Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2021 – 11:12 am GMT

PDB ID	:	7B1W
Title	:	Crystal structure of plastidial ribulose epimerase RPE1 from the model alga Chlamydomonas reinhardtii
Authors	:	Henri, J.; Zaffagnini, M.; Tedesco, D.; Crozet, P.; Lemaire, S.D.
Deposited on	:	2020-11-25
Resolution	:	1.94 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:

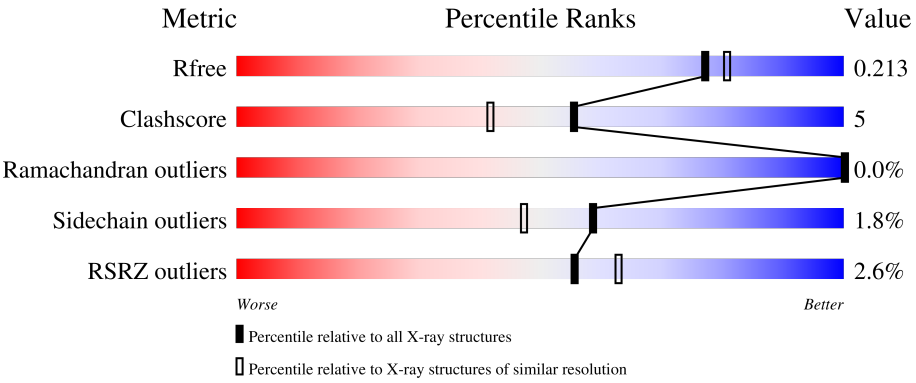
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 <=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	247	2% 84% 9% 7%
1	B	247	82% 11% 7%
1	C	247	83% 9% 7%
1	D	247	82% 11% • 6%
1	E	247	2% 82% 10% • 7%

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Mol	Chain	Length	Quality of chain
1	F	247	2% 85% 9% 5%
1	G	247	2% 83% 10% 7%
1	H	247	% 81% 12% 7%
1	I	247	2% 81% 12% 7%
1	J	247	82% 10% 7%
1	K	247	5% 81% 13% 7%
1	L	247	9% 74% 18% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22618 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 Ribulose-phosphate 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	229	Total	C	N	O	S	0	0	0
			1732	1096	302	325	9			
1	A	230	Total	C	N	O	S	0	0	0
			1739	1100	303	327	9			
1	B	229	Total	C	N	O	S	0	0	0
			1732	1096	302	325	9			
1	C	229	Total	C	N	O	S	0	0	0
			1732	1096	302	325	9			
1	D	231	Total	C	N	O	S	0	0	0
			1744	1103	304	328	9			
1	E	229	Total	C	N	O	S	0	0	0
			1732	1096	302	325	9			
1	F	234	Total	C	N	O	S	0	0	0
			1768	1118	308	332	10			
1	G	230	Total	C	N	O	S	0	0	0
			1739	1100	303	327	9			
1	H	230	Total	C	N	O	S	0	0	0
			1739	1100	303	327	9			
1	I	230	Total	C	N	O	S	0	0	0
			1739	1100	303	327	9			
1	K	230	Total	C	N	O	S	0	0	0
			1739	1100	303	327	9			
1	L	229	Total	C	N	O	S	0	0	0
			1732	1096	302	325	9			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	19	MET	-	initiating methionine	UNP A8IKW6
J	20	HIS	-	expression tag	UNP A8IKW6
J	21	HIS	-	expression tag	UNP A8IKW6
J	22	HIS	-	expression tag	UNP A8IKW6
J	23	HIS	-	expression tag	UNP A8IKW6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	24	HIS	-	expression tag	UNP A8IKW6
J	25	HIS	-	expression tag	UNP A8IKW6
J	26	THR	-	expression tag	UNP A8IKW6
J	27	MET	-	expression tag	UNP A8IKW6
A	19	MET	-	initiating methionine	UNP A8IKW6
A	20	HIS	-	expression tag	UNP A8IKW6
A	21	HIS	-	expression tag	UNP A8IKW6
A	22	HIS	-	expression tag	UNP A8IKW6
A	23	HIS	-	expression tag	UNP A8IKW6
A	24	HIS	-	expression tag	UNP A8IKW6
A	25	HIS	-	expression tag	UNP A8IKW6
A	26	THR	-	expression tag	UNP A8IKW6
A	27	MET	-	expression tag	UNP A8IKW6
B	19	MET	-	initiating methionine	UNP A8IKW6
B	20	HIS	-	expression tag	UNP A8IKW6
B	21	HIS	-	expression tag	UNP A8IKW6
B	22	HIS	-	expression tag	UNP A8IKW6
B	23	HIS	-	expression tag	UNP A8IKW6
B	24	HIS	-	expression tag	UNP A8IKW6
B	25	HIS	-	expression tag	UNP A8IKW6
B	26	THR	-	expression tag	UNP A8IKW6
B	27	MET	-	expression tag	UNP A8IKW6
C	19	MET	-	initiating methionine	UNP A8IKW6
C	20	HIS	-	expression tag	UNP A8IKW6
C	21	HIS	-	expression tag	UNP A8IKW6
C	22	HIS	-	expression tag	UNP A8IKW6
C	23	HIS	-	expression tag	UNP A8IKW6
C	24	HIS	-	expression tag	UNP A8IKW6
C	25	HIS	-	expression tag	UNP A8IKW6
C	26	THR	-	expression tag	UNP A8IKW6
C	27	MET	-	expression tag	UNP A8IKW6
D	19	MET	-	initiating methionine	UNP A8IKW6
D	20	HIS	-	expression tag	UNP A8IKW6
D	21	HIS	-	expression tag	UNP A8IKW6
D	22	HIS	-	expression tag	UNP A8IKW6
D	23	HIS	-	expression tag	UNP A8IKW6
D	24	HIS	-	expression tag	UNP A8IKW6
D	25	HIS	-	expression tag	UNP A8IKW6
D	26	THR	-	expression tag	UNP A8IKW6
D	27	MET	-	expression tag	UNP A8IKW6
E	19	MET	-	initiating methionine	UNP A8IKW6
E	20	HIS	-	expression tag	UNP A8IKW6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	21	HIS	-	expression tag	UNP A8IKW6
E	22	HIS	-	expression tag	UNP A8IKW6
E	23	HIS	-	expression tag	UNP A8IKW6
E	24	HIS	-	expression tag	UNP A8IKW6
E	25	HIS	-	expression tag	UNP A8IKW6
E	26	THR	-	expression tag	UNP A8IKW6
E	27	MET	-	expression tag	UNP A8IKW6
F	19	MET	-	initiating methionine	UNP A8IKW6
F	20	HIS	-	expression tag	UNP A8IKW6
F	21	HIS	-	expression tag	UNP A8IKW6
F	22	HIS	-	expression tag	UNP A8IKW6
F	23	HIS	-	expression tag	UNP A8IKW6
F	24	HIS	-	expression tag	UNP A8IKW6
F	25	HIS	-	expression tag	UNP A8IKW6
F	26	THR	-	expression tag	UNP A8IKW6
F	27	MET	-	expression tag	UNP A8IKW6
G	19	MET	-	initiating methionine	UNP A8IKW6
G	20	HIS	-	expression tag	UNP A8IKW6
G	21	HIS	-	expression tag	UNP A8IKW6
G	22	HIS	-	expression tag	UNP A8IKW6
G	23	HIS	-	expression tag	UNP A8IKW6
G	24	HIS	-	expression tag	UNP A8IKW6
G	25	HIS	-	expression tag	UNP A8IKW6
G	26	THR	-	expression tag	UNP A8IKW6
G	27	MET	-	expression tag	UNP A8IKW6
H	19	MET	-	initiating methionine	UNP A8IKW6
H	20	HIS	-	expression tag	UNP A8IKW6
H	21	HIS	-	expression tag	UNP A8IKW6
H	22	HIS	-	expression tag	UNP A8IKW6
H	23	HIS	-	expression tag	UNP A8IKW6
H	24	HIS	-	expression tag	UNP A8IKW6
H	25	HIS	-	expression tag	UNP A8IKW6
H	26	THR	-	expression tag	UNP A8IKW6
H	27	MET	-	expression tag	UNP A8IKW6
I	19	MET	-	initiating methionine	UNP A8IKW6
I	20	HIS	-	expression tag	UNP A8IKW6
I	21	HIS	-	expression tag	UNP A8IKW6
I	22	HIS	-	expression tag	UNP A8IKW6
I	23	HIS	-	expression tag	UNP A8IKW6
I	24	HIS	-	expression tag	UNP A8IKW6
I	25	HIS	-	expression tag	UNP A8IKW6
I	26	THR	-	expression tag	UNP A8IKW6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	27	MET	-	expression tag	UNP A8IKW6
K	19	MET	-	initiating methionine	UNP A8IKW6
K	20	HIS	-	expression tag	UNP A8IKW6
K	21	HIS	-	expression tag	UNP A8IKW6
K	22	HIS	-	expression tag	UNP A8IKW6
K	23	HIS	-	expression tag	UNP A8IKW6
K	24	HIS	-	expression tag	UNP A8IKW6
K	25	HIS	-	expression tag	UNP A8IKW6
K	26	THR	-	expression tag	UNP A8IKW6
K	27	MET	-	expression tag	UNP A8IKW6
L	19	MET	-	initiating methionine	UNP A8IKW6
L	20	HIS	-	expression tag	UNP A8IKW6
L	21	HIS	-	expression tag	UNP A8IKW6
L	22	HIS	-	expression tag	UNP A8IKW6
L	23	HIS	-	expression tag	UNP A8IKW6
L	24	HIS	-	expression tag	UNP A8IKW6
L	25	HIS	-	expression tag	UNP A8IKW6
L	26	THR	-	expression tag	UNP A8IKW6
L	27	MET	-	expression tag	UNP A8IKW6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0

- Molecule 3 is water.

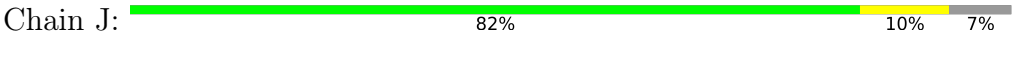
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	197	Total O 197 197	0	0
3	A	177	Total O 177 177	0	0
3	B	155	Total O 155 155	0	0
3	C	191	Total O 191 191	0	0
3	D	167	Total O 167 167	0	0
3	E	148	Total O 148 148	0	0
3	F	163	Total O 163 163	0	0
3	G	118	Total O 118 118	0	0
3	H	149	Total O 149 149	0	0
3	I	96	Total O 96 96	0	0
3	K	107	Total O 107 107	0	0
3	L	71	Total O 71 71	0	0

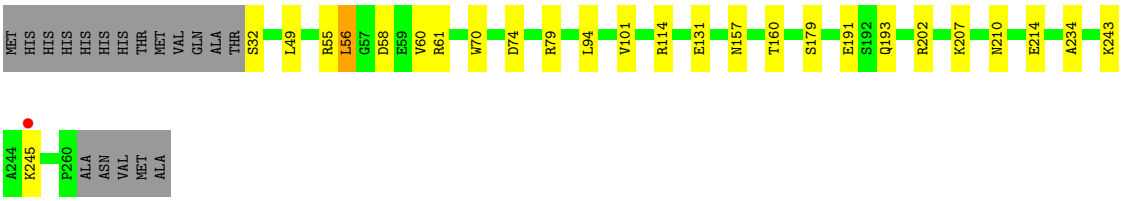
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ribulose-phosphate 3-epimerase

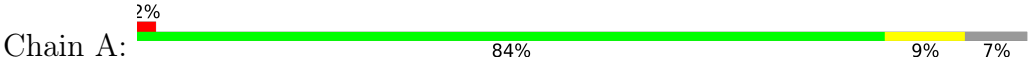
Chain J:

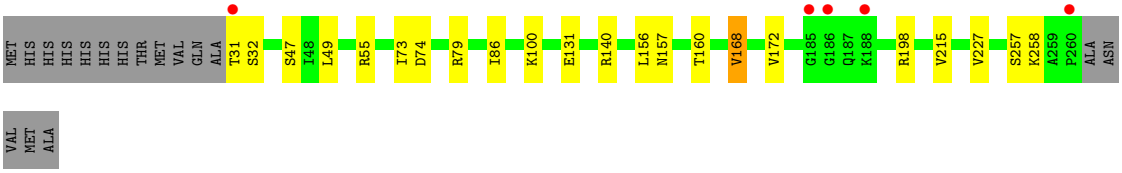




• Molecule 1: Ribulose-phosphate 3-epimerase

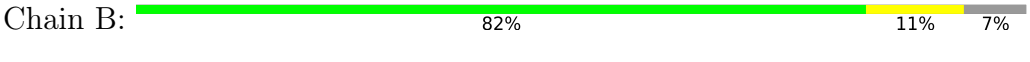
Chain A:

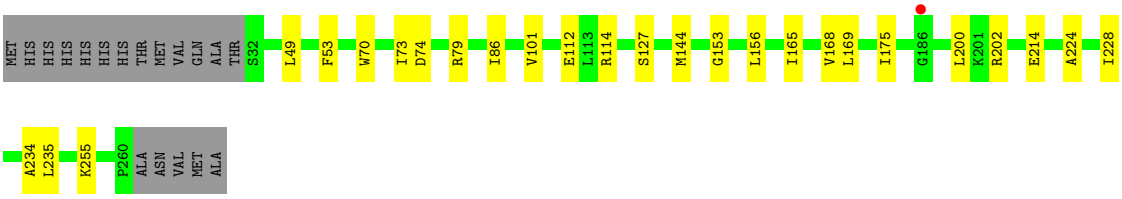




• Molecule 1: Ribulose-phosphate 3-epimerase

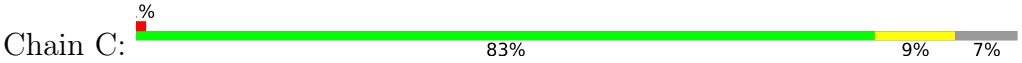
Chain B:

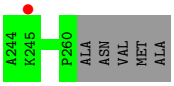




• Molecule 1: Ribulose-phosphate 3-epimerase

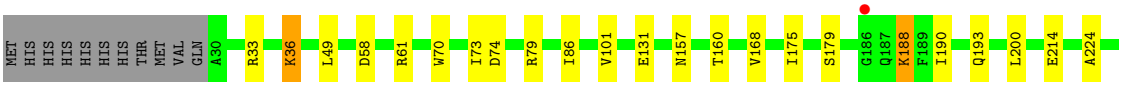
Chain C:

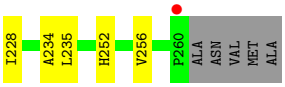




• Molecule 1: Ribulose-phosphate 3-epimerase

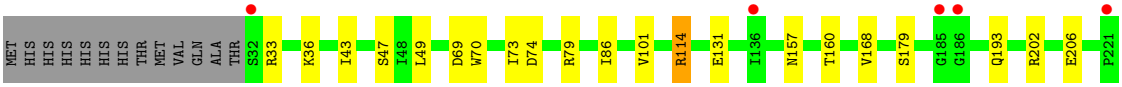
Chain D:

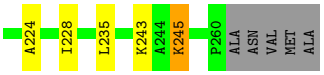




• Molecule 1: Ribulose-phosphate 3-epimerase

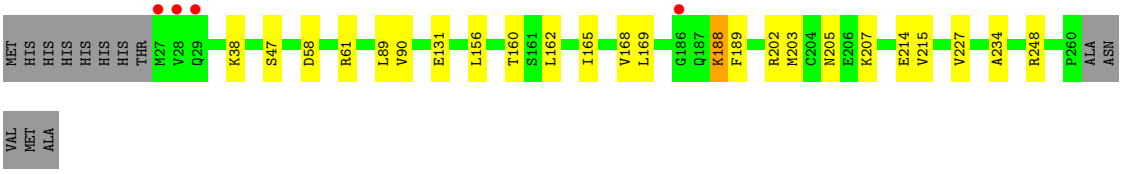
Chain E:





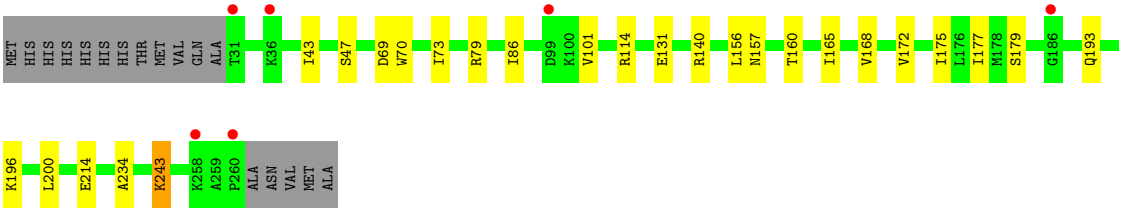
• Molecule 1: Ribulose-phosphate 3-epimerase

Chain F:



• Molecule 1: Ribulose-phosphate 3-epimerase

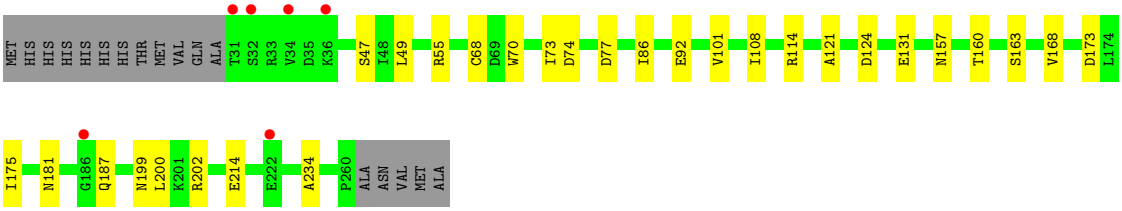
Chain G:



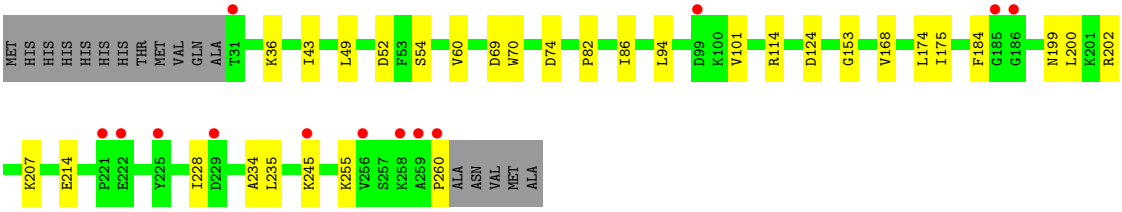
• Molecule 1: Ribulose-phosphate 3-epimerase

Chain H:

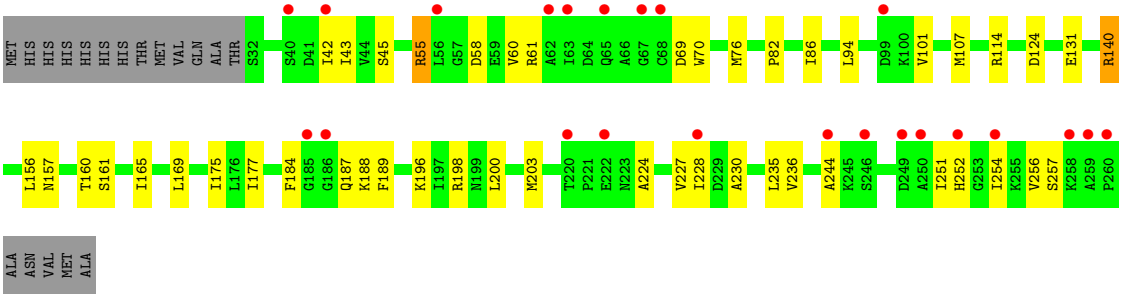
• Molecule 1: Ribulose-phosphate 3-epimerase



• Molecule 1: Ribulose-phosphate 3-epimerase



• Molecule 1: Ribulose-phosphate 3-epimerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.29Å 297.32Å 77.75Å 90.00° 116.30° 90.00°	Depositor
Resolution (Å)	49.29 – 1.94 49.55 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.29-1.94) 98.7 (49.55-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.184 , 0.214 0.184 , 0.213	Depositor DCC
R_{free} test set	2409 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22618	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	0.45	0/1767	0.61	0/2396
1	B	0.42	0/1760	0.59	0/2386
1	C	0.43	0/1760	0.60	1/2386 (0.0%)
1	D	0.41	0/1772	0.56	0/2403
1	E	0.41	0/1760	0.58	0/2386
1	F	0.42	0/1796	0.57	0/2435
1	G	0.40	0/1767	0.55	0/2396
1	H	0.40	0/1767	0.57	0/2396
1	I	0.36	0/1767	0.52	0/2396
1	J	0.45	0/1760	0.60	0/2386
1	K	0.36	0/1767	0.53	0/2396
1	L	0.36	0/1760	0.52	0/2386
All	All	0.41	0/21203	0.57	1/28748 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	188	LYS	CA-CB-CG	5.20	124.83	113.40

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	1739	0	1789	17	0
1	B	1732	0	1782	14	0
1	C	1732	0	1782	13	0
1	D	1744	0	1794	21	0
1	E	1732	0	1782	14	0
1	F	1768	0	1820	16	0
1	G	1739	0	1789	13	0
1	H	1739	0	1789	20	0
1	I	1739	0	1789	19	0
1	J	1732	0	1782	20	0
1	K	1739	0	1789	16	0
1	L	1732	0	1782	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	177	0	0	3	0
3	B	155	0	0	1	0
3	C	191	0	0	4	1
3	D	167	0	0	2	1
3	E	148	0	0	2	0
3	F	163	0	0	1	1
3	G	118	0	0	1	0
3	H	149	0	0	2	0
3	I	96	0	0	4	0
3	J	197	0	0	10	1
3	K	107	0	0	2	0
3	L	71	0	0	5	0
All	All	22618	0	21469	214	2

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 5.

All (214) 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:E:245:LYS:NZ	3:E:401:HOH:O	2.03	0.88
1:J:207:LYS:NZ	3:J:402:HOH:O	2.11	0.82
1:D:188:LYS:NZ	3:D:401:HOH:O	2.17	0.78
1:L:114:ARG:NH2	3:L:403:HOH:O	2.17	0.75
1:L:43:ILE:HG23	1:L:69:ASP:HB2	1.70	0.72
1:E:114:ARG:NH2	3:E:402:HOH:O	2.20	0.72
1:J:191:GLU:OE1	3:J:401:HOH:O	2.08	0.71
1:A:258:LYS:HE3	1:A:258:LYS:HA	1.72	0.71
1:D:131:GLU:OE2	1:D:160:THR:HG21	1.91	0.70
1:L:227:VAL:O	3:L:401:HOH:O	2.10	0.70
1:F:131:GLU:OE2	1:F:160:THR:HG21	1.91	0.70
1:J:61:ARG:NH2	3:J:404:HOH:O	2.24	0.70
1:K:199:ASN:OD1	1:K:202:ARG:NH2	2.26	0.69
1:A:257:SER:O	1:A:258:LYS:HD2	1.93	0.69
1:J:131:GLU:OE2	1:J:160:THR:HG21	1.94	0.68
1:J:202:ARG:NH1	3:J:403:HOH:O	2.23	0.67
1:A:198:ARG:NH1	3:A:401:HOH:O	2.27	0.67
1:A:55:ARG:NH2	3:A:402:HOH:O	2.28	0.66
1:B:156:LEU:HD11	1:B:165:ILE:HD13	1.78	0.66
1:E:73:ILE:HG23	1:E:86:ILE:HD11	1.76	0.66
1:I:199:ASN:OD1	1:I:202:ARG:NH2	2.29	0.66
1:K:175:ILE:HD13	1:K:200:LEU:HD11	1.78	0.65
1:I:92:GLU:HB2	3:I:408:HOH:O	1.97	0.64
1:E:131:GLU:OE2	1:E:160:THR:HG21	1.97	0.63
1:D:79:ARG:HG3	1:G:79:ARG:HG3	1.80	0.63
1:L:198:ARG:HG3	1:L:230:ALA:HB1	1.81	0.63
1:L:131:GLU:OE2	1:L:160:THR:HG21	1.97	0.63
1:A:131:GLU:OE2	1:A:160:THR:HG21	1.99	0.63
1:G:131:GLU:OE2	1:G:160:THR:HG21	1.98	0.62
1:L:224:ALA:HB2	1:L:254:ILE:CD1	2.29	0.62
1:E:33:ARG:HA	1:E:36:LYS:HE3	1.80	0.62
1:C:131:GLU:OE2	1:C:160:THR:HG21	2.00	0.61
1:D:228:ILE:HD11	1:D:235:LEU:HD21	1.82	0.61
1:D:224:ALA:O	1:D:228:ILE:HG12	2.00	0.61
1:I:55:ARG:NH2	3:I:405:HOH:O	2.32	0.61
1:J:79:ARG:HG3	1:E:79:ARG:HG3	1.81	0.60
1:L:42:ILE:HD13	1:L:228:ILE:HD12	1.82	0.60
1:F:215:VAL:HG21	1:F:227:VAL:HG13	1.84	0.59
1:B:112:GLU:HA	1:B:144:MET:HE1	1.84	0.59
1:D:157:ASN:HB2	1:D:160:THR:HG23	1.84	0.59
1:H:61:ARG:NH2	3:H:403:HOH:O	2.36	0.59
1:L:224:ALA:HB2	1:L:254:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:HD2	1:H:229:ASP:OD1	2.02	0.59
1:L:224:ALA:O	1:L:227:VAL:N	2.36	0.59
1:K:228:ILE:HD11	1:K:235:LEU:HD11	1.86	0.57
1:F:58:ASP:OD1	1:F:61:ARG:NH1	2.37	0.57
1:L:244:ALA:O	3:L:402:HOH:O	2.17	0.57
1:C:73:ILE:HG23	1:C:86:ILE:HD11	1.86	0.56
1:I:49:LEU:HG	1:I:74:ASP:HB2	1.87	0.56
1:A:79:ARG:HG3	1:B:79:ARG:HG3	1.88	0.56
1:L:230:ALA:HB3	3:L:401:HOH:O	2.06	0.56
1:L:76:MET:HG2	1:L:107:MET:HE3	1.87	0.55
1:L:228:ILE:HD11	1:L:235:LEU:HD11	1.88	0.55
1:L:198:ARG:HG3	1:L:230:ALA:CB	2.36	0.55
1:F:162:LEU:HB3	1:F:203:MET:HE1	1.88	0.55
1:H:157:ASN:HB2	1:H:160:THR:HG23	1.88	0.55
1:E:157:ASN:HB2	1:E:160:THR:HG23	1.88	0.54
1:F:89:LEU:HD12	1:F:90:VAL:HG23	1.88	0.54
1:I:157:ASN:HB2	1:I:160:THR:HG23	1.88	0.54
1:B:228:ILE:HD11	1:B:235:LEU:HD11	1.90	0.54
1:I:131:GLU:OE2	1:I:160:THR:HG21	2.08	0.54
1:L:188:LYS:HE3	1:L:189:PHE:H	1.72	0.54
1:J:55:ARG:NE	3:J:406:HOH:O	2.31	0.54
1:L:45:SER:O	1:L:236:VAL:HA	2.07	0.54
1:L:86:ILE:C	1:L:86:ILE:HD12	2.27	0.53
1:A:55:ARG:NH1	3:A:408:HOH:O	2.42	0.52
1:K:70:TRP:CD1	1:K:101:VAL:HB	2.44	0.52
1:L:175:ILE:HD13	1:L:200:LEU:HD11	1.91	0.52
1:H:31:THR:N	3:H:407:HOH:O	2.42	0.52
1:J:58:ASP:OD1	1:J:61:ARG:NH1	2.42	0.52
1:L:70:TRP:CD1	1:L:101:VAL:HB	2.44	0.52
1:D:190:ILE:HG23	3:D:416:HOH:O	2.09	0.52
1:L:187:GLN:O	3:L:404:HOH:O	2.18	0.51
1:A:157:ASN:HB2	1:A:160:THR:HG23	1.92	0.51
1:C:55:ARG:NE	3:C:408:HOH:O	2.43	0.51
1:F:205:ASN:ND2	3:F:405:HOH:O	2.42	0.51
1:D:58:ASP:OD1	1:D:61:ARG:NH1	2.43	0.51
1:H:131:GLU:OE2	1:H:160:THR:HG21	2.10	0.51
1:H:187:GLN:HE22	1:L:140:ARG:NH1	2.09	0.51
1:K:260:PRO:O	3:K:401:HOH:O	2.19	0.51
1:F:215:VAL:HG21	1:F:227:VAL:CG1	2.41	0.51
1:J:157:ASN:HB2	1:J:160:THR:HG23	1.91	0.51
1:B:49:LEU:HG	1:B:74:ASP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:ILE:HD13	1:H:200:LEU:HD11	1.93	0.49
1:L:82:PRO:HG3	1:L:184:PHE:CE2	2.47	0.49
1:J:179:SER:HA	1:J:193:GLN:HG3	1.95	0.49
1:L:169:LEU:HD11	1:L:203:MET:HE3	1.95	0.49
1:K:49:LEU:HG	1:K:74:ASP:HB2	1.95	0.49
1:I:181:ASN:HB2	1:I:187:GLN:HE22	1.77	0.49
1:D:175:ILE:HD13	1:D:200:LEU:HD11	1.94	0.49
1:J:214:GLU:HA	1:J:234:ALA:O	2.14	0.48
1:I:163:SER:O	1:L:161:SER:HB2	2.12	0.48
1:L:60:VAL:HG21	1:L:94:LEU:HD22	1.94	0.48
1:H:228:ILE:HD11	1:H:235:LEU:HD21	1.95	0.48
1:L:55:ARG:HH11	1:L:55:ARG:HG2	1.78	0.48
1:A:73:ILE:HG23	1:A:86:ILE:HD11	1.94	0.48
1:G:214:GLU:HA	1:G:234:ALA:O	2.14	0.48
1:A:73:ILE:CG2	1:A:86:ILE:HD11	2.44	0.48
1:F:214:GLU:HA	1:F:234:ALA:O	2.14	0.48
1:G:175:ILE:HD13	1:G:200:LEU:HD11	1.96	0.48
1:G:157:ASN:HB2	1:G:160:THR:HG23	1.95	0.48
1:C:188:LYS:NZ	3:C:402:HOH:O	2.26	0.47
1:E:43:ILE:HG23	1:E:69:ASP:HB2	1.95	0.47
1:D:70:TRP:CD1	1:D:101:VAL:HB	2.50	0.47
1:H:70:TRP:CD1	1:H:101:VAL:HB	2.49	0.47
1:K:52:ASP:OD1	1:K:54:SER:OG	2.24	0.47
1:J:207:LYS:O	1:J:207:LYS:HG2	2.15	0.47
1:G:70:TRP:CD1	1:G:101:VAL:HB	2.49	0.47
1:J:32:SER:N	3:J:411:HOH:O	2.48	0.47
1:A:215:VAL:HG21	1:A:227:VAL:HG13	1.95	0.46
1:K:214:GLU:HA	1:K:234:ALA:O	2.14	0.46
3:J:408:HOH:O	1:F:202:ARG:NE	2.38	0.46
1:C:70:TRP:CD1	1:C:101:VAL:HB	2.50	0.46
1:H:127:SER:HB3	1:H:153:GLY:HA3	1.96	0.46
1:C:243:LYS:HE3	3:C:469:HOH:O	2.16	0.46
1:I:175:ILE:HD13	1:I:200:LEU:HD11	1.97	0.46
1:D:228:ILE:CD1	1:D:235:LEU:HD21	2.44	0.46
1:I:101:VAL:HG13	1:I:124:ASP:HB2	1.98	0.46
1:J:70:TRP:CD1	1:J:101:VAL:HB	2.51	0.46
1:J:243:LYS:HE3	3:J:468:HOH:O	2.16	0.46
1:D:73:ILE:HG23	1:D:86:ILE:HD11	1.97	0.45
1:B:73:ILE:CG2	1:B:86:ILE:HD11	2.46	0.45
1:J:49:LEU:HG	1:J:74:ASP:HB2	1.98	0.45
1:H:168:VAL:HG13	1:H:172:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:VAL:HG13	1:L:124:ASP:HB2	1.99	0.45
1:C:224:ALA:O	1:C:228:ILE:HG12	2.17	0.45
1:I:70:TRP:CD1	1:I:101:VAL:HB	2.52	0.45
1:L:86:ILE:HD12	1:L:86:ILE:O	2.17	0.45
1:L:251:ILE:O	1:L:254:ILE:HG22	2.17	0.45
1:G:168:VAL:HG13	1:G:172:VAL:HG13	1.99	0.45
1:L:224:ALA:HB2	1:L:254:ILE:HD12	1.99	0.45
1:K:101:VAL:HG13	1:K:124:ASP:HB2	1.99	0.45
1:A:49:LEU:HG	1:A:74:ASP:HB2	1.98	0.45
1:C:61:ARG:NH2	3:C:416:HOH:O	2.49	0.45
1:L:58:ASP:OD1	1:L:61:ARG:NH1	2.50	0.45
1:H:58:ASP:OD1	1:H:61:ARG:NH1	2.50	0.44
1:L:156:LEU:HD11	1:L:165:ILE:HD13	1.99	0.44
1:D:49:LEU:HG	1:D:74:ASP:HB2	2.00	0.44
1:J:210:ASN:ND2	3:J:408:HOH:O	2.38	0.44
1:E:228:ILE:HD11	1:E:235:LEU:HD21	1.99	0.44
1:L:252:HIS:HE1	1:L:256:VAL:HG11	1.83	0.44
1:D:33:ARG:HA	1:D:36:LYS:HE2	1.99	0.44
1:K:43:ILE:HG23	1:K:69:ASP:HB2	2.00	0.44
1:A:31:THR:OG1	1:D:252:HIS:CG	2.71	0.44
1:I:121:ALA:HA	3:I:408:HOH:O	2.16	0.44
1:I:181:ASN:H	1:I:187:GLN:CD	2.18	0.44
1:F:38:LYS:HB2	1:F:38:LYS:HE2	1.78	0.43
1:F:207:LYS:HG3	1:F:207:LYS:O	2.18	0.43
1:K:60:VAL:HG21	1:K:94:LEU:HD22	1.99	0.43
1:H:187:GLN:HE22	1:L:140:ARG:HH11	1.64	0.43
1:K:86:ILE:HD12	1:K:86:ILE:O	2.17	0.43
1:B:214:GLU:HA	1:B:234:ALA:O	2.19	0.43
1:I:73:ILE:HG23	1:I:86:ILE:HD11	1.98	0.43
1:J:245:LYS:HG2	3:J:471:HOH:O	2.18	0.43
1:B:70:TRP:CD1	1:B:101:VAL:HB	2.54	0.43
1:B:224:ALA:O	1:B:228:ILE:HG12	2.18	0.43
1:E:179:SER:HA	1:E:193:GLN:HG3	2.01	0.43
1:K:255:LYS:NZ	3:K:418:HOH:O	2.52	0.43
1:G:43:ILE:HG23	1:G:69:ASP:HB2	2.00	0.43
1:J:60:VAL:HG21	1:J:94:LEU:HD22	1.99	0.43
1:G:156:LEU:HD11	1:G:165:ILE:HD13	2.01	0.43
1:F:203:MET:HB3	1:F:203:MET:HE3	1.75	0.42
1:H:43:ILE:HG23	1:H:69:ASP:HB2	2.00	0.42
1:H:157:ASN:HB2	1:H:160:THR:CG2	2.49	0.42
1:K:82:PRO:HG3	1:K:184:PHE:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD12	1:A:156:LEU:N	2.35	0.42
1:C:58:ASP:OD1	1:C:61:ARG:NH1	2.49	0.42
1:E:224:ALA:O	1:E:228:ILE:HG12	2.19	0.42
1:F:156:LEU:HD11	1:F:165:ILE:HD13	2.02	0.42
1:A:215:VAL:HG21	1:A:227:VAL:CG1	2.49	0.42
1:E:70:TRP:CD1	1:E:101:VAL:HB	2.55	0.42
1:L:157:ASN:HB2	1:L:160:THR:HG23	2.00	0.42
1:B:255:LYS:NZ	3:B:414:HOH:O	2.51	0.42
1:D:252:HIS:O	1:D:256:VAL:HG22	2.18	0.42
1:I:173:ASP:OD1	3:I:401:HOH:O	2.21	0.42
1:K:43:ILE:HG21	1:K:70:TRP:CE2	2.55	0.42
1:L:177:ILE:HD12	1:L:196:LYS:HD3	2.01	0.42
1:C:127:SER:HB3	1:C:153:GLY:HA3	2.01	0.42
1:E:49:LEU:HG	1:E:74:ASP:HB2	2.02	0.42
1:H:49:LEU:HG	1:H:74:ASP:HB2	2.01	0.42
1:H:202:ARG:O	1:H:206:GLU:HG2	2.20	0.42
1:I:214:GLU:HA	1:I:234:ALA:O	2.20	0.42
1:L:188:LYS:HD2	1:L:188:LYS:HA	1.89	0.42
1:E:202:ARG:O	1:E:206:GLU:HG3	2.20	0.41
1:B:169:LEU:HD23	1:B:169:LEU:HA	1.93	0.41
1:G:73:ILE:HG23	1:G:86:ILE:HD11	2.02	0.41
1:B:175:ILE:HD13	1:B:200:LEU:HD11	2.01	0.41
1:D:214:GLU:HA	1:D:234:ALA:O	2.21	0.41
1:G:243:LYS:HE3	3:G:405:HOH:O	2.21	0.41
1:H:169:LEU:HD23	1:H:169:LEU:HA	1.93	0.41
1:C:180:VAL:HB	1:C:187:GLN:HB3	2.03	0.41
1:D:33:ARG:O	1:D:36:LYS:HG3	2.21	0.41
1:A:140:ARG:HD3	1:A:140:ARG:C	2.41	0.41
1:D:73:ILE:CG2	1:D:86:ILE:HD11	2.50	0.41
1:D:188:LYS:H	1:D:188:LYS:HG3	1.78	0.41
1:F:89:LEU:HD12	1:F:90:VAL:N	2.36	0.41
1:G:177:ILE:HD12	1:G:196:LYS:HD3	2.02	0.41
1:H:56:LEU:HD23	1:H:56:LEU:HA	1.82	0.41
1:B:127:SER:HB3	1:B:153:GLY:HA3	2.03	0.41
1:I:77:ASP:HB3	1:I:108:ILE:HG22	2.02	0.41
1:D:179:SER:HA	1:D:193:GLN:HG3	2.03	0.40
1:C:214:GLU:HA	1:C:234:ALA:O	2.21	0.40
1:F:169:LEU:HD23	1:F:169:LEU:HA	1.91	0.40
1:G:179:SER:HA	1:G:193:GLN:HG3	2.04	0.40
1:I:181:ASN:N	1:I:187:GLN:OE1	2.33	0.40
1:C:53:PHE:CE2	1:C:56:LEU:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:LYS:HD3	1:F:189:PHE:O	2.20	0.40
1:H:214:GLU:HA	1:H:234:ALA:O	2.20	0.40
1:L:224:ALA:HB3	1:L:257:SER:HB3	2.04	0.40
1:J:56:LEU:HD23	1:J:56:LEU:HA	1.89	0.40
1:A:168:VAL:HG13	1:A:172:VAL:HG13	2.03	0.40
1:I:187:GLN:HE21	1:I:187:GLN:HB2	1.61	0.40
1:K:153:GLY:HA2	1:K:174:LEU:O	2.22	0.40
1:L:169:LEU:HD23	1:L:169:LEU:HA	1.81	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:508:HOH:O	3:D:411:HOH:O[1_655]	2.01	0.19
3:C:570:HOH:O	3:F:463:HOH:O[1_556]	2.19	0.01

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	228/247 (92%)	223 (98%)	4 (2%)	1 (0%)	34	24
1	B	227/247 (92%)	222 (98%)	5 (2%)	0	100	100
1	C	227/247 (92%)	221 (97%)	6 (3%)	0	100	100
1	D	229/247 (93%)	224 (98%)	5 (2%)	0	100	100
1	E	227/247 (92%)	220 (97%)	7 (3%)	0	100	100
1	F	232/247 (94%)	226 (97%)	6 (3%)	0	100	100
1	G	228/247 (92%)	223 (98%)	5 (2%)	0	100	100
1	H	228/247 (92%)	223 (98%)	5 (2%)	0	100	100
1	I	228/247 (92%)	222 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	227/247 (92%)	222 (98%)	5 (2%)	0	100	100
1	K	228/247 (92%)	221 (97%)	7 (3%)	0	100	100
1	L	227/247 (92%)	220 (97%)	7 (3%)	0	100	100
All	All	2736/2964 (92%)	2667 (98%)	68 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	SER

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	194/208 (93%)	191 (98%)	3 (2%)	65	56
1	B	193/208 (93%)	190 (98%)	3 (2%)	62	52
1	C	193/208 (93%)	190 (98%)	3 (2%)	62	52
1	D	194/208 (93%)	191 (98%)	3 (2%)	65	56
1	E	193/208 (93%)	188 (97%)	5 (3%)	46	32
1	F	197/208 (95%)	193 (98%)	4 (2%)	55	42
1	G	194/208 (93%)	190 (98%)	4 (2%)	53	41
1	H	194/208 (93%)	191 (98%)	3 (2%)	65	56
1	I	194/208 (93%)	190 (98%)	4 (2%)	53	41
1	J	193/208 (93%)	191 (99%)	2 (1%)	76	71
1	K	194/208 (93%)	189 (97%)	5 (3%)	46	32
1	L	193/208 (93%)	191 (99%)	2 (1%)	76	71
All	All	2326/2496 (93%)	2285 (98%)	41 (2%)	59	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	56	LEU
1	J	114	ARG
1	A	47	SER
1	A	100	LYS
1	A	168	VAL
1	B	53	PHE
1	B	114	ARG
1	B	168	VAL
1	C	47	SER
1	C	168	VAL
1	C	188	LYS
1	D	36	LYS
1	D	168	VAL
1	D	188	LYS
1	E	47	SER
1	E	114	ARG
1	E	168	VAL
1	E	243	LYS
1	E	245	LYS
1	F	47	SER
1	F	168	VAL
1	F	188	LYS
1	F	248	ARG
1	G	47	SER
1	G	114	ARG
1	G	140	ARG
1	G	243	LYS
1	H	47	SER
1	H	53	PHE
1	H	168	VAL
1	I	47	SER
1	I	68	CYS
1	I	114	ARG
1	I	168	VAL
1	K	36	LYS
1	K	114	ARG
1	K	168	VAL
1	K	207	LYS
1	K	245	LYS
1	L	55	ARG
1	L	140	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	252	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	230/247 (93%)	-0.18	5 (2%)	62	69	19, 28, 43, 56	0
1	B	229/247 (92%)	-0.14	1 (0%)	92	95	21, 30, 46, 57	0
1	C	229/247 (92%)	-0.14	3 (1%)	77	81	21, 29, 42, 53	0
1	D	231/247 (93%)	-0.17	2 (0%)	84	87	21, 30, 44, 57	0
1	E	229/247 (92%)	-0.10	5 (2%)	62	69	19, 30, 46, 60	0
1	F	234/247 (94%)	-0.20	4 (1%)	70	75	22, 30, 43, 59	0
1	G	230/247 (93%)	0.08	6 (2%)	56	63	22, 34, 50, 70	0
1	H	230/247 (93%)	-0.12	3 (1%)	77	81	24, 33, 45, 65	0
1	I	230/247 (93%)	0.24	6 (2%)	56	63	24, 40, 54, 69	0
1	J	229/247 (92%)	-0.14	1 (0%)	92	95	19, 26, 39, 49	0
1	K	230/247 (93%)	0.34	13 (5%)	23	30	26, 40, 57, 68	0
1	L	229/247 (92%)	0.65	23 (10%)	7	10	27, 47, 60, 72	0
All	All	2760/2964 (93%)	0.01	72 (2%)	56	63	19, 32, 53, 72	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	31	THR	7.5
1	I	31	THR	6.3
1	H	31	THR	6.3
1	L	259	ALA	5.4
1	K	260	PRO	5.2
1	I	186	GLY	5.2
1	K	186	GLY	5.1
1	A	185	GLY	5.1
1	L	186	GLY	4.9
1	K	185	GLY	4.5
1	D	186	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	185	GLY	4.4
1	A	31	THR	4.4
1	G	186	GLY	4.1
1	L	250	ALA	4.0
1	K	259	ALA	3.9
1	L	68	CYS	3.4
1	A	186	GLY	3.4
1	G	260	PRO	3.3
1	E	185	GLY	3.3
1	K	31	THR	3.2
1	L	252	HIS	3.2
1	K	258	LYS	3.2
1	L	246	SER	3.1
1	L	63	ILE	3.0
1	L	40	SER	3.0
1	L	220	THR	2.9
1	E	186	GLY	2.9
1	K	225	TYR	2.8
1	L	42	ILE	2.8
1	L	185	GLY	2.8
1	H	186	GLY	2.8
1	L	228	ILE	2.8
1	F	28	VAL	2.7
1	I	32	SER	2.7
1	I	222	GLU	2.7
1	G	36	LYS	2.6
1	I	34	VAL	2.6
1	A	260	PRO	2.6
1	L	260	PRO	2.5
1	L	258	LYS	2.5
1	K	245	LYS	2.5
1	L	249	ASP	2.5
1	F	27	MET	2.5
1	G	99	ASP	2.5
1	K	222	GLU	2.4
1	L	65	GLN	2.4
1	L	56	LEU	2.4
1	K	229	ASP	2.3
1	J	245	LYS	2.3
1	D	260	PRO	2.3
1	E	221	PRO	2.3
1	C	245	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	258	LYS	2.3
1	C	188	LYS	2.3
1	L	67	GLY	2.3
1	K	99	ASP	2.3
1	L	254	ILE	2.3
1	I	36	LYS	2.2
1	L	62	ALA	2.2
1	E	136	ILE	2.2
1	E	32	SER	2.2
1	K	256	VAL	2.2
1	B	186	GLY	2.2
1	A	188	LYS	2.2
1	L	244	ALA	2.2
1	F	186	GLY	2.2
1	K	221	PRO	2.1
1	F	29	GLN	2.1
1	L	222	GLU	2.1
1	L	99	ASP	2.1
1	H	37	CYS	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	L	301	1/1	0.94	0.17	83,83,83,83	0
2	ZN	I	301	1/1	0.95	0.14	74,74,74,74	0
2	ZN	H	301	1/1	0.95	0.12	73,73,73,73	0
2	ZN	E	301	1/1	0.96	0.08	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	G	301	1/1	0.98	0.12	75,75,75,75	0
2	ZN	J	301	1/1	0.99	0.11	46,46,46,46	0
2	ZN	F	301	1/1	0.99	0.10	55,55,55,55	0
2	ZN	A	301	1/1	0.99	0.14	58,58,58,58	0
2	ZN	B	301	1/1	0.99	0.14	57,57,57,57	0
2	ZN	C	301	1/1	0.99	0.14	54,54,54,54	0
2	ZN	K	301	1/1	0.99	0.21	73,73,73,73	0
2	ZN	D	301	1/1	0.99	0.13	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.