	TRP
1	E	163	TYR
1	E	183	ASP
1	E	185	LYS
1	E	201	MET
1	E	202	SER
1	F	14	ARG
1	F	62	ARG
1	F	77	LEU
1	F	139	LEU
1	F	144	TRP
1	F	163	TYR

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Mol	Chain	Res	Type
1	F	183	ASP
1	F	201	MET
1	F	202	SER
1	F	206	LYS
1	F	242	LYS
1	G	14	ARG
1	G	62	ARG
1	G	77	LEU
1	G	139	LEU
1	G	144	TRP
1	G	163	TYR
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	14	ARG
1	H	15	ARG
1	H	62	ARG
1	H	77	LEU
1	H	139	LEU
1	H	144	TRP
1	H	163	TYR
1	H	183	ASP
1	H	201	MET
1	H	202	SER
1	I	14	ARG
1	I	62	ARG
1	I	77	LEU
1	I	139	LEU
1	I	144	TRP
1	I	163	TYR
1	I	183	ASP
1	I	201	MET
1	I	202	SER
1	I	210	GLU
1	I	242	LYS
1	J	14	ARG
1	J	62	ARG
1	J	77	LEU
1	J	139	LEU

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Mol	Chain	Res	Type
1	J	144	TRP
1	J	163	TYR
1	J	183	ASP
1	J	201	MET
1	J	202	SER
1	J	242	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	GLN
1	C	25	HIS
1	D	29	HIS
1	E	25	HIS
1	H	25	HIS
1	H	29	HIS
1	I	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.36	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
2	GOL	A	264	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) 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-C3
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 [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	254/263 (96%)	0.17	9 (3%) 44 43	6, 17, 35, 45	0
1	B	252/263 (95%)	-0.00	7 (2%) 53 51	6, 17, 35, 45	0
1	C	252/263 (95%)	0.18	12 (4%) 30 29	6, 17, 35, 46	0
1	D	252/263 (95%)	0.00	9 (3%) 42 42	6, 16, 34, 45	0
1	E	252/263 (95%)	-0.13	9 (3%) 42 42	6, 17, 35, 45	0
1	F	252/263 (95%)	0.12	11 (4%) 34 33	6, 16, 35, 45	0
1	G	252/263 (95%)	-0.06	8 (3%) 47 46	6, 17, 35, 46	0
1	H	252/263 (95%)	0.22	21 (8%) 11 10	6, 17, 35, 47	0
1	I	252/263 (95%)	0.02	8 (3%) 47 46	6, 17, 34, 45	0
1	J	252/263 (95%)	-0.15	12 (4%) 30 29	6, 17, 35, 45	0
All	All	2522/2630 (95%)	0.04	106 (4%) 36 35	6, 17, 35, 47	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLY	5.8
1	H	253	GLY	5.2
1	J	36	ASP	5.1
1	H	205	PRO	4.8
1	F	2	ALA	4.7
1	D	2	ALA	4.4
1	C	36	ASP	4.1
1	E	2	ALA	4.1
1	H	207	THR	4.1
1	G	207	THR	3.9
1	C	2	ALA	3.9
1	G	36	ASP	3.9
1	H	182	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	255	LYS	3.8
1	C	207	THR	3.8
1	G	2	ALA	3.8
1	I	2	ALA	3.6
1	A	2	ALA	3.6
1	J	209	THR	3.4
1	H	245	ARG	3.4
1	I	207	THR	3.4
1	J	32	ALA	3.4
1	D	207	THR	3.3
1	H	186	THR	3.3
1	B	207	THR	3.3
1	H	204	GLY	3.2
1	D	209	THR	3.2
1	I	205	PRO	3.2
1	E	207	THR	3.1
1	A	207	THR	3.1
1	F	209	THR	3.1
1	B	204	GLY	3.1
1	C	203	GLY	3.1
1	C	249	GLU	3.1
1	J	2	ALA	3.1
1	F	36	ASP	3.1
1	C	205	PRO	3.0
1	H	36	ASP	3.0
1	F	246	ALA	3.0
1	H	219	GLY	3.0
1	B	211	GLU	2.9
1	C	202	SER	2.9
1	C	206	LYS	2.9
1	I	33	ASP	2.8
1	E	3	ASN	2.8
1	C	209	THR	2.8
1	B	205	PRO	2.8
1	A	234	VAL	2.7
1	J	208	LYS	2.7
1	D	36	ASP	2.7
1	J	38	PRO	2.7
1	G	209	THR	2.7
1	I	208	LYS	2.6
1	F	3	ASN	2.6
1	A	33	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	33	ASP	2.6
1	H	202	SER	2.5
1	I	212	ASP	2.5
1	H	212	ASP	2.5
1	A	204	GLY	2.5
1	J	204	GLY	2.5
1	H	248	ALA	2.5
1	J	205	PRO	2.5
1	I	203	GLY	2.5
1	I	87	ASN	2.4
1	D	203	GLY	2.4
1	H	203	GLY	2.4
1	D	208	LYS	2.4
1	E	33	ASP	2.4
1	G	242	LYS	2.4
1	F	205	PRO	2.4
1	J	234	VAL	2.3
1	F	207	THR	2.3
1	C	119	PHE	2.3
1	H	209	THR	2.2
1	F	21	LEU	2.2
1	J	33	ASP	2.2
1	D	38	PRO	2.2
1	F	208	LYS	2.2
1	A	209	THR	2.2
1	B	2	ALA	2.2
1	E	211	GLU	2.2
1	D	54	GLY	2.2
1	H	208	LYS	2.2
1	H	242	LYS	2.2
1	H	2	ALA	2.2
1	J	35	MET	2.1
1	J	207	THR	2.1
1	F	38	PRO	2.1
1	C	25	HIS	2.1
1	H	246	ALA	2.1
1	G	230	VAL	2.1
1	H	250	LEU	2.1
1	G	208	LYS	2.1
1	D	48	ARG	2.1
1	H	119	PHE	2.1
1	E	249	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	205	PRO	2.1
1	H	206	LYS	2.1
1	B	209	THR	2.0
1	E	203	GLY	2.0
1	F	14	ARG	2.0
1	A	211	GLU	2.0
1	E	208	LYS	2.0
1	G	211	GLU	2.0
1	C	33	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
2	GOL	A	264	6/6	0.55	0.22	75,77,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.