



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:23 PM GMT

PDB ID : 1OJX
Title : CRYSTAL STRUCTURE OF AN ARCHAEL FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE
Authors : Lorentzen, E.; Zwart, P.; Stark, A.; Hensel, R.; Siebers, B.; Pohl, E.
Deposited on : 2003-07-16
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

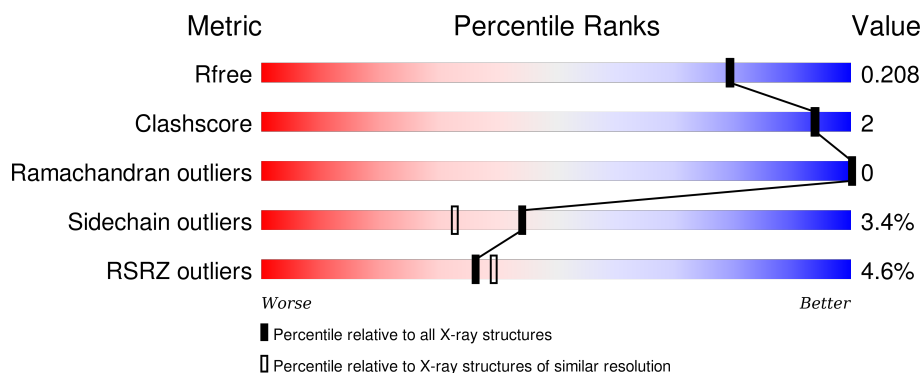
1 Overall quality at a glance ⓘ

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>8%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	B	263	<div> <div>2%</div> <div>89%</div> <div>7%</div> <div>5%</div> </div>
1	C	263	<div> <div>8%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	D	263	<div> <div>7%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	E	263	<div> <div>3%</div> <div>92%</div> <div>.</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	263	<div><div></div><div>6%</div><div>91%</div><div>5%</div></div>
1	G	263	<div><div></div><div>2%</div><div>89%</div><div>6% • 5%</div></div>
1	H	263	<div><div></div><div>5%</div><div>87%</div><div>7% • 5%</div></div>
1	I	263	<div><div></div><div>4%</div><div>88%</div><div>7% 5%</div></div>
1	J	263	<div><div></div><div>%</div><div>89%</div><div>7% 5%</div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 21474 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	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	B	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	C	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	D	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	E	253	Total 1944	C 1251	N 331	O 357	S 5	0	0	1
1	F	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	G	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	H	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	I	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1
1	J	251	Total 1936	C 1247	N 329	O 355	S 5	0	0	1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	208	Total 208	O 208	0	0
2	B	237	Total 237	O 237	0	0
2	C	173	Total 173	O 173	0	0
2	D	182	Total 182	O 182	0	0

Continued on next page...

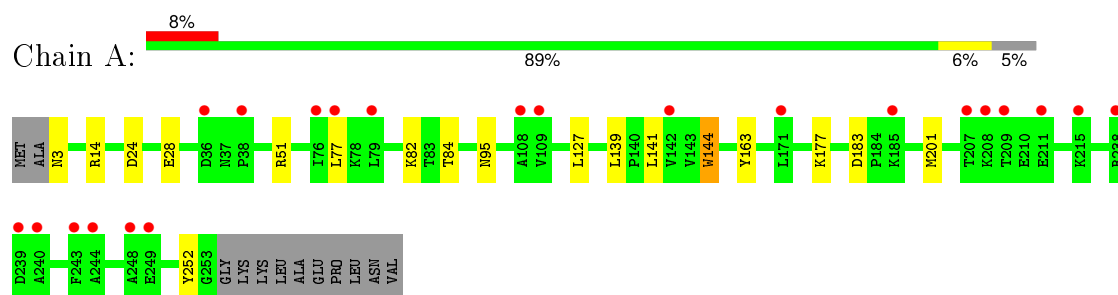
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	230	Total 230	O 230	0	0
2	F	189	Total 189	O 189	0	0
2	G	216	Total 216	O 216	0	0
2	H	216	Total 216	O 216	0	0
2	I	210	Total 210	O 210	0	0
2	J	245	Total 245	O 245	0	0

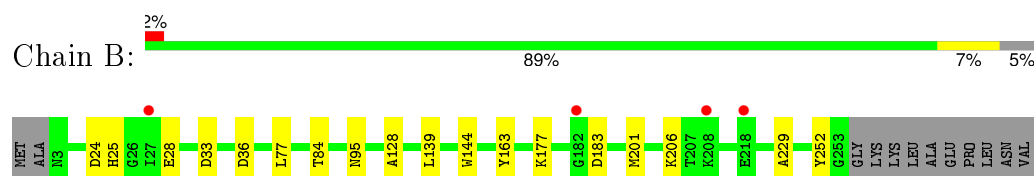
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

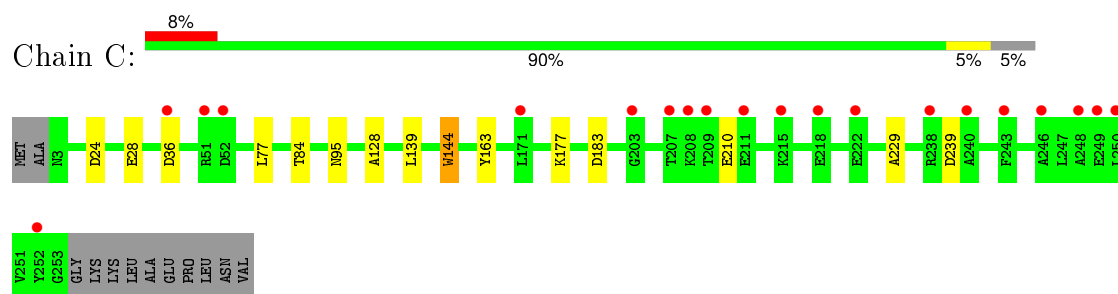
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



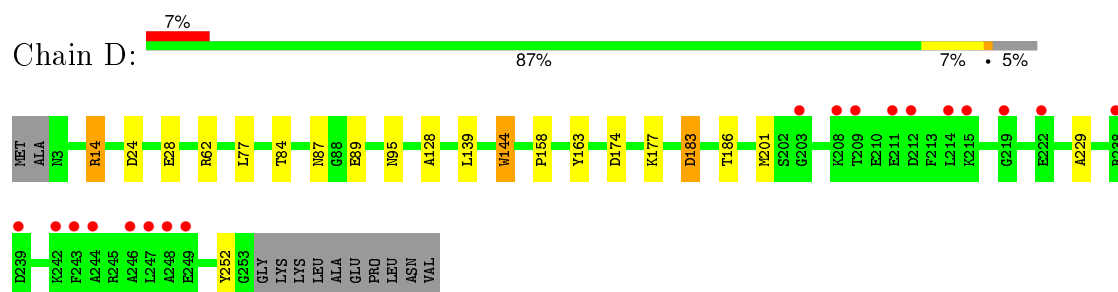
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



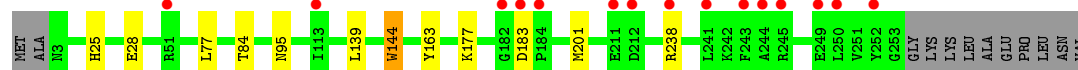
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

Chain E: 




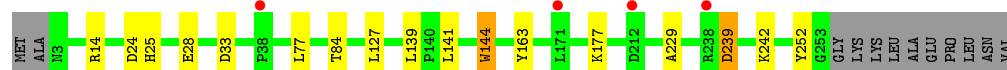
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

Chain F: 




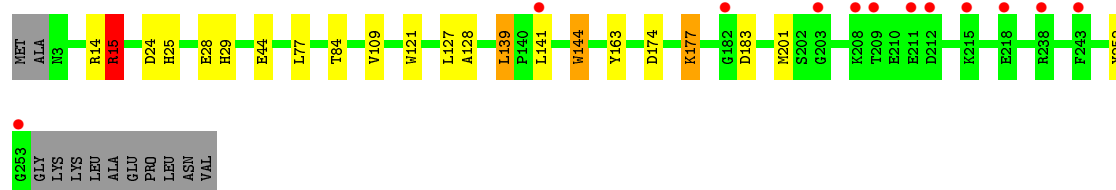
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

Chain G: 




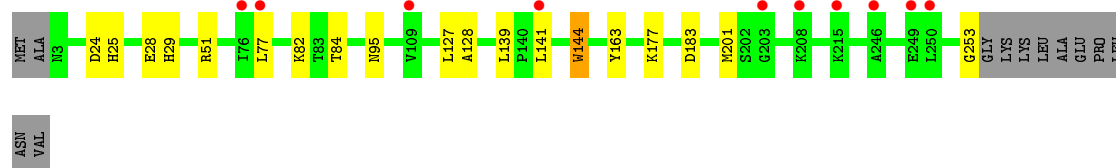
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

Chain H: 




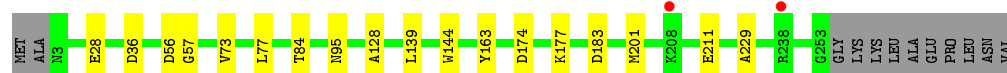
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

Chain I: 



- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.30Å 158.97Å 102.99Å 90.00° 108.11° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 38.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	0.9 (40.00-1.90) 94.8 (38.41-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.179 0.190 , 0.208	Depositor DCC
R_{free} test set	4721 reflections (2.51%)	DCC
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 188243 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21474	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.55	1/1979 (0.1%)	0.77	2/2680 (0.1%)
1	B	0.55	0/1979	0.76	2/2680 (0.1%)
1	C	0.54	0/1979	0.77	3/2680 (0.1%)
1	D	0.55	1/1979 (0.1%)	0.75	4/2680 (0.1%)
1	E	0.55	0/1987	0.76	1/2690 (0.0%)
1	F	0.53	0/1979	0.75	1/2680 (0.0%)
1	G	0.55	1/1979 (0.1%)	0.77	2/2680 (0.1%)
1	H	0.55	1/1979 (0.1%)	0.77	3/2680 (0.1%)
1	I	0.56	0/1979	0.76	2/2680 (0.1%)
1	J	0.58	0/1979	0.79	3/2680 (0.1%)
All	All	0.55	4/19798 (0.0%)	0.76	23/26810 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	252	TYR	C-N	-5.11	1.23	1.33
1	A	252	TYR	C-N	-5.07	1.24	1.33
1	D	252	TYR	C-N	-5.04	1.24	1.33
1	G	252	TYR	C-N	-5.01	1.24	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ASP	CB-CG-OD2	6.27	123.94	118.30
1	H	24	ASP	CB-CG-OD2	6.09	123.78	118.30
1	I	24	ASP	CB-CG-OD2	5.77	123.49	118.30
1	G	24	ASP	CB-CG-OD2	5.73	123.46	118.30
1	F	183	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	174	ASP	CB-CG-OD2	5.63	123.36	118.30
1	G	239	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	24	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	174	ASP	CB-CG-OD2	5.59	123.33	118.30
1	J	174	ASP	CB-CG-OD2	5.44	123.19	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	183	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	62	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	252	TYR	O-C-N	-5.24	114.30	123.20
1	D	183	ASP	CB-CG-OD2	5.23	123.01	118.30
1	J	36	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	36	ASP	CB-CG-OD2	5.21	122.98	118.30
1	H	174	ASP	CB-CG-OD2	5.19	122.97	118.30
1	H	15	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	24	ASP	CB-CG-OD2	5.08	122.87	118.30
1	J	56	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	24	ASP	CB-CG-OD2	5.05	122.85	118.30
1	I	183	ASP	CB-CG-OD2	5.02	122.82	118.30

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	1936	0	1949	7	0
1	B	1936	0	1949	8	0
1	C	1936	0	1949	8	0
1	D	1936	0	1949	10	0
1	E	1944	0	1955	6	0
1	F	1936	0	1949	4	0
1	G	1936	0	1949	9	0
1	H	1936	0	1949	12	0
1	I	1936	0	1949	9	0
1	J	1936	0	1949	5	0
2	A	208	0	0	1	0
2	B	237	0	0	1	0
2	C	173	0	0	0	0
2	D	182	0	0	3	0
2	E	230	0	0	1	0
2	F	189	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	216	0	0	1	0
2	H	216	0	0	5	0
2	I	210	0	0	1	0
2	J	245	0	0	0	0
All	All	21474	0	19496	71	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 2.

All (71) 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:H:44:GLU:OE1	2:H:2059:HOH:O	2.06	0.73
1:D:89:GLU:OE1	2:D:2080:HOH:O	2.07	0.71
1:C:144:TRP:NE1	1:C:177:LYS:HE3	2.09	0.67
1:D:28:GLU:O	1:D:84:THR:HG23	1.96	0.65
1:I:253:GLY:N	2:I:2210:HOH:O	2.29	0.65
1:C:177:LYS:HD2	1:C:229:ALA:HB3	1.80	0.63
1:D:144:TRP:NE1	1:D:177:LYS:HE3	2.15	0.62
1:A:3:ASN:N	2:A:2001:HOH:O	2.35	0.60
1:B:144:TRP:NE1	1:B:177:LYS:HE3	2.17	0.60
1:C:144:TRP:CD1	1:C:177:LYS:HE3	2.37	0.60
1:G:28:GLU:O	1:G:84:THR:HG23	2.03	0.58
1:E:144:TRP:HE1	1:E:177:LYS:HZ3	1.51	0.57
1:A:28:GLU:O	1:A:84:THR:HG23	2.05	0.57
1:B:144:TRP:CE2	1:B:177:LYS:HE3	2.42	0.55
1:H:28:GLU:O	1:H:84:THR:HG23	2.07	0.54
1:G:25:HIS:HE1	1:G:33:ASP:HB2	1.74	0.53
1:G:144:TRP:CD1	1:G:177:LYS:HE3	2.44	0.53
1:A:144:TRP:NE1	1:A:177:LYS:HE3	2.25	0.52
1:H:121:TRP:HD1	2:H:2129:HOH:O	1.91	0.52
1:G:144:TRP:NE1	1:G:177:LYS:HE3	2.26	0.51
1:J:57:GLY:HA2	1:J:73:VAL:HG12	1.93	0.51
1:C:28:GLU:O	1:C:84:THR:HG23	2.11	0.50
1:D:177:LYS:HD2	1:D:229:ALA:HB3	1.93	0.50
1:H:25:HIS:HE1	2:H:2045:HOH:O	1.93	0.50
1:I:28:GLU:O	1:I:84:THR:HG23	2.11	0.50
1:I:144:TRP:NE1	1:I:177:LYS:HE3	2.27	0.50
1:C:144:TRP:NE1	1:C:177:LYS:CE	2.75	0.50
1:G:144:TRP:NE1	1:G:177:LYS:CE	2.75	0.49
1:H:15:ARG:HD3	2:H:2075:HOH:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:ARG:NH1	2:D:2020:HOH:O	2.46	0.48
1:A:144:TRP:CD1	1:A:177:LYS:HE3	2.49	0.48
1:F:144:TRP:NE1	1:F:177:LYS:HE3	2.29	0.48
1:B:28:GLU:O	1:B:84:THR:HG23	2.13	0.48
1:E:144:TRP:HE1	1:E:177:LYS:NZ	2.12	0.47
1:I:144:TRP:CD1	1:I:177:LYS:HE3	2.49	0.47
1:A:127:LEU:HD11	1:A:141:LEU:HD21	1.96	0.47
1:I:25:HIS:CE1	1:I:29:HIS:HB2	2.49	0.47
1:G:25:HIS:CE1	1:G:33:ASP:HB2	2.49	0.47
1:H:144:TRP:NE1	1:H:177:LYS:HE3	2.29	0.47
1:E:82:LYS:HE2	2:E:2102:HOH:O	2.15	0.47
1:I:144:TRP:NE1	1:I:177:LYS:CE	2.79	0.46
1:G:239:ASP:OD2	2:G:2207:HOH:O	2.21	0.46
1:F:28:GLU:O	1:F:84:THR:HG23	2.15	0.46
1:E:28:GLU:O	1:E:84:THR:HG23	2.15	0.45
1:H:144:TRP:CE2	1:H:177:LYS:HE3	2.51	0.45
1:C:210:GLU:OE2	1:C:239:ASP:OD2	2.33	0.45
1:I:127:LEU:HD11	1:I:141:LEU:HD21	1.98	0.45
1:A:144:TRP:NE1	1:A:177:LYS:CE	2.80	0.45
1:H:127:LEU:HD11	1:H:141:LEU:HD21	1.98	0.45
1:D:144:TRP:CD1	1:D:177:LYS:HE3	2.53	0.44
1:C:95:ASN:HA	1:D:128:ALA:HB2	1.98	0.44
1:D:95:ASN:HA	1:E:128:ALA:HB2	1.99	0.44
1:F:25:HIS:HB2	2:F:2026:HOH:O	2.18	0.44
1:J:28:GLU:O	1:J:84:THR:HG23	2.19	0.43
1:H:25:HIS:HB2	2:H:2035:HOH:O	2.17	0.43
1:E:144:TRP:NE1	1:E:177:LYS:NZ	2.63	0.43
1:D:177:LYS:NZ	2:D:2148:HOH:O	2.52	0.43
1:A:95:ASN:HA	1:B:128:ALA:HB2	2.00	0.43
1:B:206:LYS:NZ	2:B:2211:HOH:O	2.45	0.42
1:G:127:LEU:HD11	1:G:141:LEU:HD21	2.02	0.42
1:J:177:LYS:CD	1:J:229:ALA:HB3	2.50	0.42
1:I:128:ALA:HB2	1:J:95:ASN:HA	2.02	0.42
1:F:95:ASN:HA	1:J:128:ALA:HB2	2.02	0.41
1:B:177:LYS:HD2	1:B:229:ALA:HB3	2.02	0.41
1:H:128:ALA:HB2	1:I:95:ASN:HA	2.02	0.41
1:G:177:LYS:HD2	1:G:229:ALA:HB3	2.02	0.41
1:D:158:PRO:HB3	1:D:186:THR:HB	2.03	0.41
1:H:109:VAL:HG13	1:H:139:LEU:HD23	2.03	0.41
1:B:25:HIS:NE2	1:B:33:ASP:HB2	2.36	0.41
1:B:95:ASN:HA	1:C:128:ALA:HB2	2.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:HIS:CE1	1:H:29:HIS:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	B	249/263 (95%)	243 (98%)	6 (2%)	0	100	100
1	C	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	D	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	E	251/263 (95%)	246 (98%)	5 (2%)	0	100	100
1	F	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	G	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	H	249/263 (95%)	242 (97%)	7 (3%)	0	100	100
1	I	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	J	249/263 (95%)	243 (98%)	6 (2%)	0	100	100
All	All	2492/2630 (95%)	2438 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	197/206 (96%)	189 (96%)	8 (4%)	37	25
1	B	197/206 (96%)	191 (97%)	6 (3%)	48	38
1	C	197/206 (96%)	193 (98%)	4 (2%)	63	57
1	D	197/206 (96%)	189 (96%)	8 (4%)	37	25
1	E	197/206 (96%)	192 (98%)	5 (2%)	55	47
1	F	197/206 (96%)	191 (97%)	6 (3%)	48	38
1	G	197/206 (96%)	191 (97%)	6 (3%)	48	38
1	H	197/206 (96%)	188 (95%)	9 (5%)	33	21
1	I	197/206 (96%)	190 (96%)	7 (4%)	42	30
1	J	197/206 (96%)	190 (96%)	7 (4%)	42	30
All	All	1970/2060 (96%)	1904 (97%)	66 (3%)	44	33

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	51	ARG
1	A	77	LEU
1	A	82	LYS
1	A	139	LEU
1	A	144	TRP
1	A	163	TYR
1	A	201	MET
1	B	36	ASP
1	B	77	LEU
1	B	139	LEU
1	B	163	TYR
1	B	183	ASP
1	B	201	MET
1	C	77	LEU
1	C	139	LEU
1	C	144	TRP
1	C	163	TYR
1	D	14	ARG
1	D	77	LEU
1	D	87	ASN
1	D	139	LEU
1	D	144	TRP
1	D	163	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	183	ASP
1	D	201	MET
1	E	77	LEU
1	E	139	LEU
1	E	144	TRP
1	E	163	TYR
1	E	201	MET
1	F	77	LEU
1	F	139	LEU
1	F	144	TRP
1	F	163	TYR
1	F	201	MET
1	F	238	ARG
1	G	14	ARG
1	G	77	LEU
1	G	139	LEU
1	G	144	TRP
1	G	163	TYR
1	G	242	LYS
1	H	14	ARG
1	H	15	ARG
1	H	77	LEU
1	H	139	LEU
1	H	144	TRP
1	H	163	TYR
1	H	177	LYS
1	H	183	ASP
1	H	201	MET
1	I	51	ARG
1	I	77	LEU
1	I	82	LYS
1	I	139	LEU
1	I	144	TRP
1	I	163	TYR
1	I	201	MET
1	J	77	LEU
1	J	139	LEU
1	J	144	TRP
1	J	163	TYR
1	J	183	ASP
1	J	201	MET
1	J	211	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	D	87	ASN
1	G	25	HIS
1	H	25	HIS
1	I	25	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	251/263 (95%)	0.35	22 (8%) 12 14	7, 12, 23, 28	0
1	B	251/263 (95%)	-0.02	4 (1%) 74 78	8, 12, 22, 27	0
1	C	251/263 (95%)	0.26	20 (7%) 15 17	8, 12, 22, 27	0
1	D	251/263 (95%)	0.03	18 (7%) 18 20	8, 12, 22, 28	0
1	E	253/263 (96%)	0.12	8 (3%) 51 54	8, 12, 23, 31	0
1	F	251/263 (95%)	0.14	15 (5%) 25 28	8, 12, 22, 27	0
1	G	251/263 (95%)	-0.11	4 (1%) 74 78	8, 12, 22, 28	0
1	H	251/263 (95%)	0.25	12 (4%) 34 37	8, 12, 22, 27	0
1	I	251/263 (95%)	0.13	10 (3%) 42 46	8, 12, 22, 27	0
1	J	251/263 (95%)	-0.08	2 (0%) 87 88	8, 12, 22, 29	0
All	All	2512/2630 (95%)	0.11	115 (4%) 36 39	7, 12, 22, 31	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	255	LYS	9.8
1	E	208	LYS	5.2
1	J	208	LYS	4.1
1	D	208	LYS	4.0
1	C	243	PHE	3.8
1	H	203	GLY	3.6
1	H	243	PHE	3.6
1	F	252	TYR	3.5
1	H	208	LYS	3.5
1	H	182	GLY	3.5
1	D	203	GLY	3.5
1	E	36	ASP	3.3
1	C	249	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	243	PHE	3.3
1	A	238	ARG	3.2
1	E	238	ARG	3.1
1	A	79	LEU	3.1
1	D	243	PHE	3.1
1	C	215	LYS	3.1
1	D	246	ALA	3.0
1	C	209	THR	3.0
1	C	203	GLY	3.0
1	I	215	LYS	3.0
1	D	247	LEU	2.9
1	B	208	LYS	2.9
1	C	36	ASP	2.9
1	D	212	ASP	2.9
1	C	240	ALA	2.9
1	G	238	ARG	2.9
1	C	218	GLU	2.8
1	I	249	GLU	2.8
1	A	36	ASP	2.8
1	C	207	THR	2.8
1	A	208	LYS	2.8
1	D	238	ARG	2.8
1	D	215	LYS	2.8
1	F	243	PHE	2.7
1	C	250	LEU	2.7
1	D	249	GLU	2.7
1	F	249	GLU	2.7
1	F	183	ASP	2.7
1	H	209	THR	2.6
1	C	246	ALA	2.6
1	I	203	GLY	2.6
1	E	207	THR	2.6
1	D	211	GLU	2.6
1	C	208	LYS	2.6
1	J	238	ARG	2.6
1	H	218	GLU	2.6
1	E	215	LYS	2.6
1	F	212	ASP	2.6
1	B	182	GLY	2.5
1	C	248	ALA	2.5
1	A	109	VAL	2.5
1	H	211	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	51	ARG	2.5
1	C	52	ASP	2.5
1	H	238	ARG	2.5
1	A	171	LEU	2.5
1	C	211	GLU	2.4
1	A	239	ASP	2.4
1	I	208	LYS	2.4
1	A	142	VAL	2.4
1	G	212	ASP	2.4
1	H	212	ASP	2.4
1	H	215	LYS	2.4
1	A	38	PRO	2.4
1	I	77	LEU	2.4
1	D	209	THR	2.3
1	D	239	ASP	2.3
1	F	238	ARG	2.3
1	E	218	GLU	2.3
1	F	241	LEU	2.3
1	A	244	ALA	2.3
1	A	108	ALA	2.3
1	C	238	ARG	2.3
1	F	51	ARG	2.3
1	I	141	LEU	2.3
1	C	222	GLU	2.3
1	G	171	LEU	2.3
1	A	215	LYS	2.3
1	C	252	TYR	2.3
1	D	214	LEU	2.2
1	D	219	GLY	2.2
1	B	27	ILE	2.2
1	A	77	LEU	2.2
1	I	109	VAL	2.2
1	A	185	LYS	2.2
1	I	250	LEU	2.2
1	F	182	GLY	2.2
1	D	222	GLU	2.2
1	D	242	LYS	2.2
1	F	250	LEU	2.2
1	F	244	ALA	2.1
1	F	245	ARG	2.1
1	A	211	GLU	2.1
1	F	184	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	113	ILE	2.1
1	E	211	GLU	2.1
1	F	211	GLU	2.1
1	A	240	ALA	2.1
1	D	244	ALA	2.1
1	D	248	ALA	2.1
1	B	218	GLU	2.1
1	H	253	GLY	2.1
1	G	38	PRO	2.1
1	A	248	ALA	2.1
1	C	171	LEU	2.1
1	A	76	ILE	2.0
1	H	141	LEU	2.0
1	A	207	THR	2.0
1	A	249	GLU	2.0
1	I	246	ALA	2.0
1	A	209	THR	2.0
1	I	76	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.