



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:07 PM GMT

PDB ID : 3D2C
Title : Structure of 4D3, a thermostable mutant of Bacillus subtilis lipase obtained through directed evolution
Authors : Sankaranarayanan, R.; Kamal, M.Z.
Deposited on : 2008-05-08
Resolution : 2.18 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

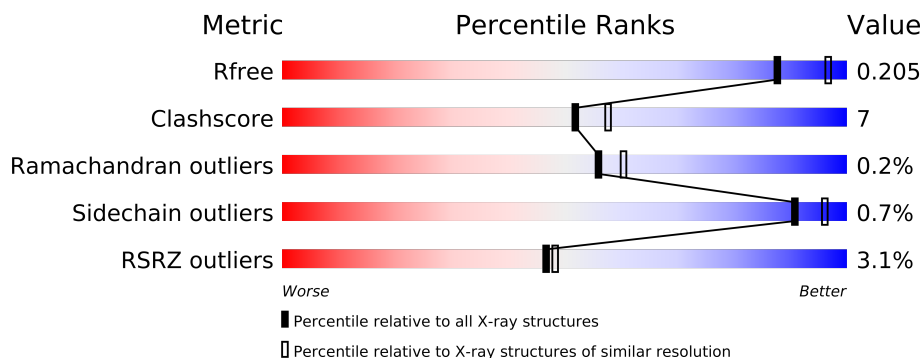
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.18 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}	66092	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	181	
1	B	181	
1	C	181	
1	D	181	
1	E	181	
1	F	181	
1	G	181	
1	H	181	
1	I	181	
1	J	181	
1	K	181	
1	L	181	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17510 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	B	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	C	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	D	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	E	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	F	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	G	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	H	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	I	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	J	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	K	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			
1	L	179	Total	C	N	O	S	0	0	0
			1365	857	238	265	5			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	ALA	ENGINEERED	UNP P37957
A	17	SER	PHE	ENGINEERED	UNP P37957
A	20	GLU	ALA	ENGINEERED	UNP P37957
A	89	TYR	ASN	ENGINEERED	UNP P37957
A	111	ASP	GLY	ENGINEERED	UNP P37957

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Chain	Residue	Modelled	Actual	Comment	Reference
A	114	PRO	LEU	ENGINEERED	UNP P37957
A	132	ASP	ALA	ENGINEERED	UNP P37957
A	157	MET	ILE	ENGINEERED	UNP P37957
A	166	TYR	ASN	ENGINEERED	UNP P37957
B	15	SER	ALA	ENGINEERED	UNP P37957
B	17	SER	PHE	ENGINEERED	UNP P37957
B	20	GLU	ALA	ENGINEERED	UNP P37957
B	89	TYR	ASN	ENGINEERED	UNP P37957
B	111	ASP	GLY	ENGINEERED	UNP P37957
B	114	PRO	LEU	ENGINEERED	UNP P37957
B	132	ASP	ALA	ENGINEERED	UNP P37957
B	157	MET	ILE	ENGINEERED	UNP P37957
B	166	TYR	ASN	ENGINEERED	UNP P37957
C	15	SER	ALA	ENGINEERED	UNP P37957
C	17	SER	PHE	ENGINEERED	UNP P37957
C	20	GLU	ALA	ENGINEERED	UNP P37957
C	89	TYR	ASN	ENGINEERED	UNP P37957
C	111	ASP	GLY	ENGINEERED	UNP P37957
C	114	PRO	LEU	ENGINEERED	UNP P37957
C	132	ASP	ALA	ENGINEERED	UNP P37957
C	157	MET	ILE	ENGINEERED	UNP P37957
C	166	TYR	ASN	ENGINEERED	UNP P37957
D	15	SER	ALA	ENGINEERED	UNP P37957
D	17	SER	PHE	ENGINEERED	UNP P37957
D	20	GLU	ALA	ENGINEERED	UNP P37957
D	89	TYR	ASN	ENGINEERED	UNP P37957
D	111	ASP	GLY	ENGINEERED	UNP P37957
D	114	PRO	LEU	ENGINEERED	UNP P37957
D	132	ASP	ALA	ENGINEERED	UNP P37957
D	157	MET	ILE	ENGINEERED	UNP P37957
D	166	TYR	ASN	ENGINEERED	UNP P37957
E	15	SER	ALA	ENGINEERED	UNP P37957
E	17	SER	PHE	ENGINEERED	UNP P37957
E	20	GLU	ALA	ENGINEERED	UNP P37957
E	89	TYR	ASN	ENGINEERED	UNP P37957
E	111	ASP	GLY	ENGINEERED	UNP P37957
E	114	PRO	LEU	ENGINEERED	UNP P37957
E	132	ASP	ALA	ENGINEERED	UNP P37957
E	157	MET	ILE	ENGINEERED	UNP P37957
E	166	TYR	ASN	ENGINEERED	UNP P37957
F	15	SER	ALA	ENGINEERED	UNP P37957
F	17	SER	PHE	ENGINEERED	UNP P37957

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Chain	Residue	Modelled	Actual	Comment	Reference
F	20	GLU	ALA	ENGINEERED	UNP P37957
F	89	TYR	ASN	ENGINEERED	UNP P37957
F	111	ASP	GLY	ENGINEERED	UNP P37957
F	114	PRO	LEU	ENGINEERED	UNP P37957
F	132	ASP	ALA	ENGINEERED	UNP P37957
F	157	MET	ILE	ENGINEERED	UNP P37957
F	166	TYR	ASN	ENGINEERED	UNP P37957
G	15	SER	ALA	ENGINEERED	UNP P37957
G	17	SER	PHE	ENGINEERED	UNP P37957
G	20	GLU	ALA	ENGINEERED	UNP P37957
G	89	TYR	ASN	ENGINEERED	UNP P37957
G	111	ASP	GLY	ENGINEERED	UNP P37957
G	114	PRO	LEU	ENGINEERED	UNP P37957
G	132	ASP	ALA	ENGINEERED	UNP P37957
G	157	MET	ILE	ENGINEERED	UNP P37957
G	166	TYR	ASN	ENGINEERED	UNP P37957
H	15	SER	ALA	ENGINEERED	UNP P37957
H	17	SER	PHE	ENGINEERED	UNP P37957
H	20	GLU	ALA	ENGINEERED	UNP P37957
H	89	TYR	ASN	ENGINEERED	UNP P37957
H	111	ASP	GLY	ENGINEERED	UNP P37957
H	114	PRO	LEU	ENGINEERED	UNP P37957
H	132	ASP	ALA	ENGINEERED	UNP P37957
H	157	MET	ILE	ENGINEERED	UNP P37957
H	166	TYR	ASN	ENGINEERED	UNP P37957
I	15	SER	ALA	ENGINEERED	UNP P37957
I	17	SER	PHE	ENGINEERED	UNP P37957
I	20	GLU	ALA	ENGINEERED	UNP P37957
I	89	TYR	ASN	ENGINEERED	UNP P37957
I	111	ASP	GLY	ENGINEERED	UNP P37957
I	114	PRO	LEU	ENGINEERED	UNP P37957
I	132	ASP	ALA	ENGINEERED	UNP P37957
I	157	MET	ILE	ENGINEERED	UNP P37957
I	166	TYR	ASN	ENGINEERED	UNP P37957
J	15	SER	ALA	ENGINEERED	UNP P37957
J	17	SER	PHE	ENGINEERED	UNP P37957
J	20	GLU	ALA	ENGINEERED	UNP P37957
J	89	TYR	ASN	ENGINEERED	UNP P37957
J	111	ASP	GLY	ENGINEERED	UNP P37957
J	114	PRO	LEU	ENGINEERED	UNP P37957
J	132	ASP	ALA	ENGINEERED	UNP P37957
J	157	MET	ILE	ENGINEERED	UNP P37957

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Chain	Residue	Modelled	Actual	Comment	Reference
J	166	TYR	ASN	ENGINEERED	UNP P37957
K	15	SER	ALA	ENGINEERED	UNP P37957
K	17	SER	PHE	ENGINEERED	UNP P37957
K	20	GLU	ALA	ENGINEERED	UNP P37957
K	89	TYR	ASN	ENGINEERED	UNP P37957
K	111	ASP	GLY	ENGINEERED	UNP P37957
K	114	PRO	LEU	ENGINEERED	UNP P37957
K	132	ASP	ALA	ENGINEERED	UNP P37957
K	157	MET	ILE	ENGINEERED	UNP P37957
K	166	TYR	ASN	ENGINEERED	UNP P37957
L	15	SER	ALA	ENGINEERED	UNP P37957
L	17	SER	PHE	ENGINEERED	UNP P37957
L	20	GLU	ALA	ENGINEERED	UNP P37957
L	89	TYR	ASN	ENGINEERED	UNP P37957
L	111	ASP	GLY	ENGINEERED	UNP P37957
L	114	PRO	LEU	ENGINEERED	UNP P37957
L	132	ASP	ALA	ENGINEERED	UNP P37957
L	157	MET	ILE	ENGINEERED	UNP P37957
L	166	TYR	ASN	ENGINEERED	UNP P37957

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	97	Total O 97 97	0	0
2	B	83	Total O 83 83	0	0
2	C	107	Total O 107 107	0	0
2	D	90	Total O 90 90	0	0
2	E	97	Total O 97 97	0	0
2	F	90	Total O 90 90	0	0
2	G	94	Total O 94 94	0	0
2	H	83	Total O 83 83	0	0
2	I	99	Total O 99 99	0	0
2	J	92	Total O 92 92	0	0

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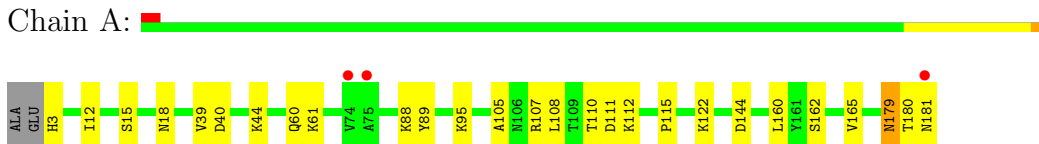
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	93	Total 93	O 93	0	0
2	L	105	Total 105	O 105	0	0

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.

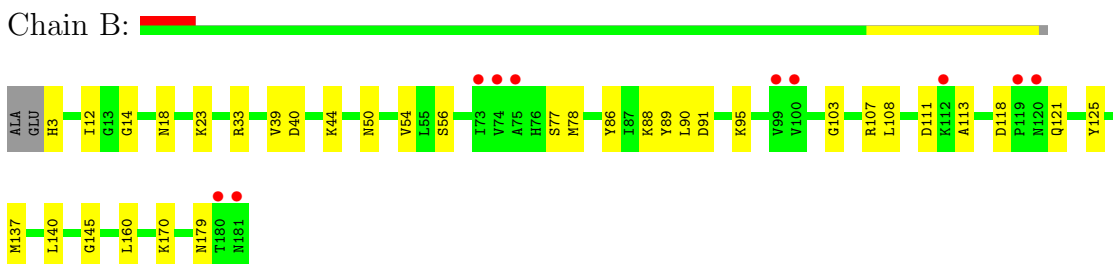
• Molecule 1: Lipase

Chain A:



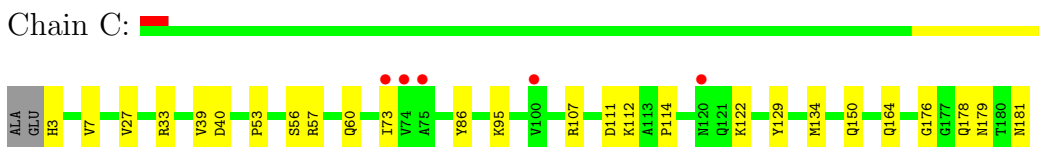
• Molecule 1: Lipase

Chain B:



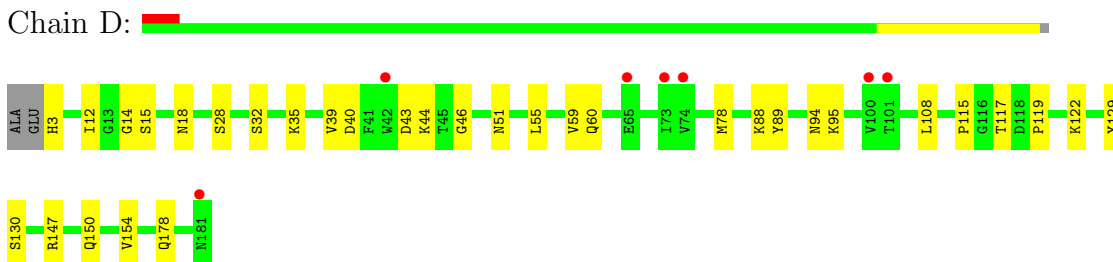
• Molecule 1: Lipase

Chain C:



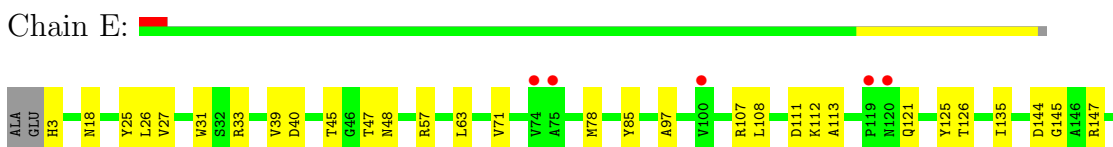
• Molecule 1: Lipase

Chain D:



• Molecule 1: Lipase

Chain E:





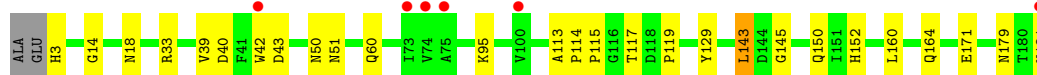
- Molecule 1: Lipase

Chain F:



- Molecule 1: Lipase

Chain G:



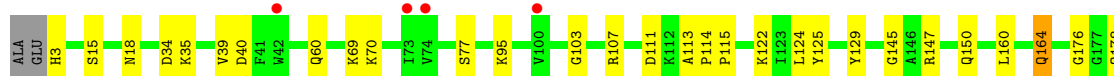
- Molecule 1: Lipase

Chain H:



- Molecule 1: Lipase

Chain I:



- Molecule 1: Lipase

Chain J:

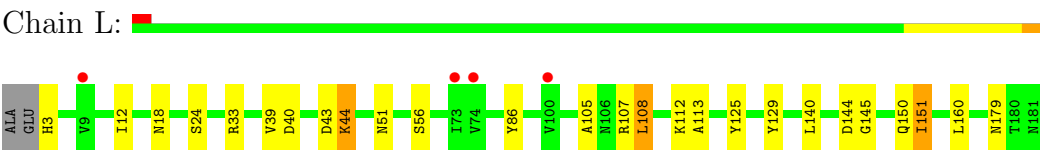


- Molecule 1: Lipase

Chain K:



- Molecule 1: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.28Å 198.04Å 197.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.18 24.89 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-2.18) 98.8 (24.89-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.17Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.245 0.204 , 0.205	Depositor DCC
R_{free} test set	6669 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 133208 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17510	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.31	0/1392	0.59	0/1884
1	B	0.32	0/1392	0.59	0/1884
1	C	0.33	0/1392	0.60	0/1884
1	D	0.32	0/1392	0.59	0/1884
1	E	0.31	0/1392	0.58	0/1884
1	F	0.32	0/1392	0.61	0/1884
1	G	0.32	0/1392	0.58	0/1884
1	H	0.31	0/1392	0.60	0/1884
1	I	0.32	0/1392	0.60	0/1884
1	J	0.31	0/1392	0.58	0/1884
1	K	0.32	0/1392	0.61	0/1884
1	L	0.33	0/1392	0.60	0/1884
All	All	0.32	0/16704	0.59	0/22608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1365	0	1339	24	0
1	B	1365	0	1339	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1365	0	1339	19	0
1	D	1365	0	1339	25	0
1	E	1365	0	1339	24	0
1	F	1365	0	1339	19	0
1	G	1365	0	1339	17	0
1	H	1365	0	1339	16	0
1	I	1365	0	1339	22	0
1	J	1365	0	1339	24	0
1	K	1365	0	1339	12	0
1	L	1365	0	1339	18	0
2	A	97	0	0	3	0
2	B	83	0	0	4	0
2	C	107	0	0	3	0
2	D	90	0	0	4	0
2	E	97	0	0	4	0
2	F	90	0	0	4	0
2	G	94	0	0	2	0
2	H	83	0	0	6	0
2	I	99	0	0	3	0
2	J	92	0	0	2	0
2	K	93	0	0	3	0
2	L	105	0	0	2	0
All	All	17510	0	16068	233	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (233) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:69:LYS:HG2	1:I:70:LYS:HG3	1.48	0.92
1:I:147:ARG:HB2	1:I:178:GLN:HG2	1.60	0.84
1:D:147:ARG:HB2	1:D:178:GLN:HG2	1.66	0.77
1:H:112:LYS:HG2	1:H:144:ASP:HB2	1.67	0.76
1:L:112:LYS:HG2	1:L:144:ASP:HB2	1.67	0.74
1:D:15:SER:H	1:D:18:ASN:ND2	1.84	0.74
1:E:156:HIS:HB3	1:F:137:MET:HE1	1.71	0.72
1:L:44:LYS:HE3	1:L:44:LYS:HA	1.72	0.71
1:L:107:ARG:HG3	1:L:140:LEU:HA	1.73	0.70
1:J:18:ASN:HB3	1:J:160:LEU:HD13	1.73	0.70
1:A:107:ARG:NH1	1:A:111:ASP:HB2	2.09	0.68
1:B:107:ARG:HG3	1:B:140:LEU:HA	1.74	0.68
1:F:33:ARG:HD2	2:F:269:HOH:O	1.93	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:129:TYR:O	1:L:151:ILE:HD13	1.96	0.66
1:B:18:ASN:HB3	1:B:160:LEU:HD13	1.76	0.66
1:J:145:GLY:O	1:J:179:ASN:HA	1.97	0.65
1:D:12:ILE:HD11	1:D:78:MET:HG3	1.79	0.65
1:C:107:ARG:NH1	1:C:111:ASP:HB2	2.12	0.65
1:L:18:ASN:HB3	1:L:160:LEU:HD13	1.79	0.64
1:B:3:HIS:HE1	2:B:183:HOH:O	1.80	0.64
1:F:3:HIS:HD2	2:F:188:HOH:O	1.81	0.63
1:A:60:GLN:NE2	1:A:95:LYS:NZ	2.47	0.63
1:A:88:LYS:HD3	1:A:89:TYR:CE1	2.34	0.62
1:D:78:MET:SD	1:D:108:LEU:HD12	2.40	0.62
1:K:3:HIS:HD2	2:K:249:HOH:O	1.82	0.61
1:E:107:ARG:HD3	1:E:111:ASP:OD1	2.00	0.61
1:D:115:PRO:HB3	1:D:122:LYS:HD2	1.81	0.61
1:E:135:ILE:HG13	1:F:137:MET:HE3	1.82	0.61
1:I:3:HIS:HE1	2:I:192:HOH:O	1.83	0.61
1:I:176:GLY:O	1:K:24:SER:HB3	2.00	0.60
1:D:12:ILE:HG12	2:D:271:HOH:O	2.02	0.59
1:C:164:GLN:HG2	2:C:239:HOH:O	2.02	0.59
1:H:78:MET:SD	1:H:108:LEU:HD12	2.42	0.59
1:K:60:GLN:NE2	1:K:95:LYS:NZ	2.51	0.59
1:J:107:ARG:NH1	1:J:111:ASP:HB2	2.17	0.59
1:K:60:GLN:NE2	1:K:95:LYS:HZ3	2.01	0.59
1:J:15:SER:H	1:J:18:ASN:ND2	2.01	0.58
1:D:60:GLN:NE2	1:D:95:LYS:HZ3	2.01	0.58
1:H:3:HIS:HD2	2:H:212:HOH:O	1.85	0.58
1:B:3:HIS:HD2	2:B:187:HOH:O	1.85	0.58
1:D:44:LYS:HB2	2:K:230:HOH:O	2.02	0.58
1:I:3:HIS:HD2	2:I:203:HOH:O	1.86	0.58
1:L:3:HIS:HD2	2:L:285:HOH:O	1.87	0.58
1:C:53:PRO:O	1:C:57:ARG:HD3	2.03	0.58
1:J:45:THR:OG1	1:J:47:THR:HG23	2.03	0.58
1:E:178:GLN:NE2	2:E:217:HOH:O	2.37	0.58
1:F:39:VAL:HG22	1:F:40:ASP:N	2.18	0.58
1:J:122:LYS:HD2	1:J:179:ASN:HB3	1.87	0.57
1:B:12:ILE:HG23	1:B:44:LYS:O	2.03	0.57
1:J:60:GLN:NE2	1:J:95:LYS:HZ3	2.04	0.56
1:C:60:GLN:NE2	1:C:95:LYS:NZ	2.54	0.56
1:I:15:SER:H	1:I:18:ASN:ND2	2.03	0.56
1:F:3:HIS:HE1	2:F:185:HOH:O	1.89	0.56
1:I:122:LYS:NZ	1:I:181:ASN:O	2.34	0.56
1:C:3:HIS:HD2	2:C:222:HOH:O	1.89	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:63:LEU:HD21	1:J:71:VAL:HG13	1.86	0.56
1:A:60:GLN:HE21	1:A:95:LYS:NZ	2.04	0.55
1:D:3:HIS:HE1	2:D:182:HOH:O	1.88	0.55
1:F:107:ARG:HG3	1:F:140:LEU:HA	1.89	0.55
1:B:39:VAL:HG22	1:B:40:ASP:N	2.22	0.55
1:K:27:VAL:HG21	1:K:33:ARG:HD2	1.87	0.55
1:E:3:HIS:HE1	2:E:189:HOH:O	1.90	0.55
1:A:3:HIS:HD2	2:A:209:HOH:O	1.89	0.54
1:G:33:ARG:HD2	2:G:217:HOH:O	2.06	0.54
1:B:23:LYS:HE3	2:B:214:HOH:O	2.08	0.54
1:D:60:GLN:NE2	1:D:95:LYS:NZ	2.55	0.54
1:D:3:HIS:HD2	2:D:183:HOH:O	1.89	0.54
1:D:117:THR:O	1:D:119:PRO:HD3	2.08	0.54
1:E:45:THR:OG1	1:E:47:THR:HG23	2.08	0.53
1:A:88:LYS:HD3	1:A:89:TYR:HE1	1.74	0.53
1:K:78:MET:SD	1:K:108:LEU:HD12	2.48	0.53
1:I:60:GLN:NE2	1:I:95:LYS:NZ	2.57	0.53
1:L:3:HIS:HE1	2:L:302:HOH:O	1.91	0.53
1:J:60:GLN:NE2	1:J:95:LYS:NZ	2.57	0.52
1:A:39:VAL:HG22	1:A:40:ASP:N	2.23	0.52
1:E:3:HIS:HD2	2:E:191:HOH:O	1.91	0.52
1:I:34:ASP:OD1	1:I:35:LYS:HG2	2.10	0.52
1:I:39:VAL:HG22	1:I:40:ASP:N	2.25	0.52
1:G:3:HIS:HE1	2:G:212:HOH:O	1.92	0.52
1:A:112:LYS:HG2	1:A:144:ASP:HB2	1.91	0.52
1:L:145:GLY:O	1:L:179:ASN:HA	2.10	0.52
1:I:18:ASN:HB3	1:I:160:LEU:HD13	1.92	0.52
1:E:112:LYS:HD3	1:E:144:ASP:HB2	1.92	0.52
1:E:63:LEU:HD21	1:E:71:VAL:HG13	1.90	0.52
1:B:78:MET:SD	1:B:108:LEU:HD12	2.50	0.52
1:E:39:VAL:HG22	1:E:40:ASP:N	2.25	0.51
1:F:15:SER:H	1:F:18:ASN:ND2	2.08	0.51
1:H:113:ALA:HB1	1:H:125:TYR:CD1	2.46	0.51
1:C:129:TYR:CE1	1:C:150:GLN:HB2	2.45	0.51
1:E:48:ASN:HB3	1:E:85:TYR:CG	2.47	0.50
1:E:145:GLY:HA2	1:E:180:THR:OG1	2.10	0.50
1:A:60:GLN:NE2	1:A:95:LYS:HZ1	2.09	0.50
1:J:12:ILE:HG23	1:J:44:LYS:O	2.12	0.50
1:D:43:ASP:HB3	1:D:51:ASN:HD21	1.75	0.50
1:J:108:LEU:HD21	1:L:12:ILE:CG2	2.41	0.50
1:I:145:GLY:HA3	1:I:181:ASN:ND2	2.27	0.50
1:H:44:LYS:HE2	1:H:44:LYS:HA	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:162:SER:HB3	1:F:165:VAL:HG23	1.94	0.49
1:H:178:GLN:HG2	1:H:179:ASN:N	2.27	0.49
1:B:91:ASP:OD2	1:B:95:LYS:NZ	2.44	0.49
1:C:39:VAL:HG22	1:C:40:ASP:N	2.27	0.49
1:A:60:GLN:NE2	1:A:95:LYS:HZ3	2.09	0.49
1:A:3:HIS:HE1	2:A:185:HOH:O	1.95	0.49
1:B:50:ASN:O	1:B:54:VAL:HG23	2.12	0.49
1:L:56:SER:HA	1:L:86:TYR:CE1	2.48	0.49
1:B:86:TYR:O	1:B:90:LEU:HB2	2.12	0.49
1:G:43:ASP:HB3	1:G:51:ASN:HD21	1.77	0.49
1:K:39:VAL:HG22	1:K:40:ASP:N	2.28	0.49
1:E:27:VAL:HG21	1:E:33:ARG:NH1	2.27	0.49
1:A:162:SER:HB3	1:A:165:VAL:HG23	1.95	0.49
1:E:113:ALA:HB1	1:E:125:TYR:CD1	2.48	0.48
1:D:35:LYS:HE3	2:D:188:HOH:O	2.13	0.48
1:A:18:ASN:HB3	1:A:160:LEU:HD13	1.94	0.48
1:E:18:ASN:HB3	1:E:160:LEU:HD13	1.93	0.48
1:G:60:GLN:NE2	1:G:95:LYS:HE2	2.28	0.48
1:B:113:ALA:HB1	1:B:125:TYR:CD1	2.48	0.48
1:J:39:VAL:HG22	1:J:40:ASP:N	2.28	0.48
1:J:3:HIS:HE1	2:J:269:HOH:O	1.96	0.48
1:C:176:GLY:O	1:L:24:SER:HB3	2.14	0.48
1:G:145:GLY:HA3	1:G:181:ASN:ND2	2.29	0.48
1:F:77:SER:HB3	2:F:199:HOH:O	2.13	0.48
1:L:105:ALA:O	1:L:108:LEU:HB2	2.13	0.48
1:E:25:TYR:CD2	1:E:166:TYR:HB3	2.49	0.47
1:C:33:ARG:NH2	2:C:218:HOH:O	2.47	0.47
1:A:15:SER:H	1:A:18:ASN:ND2	2.11	0.47
1:A:179:ASN:C	1:A:181:ASN:H	2.18	0.47
1:D:129:TYR:CE1	1:D:150:GLN:HB2	2.50	0.47
1:J:5:PRO:HG3	1:J:35:LYS:HE3	1.96	0.47
1:A:105:ALA:O	1:A:108:LEU:HB2	2.15	0.47
1:G:18:ASN:HB3	1:G:160:LEU:HD13	1.97	0.47
1:E:78:MET:SD	1:E:108:LEU:HD12	2.55	0.47
1:D:32:SER:HB3	1:D:35:LYS:HE2	1.97	0.47
1:C:60:GLN:HE21	1:C:95:LYS:HZ3	1.63	0.46
1:J:147:ARG:HB2	1:J:178:GLN:HB3	1.97	0.46
1:K:137:MET:HG3	2:K:306:HOH:O	2.15	0.46
1:G:114:PRO:HA	1:G:115:PRO:HD3	1.77	0.46
1:I:77:SER:HA	1:I:103:GLY:O	2.15	0.46
1:J:113:ALA:HB1	1:J:125:TYR:CD1	2.50	0.46
1:F:113:ALA:HB1	1:F:125:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:LYS:NZ	1:A:61:LYS:HB3	2.31	0.46
1:D:55:LEU:O	1:D:59:VAL:HG23	2.16	0.46
1:K:43:ASP:HB3	1:K:51:ASN:HD21	1.80	0.46
1:B:88:LYS:HD3	1:B:89:TYR:CZ	2.50	0.46
1:B:145:GLY:O	1:B:179:ASN:HA	2.15	0.46
1:B:89:TYR:O	1:B:90:LEU:HD23	2.15	0.46
1:L:113:ALA:HB1	1:L:125:TYR:CD1	2.51	0.46
1:G:14:GLY:CA	1:G:18:ASN:HD21	2.29	0.46
1:H:39:VAL:HG22	1:H:40:ASP:N	2.31	0.46
1:J:20:GLU:HA	1:J:20:GLU:OE1	2.16	0.46
1:E:97:ALA:CB	1:E:121:GLN:HE22	2.28	0.46
1:L:12:ILE:HG23	1:L:44:LYS:O	2.15	0.46
1:D:60:GLN:HE21	1:D:95:LYS:HZ3	1.62	0.45
1:C:7:VAL:HB	1:C:73:ILE:HD13	1.98	0.45
1:G:39:VAL:HG22	1:G:40:ASP:N	2.31	0.45
1:L:151:ILE:HD13	1:L:151:ILE:H	1.81	0.45
1:B:88:LYS:HD3	1:B:89:TYR:CE1	2.51	0.45
1:D:130:SER:HB2	1:D:154:VAL:HG13	1.98	0.45
1:I:114:PRO:HA	1:I:115:PRO:HD3	1.86	0.45
1:G:179:ASN:C	1:G:181:ASN:H	2.20	0.45
1:A:108:LEU:HD12	1:K:45:THR:HG22	1.98	0.45
1:K:145:GLY:O	1:K:179:ASN:HA	2.16	0.45
1:H:63:LEU:HD21	1:H:71:VAL:HG13	1.99	0.45
1:L:39:VAL:HG22	1:L:40:ASP:N	2.32	0.45
1:F:162:SER:HB3	1:F:165:VAL:CG2	2.46	0.45
1:C:27:VAL:HG21	1:C:33:ARG:HD2	1.98	0.45
1:J:59:VAL:O	1:J:63:LEU:HG	2.17	0.44
1:B:170:LYS:HE2	2:H:240:HOH:O	2.16	0.44
1:C:60:GLN:NE2	1:C:95:LYS:HZ3	2.15	0.44
1:I:60:GLN:NE2	1:I:95:LYS:HZ2	2.15	0.44
1:F:14:GLY:CA	1:F:18:ASN:HD21	2.30	0.44
1:C:56:SER:HA	1:C:86:TYR:CE1	2.52	0.44
1:D:39:VAL:HG22	1:D:40:ASP:N	2.32	0.44
1:H:43:ASP:HB3	1:H:51:ASN:HD21	1.82	0.44
1:A:162:SER:HB3	1:A:165:VAL:CG2	2.47	0.44
1:A:115:PRO:HB3	1:A:122:LYS:HG3	2.00	0.44
1:G:150:GLN:HE21	1:G:152:HIS:CE1	2.36	0.44
1:G:117:THR:O	1:G:119:PRO:HD3	2.18	0.44
1:L:43:ASP:HB3	1:L:51:ASN:HD21	1.83	0.44
1:A:115:PRO:HG2	2:A:222:HOH:O	2.17	0.43
1:H:25:TYR:O	1:H:29:GLN:HG2	2.18	0.43
1:B:77:SER:HA	1:B:103:GLY:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:124:LEU:HD22	1:I:178:GLN:HA	1.99	0.43
1:H:94:ASN:HA	2:H:189:HOH:O	2.17	0.43
1:I:34:ASP:OD1	1:I:35:LYS:HE3	2.18	0.43
1:J:44:LYS:HA	2:J:282:HOH:O	2.17	0.43
1:E:26:LEU:O	1:E:31:TRP:HB2	2.17	0.43
1:D:46:GLY:HA2	1:D:51:ASN:OD1	2.19	0.43
1:J:5:PRO:HG3	1:J:35:LYS:CE	2.48	0.43
1:G:113:ALA:N	1:G:143:LEU:HD22	2.34	0.43
1:E:135:ILE:HG13	1:F:137:MET:CE	2.48	0.43
1:L:129:TYR:CE1	1:L:150:GLN:HB2	2.54	0.43
1:G:129:TYR:CE1	1:G:150:GLN:HB2	2.54	0.43
1:B:107:ARG:NH1	1:B:111:ASP:HB3	2.33	0.43
1:D:14:GLY:O	1:D:44:LYS:HE3	2.18	0.43
1:C:60:GLN:HE21	1:C:95:LYS:NZ	2.14	0.43
1:A:107:ARG:HA	1:A:110:THR:O	2.19	0.43
1:H:3:HIS:HE1	2:H:213:HOH:O	2.01	0.43
1:C:134:MET:HE1	1:F:134:MET:SD	2.59	0.43
1:D:88:LYS:HD3	1:D:89:TYR:CE1	2.54	0.42
1:J:126:THR:OG1	1:J:177:GLY:HA2	2.19	0.42
1:K:15:SER:H	1:K:18:ASN:ND2	2.17	0.42
1:J:105:ALA:HB1	1:J:108:LEU:HD12	2.00	0.42
1:J:177:GLY:O	1:J:178:GLN:HB2	2.20	0.42
1:B:14:GLY:CA	1:B:18:ASN:HD21	2.33	0.42
1:D:94:ASN:HB3	1:D:117:THR:OG1	2.20	0.42
1:F:114:PRO:HA	1:F:115:PRO:HD3	1.80	0.42
1:F:12:ILE:HG12	1:F:45:THR:O	2.19	0.42
1:G:42:TRP:CH2	1:G:50:ASN:HB3	2.55	0.41
1:B:137:MET:HG3	2:B:242:HOH:O	2.18	0.41
1:A:60:GLN:HE21	1:A:95:LYS:HZ3	1.67	0.41
1:H:32:SER:HB2	1:H:35:LYS:CG	2.51	0.41
1:I:113:ALA:HB1	1:I:125:TYR:CD1	2.56	0.41
1:I:164:GLN:HG2	2:I:240:HOH:O	2.19	0.41
1:H:56:SER:HA	1:H:86:TYR:CE1	2.55	0.41
1:C:112:LYS:O	1:C:114:PRO:HD3	2.20	0.41
1:B:56:SER:HA	1:B:86:TYR:CE1	2.56	0.41
1:B:118:ASP:HB3	1:B:121:GLN:O	2.21	0.41
1:D:28:SER:HB2	1:G:171:GLU:HA	2.02	0.41
1:I:107:ARG:HG2	1:I:111:ASP:OD1	2.20	0.41
1:J:122:LYS:CD	1:J:179:ASN:HB3	2.51	0.41
1:I:60:GLN:HE22	1:I:95:LYS:NZ	2.19	0.41
1:I:129:TYR:CE1	1:I:150:GLN:HB2	2.56	0.41
1:G:150:GLN:HE21	1:G:152:HIS:HE1	1.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:18:ASN:ND2	2:H:192:HOH:O	2.54	0.41
1:E:126:THR:OG1	1:E:177:GLY:HA2	2.21	0.41
1:E:156:HIS:HB3	1:F:137:MET:CE	2.47	0.40
1:F:63:LEU:HD22	1:F:68:ALA:O	2.21	0.40
1:C:122:LYS:HE2	1:C:181:ASN:O	2.22	0.40
1:H:70:LYS:HE3	2:H:189:HOH:O	2.21	0.40
1:A:12:ILE:HG23	1:A:44:LYS:O	2.22	0.40
1:C:178:GLN:HG2	1:C:179:ASN:N	2.36	0.40
1:E:147:ARG:NH2	2:E:223:HOH:O	2.55	0.40
1:E:57:ARG:HH11	1:E:57:ARG:HG3	1.87	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	177/181 (98%)	170 (96%)	5 (3%)	2 (1%)	21	15
1	B	177/181 (98%)	171 (97%)	6 (3%)	0	100	100
1	C	177/181 (98%)	172 (97%)	5 (3%)	0	100	100
1	D	177/181 (98%)	173 (98%)	4 (2%)	0	100	100
1	E	177/181 (98%)	172 (97%)	5 (3%)	0	100	100
1	F	177/181 (98%)	171 (97%)	5 (3%)	1 (1%)	33	31
1	G	177/181 (98%)	171 (97%)	6 (3%)	0	100	100
1	H	177/181 (98%)	171 (97%)	6 (3%)	0	100	100
1	I	177/181 (98%)	170 (96%)	7 (4%)	0	100	100
1	J	177/181 (98%)	167 (94%)	8 (4%)	2 (1%)	21	15
1	K	177/181 (98%)	172 (97%)	5 (3%)	0	100	100
1	L	177/181 (98%)	173 (98%)	4 (2%)	0	100	100
All	All	2124/2172 (98%)	2053 (97%)	66 (3%)	5 (0%)	56	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	180	THR
1	J	177	GLY
1	F	179	ASN
1	J	93	GLY

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	148/149 (99%)	148 (100%)	0	100	100
1	B	148/149 (99%)	147 (99%)	1 (1%)	91	96
1	C	148/149 (99%)	148 (100%)	0	100	100
1	D	148/149 (99%)	148 (100%)	0	100	100
1	E	148/149 (99%)	148 (100%)	0	100	100
1	F	148/149 (99%)	146 (99%)	2 (1%)	78	87
1	G	148/149 (99%)	146 (99%)	2 (1%)	78	87
1	H	148/149 (99%)	147 (99%)	1 (1%)	91	96
1	I	148/149 (99%)	147 (99%)	1 (1%)	91	96
1	J	148/149 (99%)	147 (99%)	1 (1%)	91	96
1	K	148/149 (99%)	147 (99%)	1 (1%)	91	96
1	L	148/149 (99%)	144 (97%)	4 (3%)	57	66
All	All	1776/1788 (99%)	1763 (99%)	13 (1%)	91	96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	33	ARG
1	F	77	SER
1	F	137	MET
1	G	143	LEU
1	G	164	GLN

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Mol	Chain	Res	Type
1	H	57	ARG
1	I	164	GLN
1	J	157	MET
1	K	40	ASP
1	L	33	ARG
1	L	44	LYS
1	L	108	LEU
1	L	151	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	18	ASN
1	A	51	ASN
1	A	60	GLN
1	A	82	ASN
1	A	178	GLN
1	B	3	HIS
1	B	18	ASN
1	B	51	ASN
1	B	60	GLN
1	B	82	ASN
1	C	3	HIS
1	C	18	ASN
1	C	51	ASN
1	C	60	GLN
1	C	82	ASN
1	C	164	GLN
1	C	178	GLN
1	D	3	HIS
1	D	18	ASN
1	D	51	ASN
1	D	60	GLN
1	D	82	ASN
1	D	174	ASN
1	D	181	ASN
1	E	3	HIS
1	E	18	ASN
1	E	51	ASN
1	E	60	GLN
1	E	82	ASN

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Mol	Chain	Res	Type
1	E	121	GLN
1	E	164	GLN
1	E	178	GLN
1	F	3	HIS
1	F	18	ASN
1	F	51	ASN
1	F	60	GLN
1	F	82	ASN
1	G	3	HIS
1	G	18	ASN
1	G	51	ASN
1	G	60	GLN
1	G	82	ASN
1	G	150	GLN
1	G	164	GLN
1	H	3	HIS
1	H	18	ASN
1	H	51	ASN
1	H	60	GLN
1	H	82	ASN
1	H	121	GLN
1	I	3	HIS
1	I	18	ASN
1	I	51	ASN
1	I	60	GLN
1	I	82	ASN
1	I	164	GLN
1	J	3	HIS
1	J	18	ASN
1	J	51	ASN
1	J	60	GLN
1	J	82	ASN
1	J	120	ASN
1	J	178	GLN
1	K	3	HIS
1	K	18	ASN
1	K	51	ASN
1	K	60	GLN
1	K	82	ASN
1	L	3	HIS
1	L	18	ASN
1	L	51	ASN

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Mol	Chain	Res	Type
1	L	60	GLN
1	L	82	ASN
1	L	121	GLN
1	L	178	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	179/181 (98%)	-0.02	3 (1%) 67 69	19, 30, 46, 59	0
1	B	179/181 (98%)	0.12	10 (5%) 24 24	21, 32, 49, 66	0
1	C	179/181 (98%)	-0.15	5 (2%) 50 52	17, 26, 39, 51	0
1	D	179/181 (98%)	-0.01	7 (3%) 37 39	19, 30, 43, 55	0
1	E	179/181 (98%)	-0.05	6 (3%) 43 44	20, 29, 42, 51	0
1	F	179/181 (98%)	-0.12	3 (1%) 67 69	20, 30, 40, 57	0
1	G	179/181 (98%)	-0.02	6 (3%) 43 44	21, 29, 43, 61	0
1	H	179/181 (98%)	-0.05	3 (1%) 67 69	20, 30, 42, 53	0
1	I	179/181 (98%)	-0.05	5 (2%) 50 52	21, 29, 42, 54	0
1	J	179/181 (98%)	0.05	8 (4%) 32 33	21, 31, 48, 59	0
1	K	179/181 (98%)	-0.09	6 (3%) 43 44	19, 28, 42, 56	0
1	L	179/181 (98%)	-0.05	4 (2%) 59 60	19, 27, 41, 52	0
All	All	2148/2172 (98%)	-0.04	66 (3%) 47 48	17, 29, 43, 66	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	ASN	4.0
1	D	100	VAL	3.8
1	G	181	ASN	3.8
1	E	181	ASN	3.6
1	K	181	ASN	3.4
1	D	181	ASN	3.3
1	I	181	ASN	3.2
1	B	73	ILE	3.2
1	F	181	ASN	3.1
1	I	100	VAL	3.1
1	B	100	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	74	VAL	3.0
1	K	73	ILE	3.0
1	B	120	ASN	2.9
1	B	119	PRO	2.9
1	J	181	ASN	2.9
1	B	74	VAL	2.8
1	D	73	ILE	2.8
1	C	75	ALA	2.7
1	C	74	VAL	2.7
1	A	181	ASN	2.6
1	B	99	VAL	2.6
1	B	75	ALA	2.5
1	H	75	ALA	2.5
1	K	100	VAL	2.5
1	E	100	VAL	2.5
1	J	100	VAL	2.5
1	C	73	ILE	2.5
1	F	100	VAL	2.5
1	A	75	ALA	2.4
1	K	75	ALA	2.4
1	J	120	ASN	2.4
1	J	73	ILE	2.4
1	D	101	THR	2.3
1	E	75	ALA	2.3
1	I	73	ILE	2.3
1	L	74	VAL	2.3
1	G	42	TRP	2.3
1	G	100	VAL	2.2
1	E	120	ASN	2.2
1	E	119	PRO	2.2
1	J	99	VAL	2.2
1	L	100	VAL	2.2
1	D	42	TRP	2.2
1	H	181	ASN	2.2
1	I	42	TRP	2.2
1	I	74	VAL	2.2
1	K	99	VAL	2.2
1	L	73	ILE	2.2
1	C	120	ASN	2.2
1	F	75	ALA	2.1
1	C	100	VAL	2.1
1	E	74	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	75	ALA	2.1
1	J	75	ALA	2.1
1	H	73	ILE	2.1
1	G	74	VAL	2.1
1	L	9	VAL	2.1
1	D	65	GLU	2.1
1	A	74	VAL	2.1
1	B	112	LYS	2.1
1	J	74	VAL	2.0
1	J	49	TYR	2.0
1	B	180	THR	2.0
1	K	69	LYS	2.0
1	G	73	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.