Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2024 – 04:11 PM JST

PDB ID	:	8KG3
Title	:	Structure of THOUSAND-GRAIN WEIGHT 6 (TGW6)
Authors	:	Akabane, T.; Suzuki, N.; Matsumura, H.; Yoshizawa, T.; Tsuchiya, W.; Katoh, E.; Hirotsu, N.
Deposited on	:	2023-08-17
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

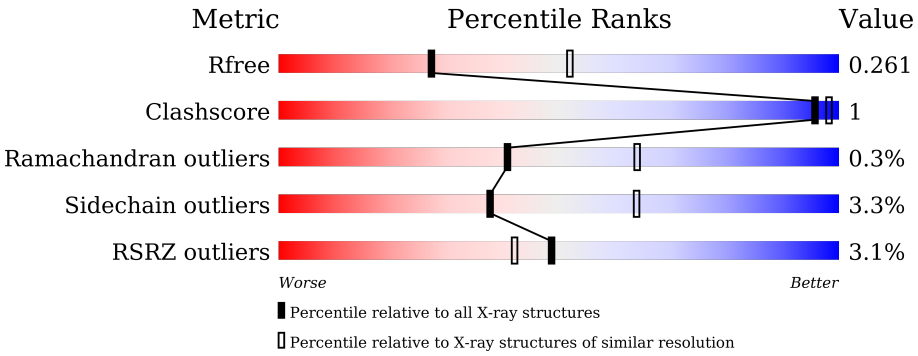
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	322	2% 91% 6% ·
1	B	322	2% 91% 6% ·
1	C	322	2% 91% 5% ·
1	D	322	2% 92% · ·
1	E	322	3% 90% 6% ·
1	F	322	2% 92% 5% ·

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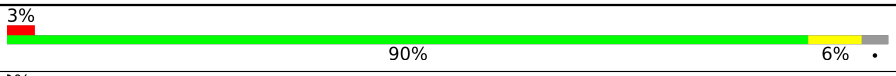
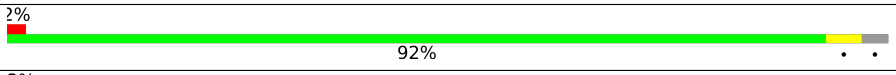
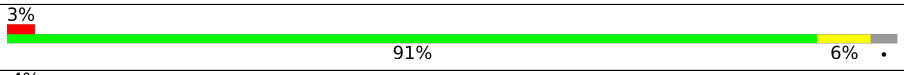
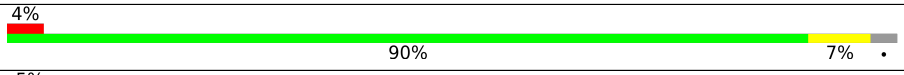
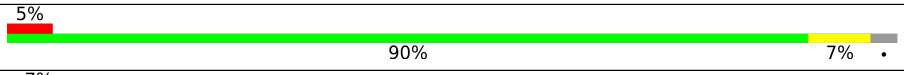
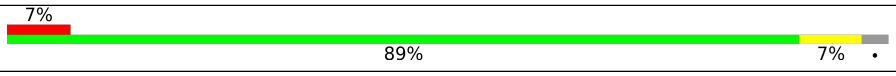
Mol	Chain	Length	Quality of chain
1	G	322	
1	H	322	
1	I	322	
1	J	322	
1	K	322	
1	L	322	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28949 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 Os06g0623700 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2404	1510	432	447	15			
1	B	311	Total	C	N	O	S	0	0	0
			2401	1508	432	447	14			
1	C	311	Total	C	N	O	S	0	0	0
			2394	1504	428	447	15			
1	D	311	Total	C	N	O	S	0	0	0
			2396	1504	430	447	15			
1	E	311	Total	C	N	O	S	0	0	0
			2383	1496	426	447	14			
1	F	311	Total	C	N	O	S	0	0	0
			2396	1504	430	447	15			
1	G	311	Total	C	N	O	S	0	0	0
			2400	1507	431	447	15			
1	H	311	Total	C	N	O	S	0	0	0
			2392	1501	429	447	15			
1	I	311	Total	C	N	O	S	0	0	0
			2382	1495	425	447	15			
1	J	311	Total	C	N	O	S	0	0	0
			2390	1501	427	447	15			
1	K	311	Total	C	N	O	S	0	0	0
			2376	1492	422	447	15			
1	L	311	Total	C	N	O	S	0	0	0
			2390	1502	428	445	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q69U01
A	30	SER	-	expression tag	UNP Q69U01
B	29	GLY	-	expression tag	UNP Q69U01
B	30	SER	-	expression tag	UNP Q69U01
C	29	GLY	-	expression tag	UNP Q69U01

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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	SER	-	expression tag	UNP Q69U01
D	29	GLY	-	expression tag	UNP Q69U01
D	30	SER	-	expression tag	UNP Q69U01
E	29	GLY	-	expression tag	UNP Q69U01
E	30	SER	-	expression tag	UNP Q69U01
F	29	GLY	-	expression tag	UNP Q69U01
F	30	SER	-	expression tag	UNP Q69U01
G	29	GLY	-	expression tag	UNP Q69U01
G	30	SER	-	expression tag	UNP Q69U01
H	29	GLY	-	expression tag	UNP Q69U01
H	30	SER	-	expression tag	UNP Q69U01
I	29	GLY	-	expression tag	UNP Q69U01
I	30	SER	-	expression tag	UNP Q69U01
J	29	GLY	-	expression tag	UNP Q69U01
J	30	SER	-	expression tag	UNP Q69U01
K	29	GLY	-	expression tag	UNP Q69U01
K	30	SER	-	expression tag	UNP Q69U01
L	29	GLY	-	expression tag	UNP Q69U01
L	30	SER	-	expression tag	UNP Q69U01

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	34	Total O 34 34	0	0
2	C	20	Total O 20 20	0	0
2	D	24	Total O 24 24	0	0
2	E	20	Total O 20 20	0	0
2	F	18	Total O 18 18	0	0
2	G	16	Total O 16 16	0	0
2	H	18	Total O 18 18	0	0
2	I	21	Total O 21 21	0	0
2	J	17	Total O 17 17	0	0

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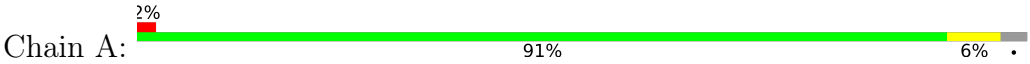
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	13	Total O 13 13	0	0
2	L	15	Total O 15 15	0	0

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.

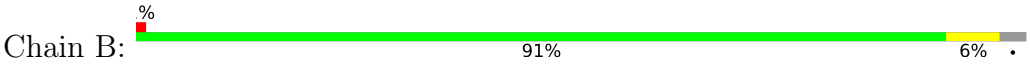
- Molecule 1: Os06g0623700 protein

Chain A:



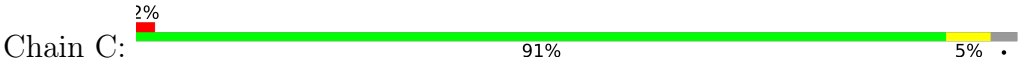
- Molecule 1: Os06g0623700 protein

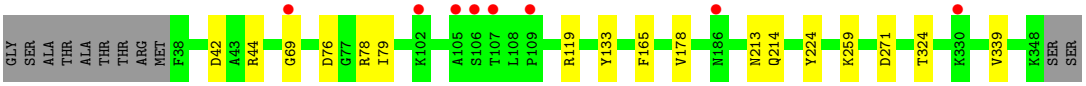
Chain B:



- Molecule 1: Os06g0623700 protein

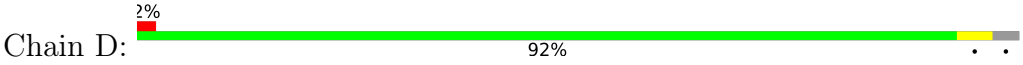
Chain C:





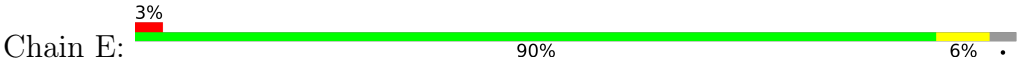
- Molecule 1: Os06g0623700 protein

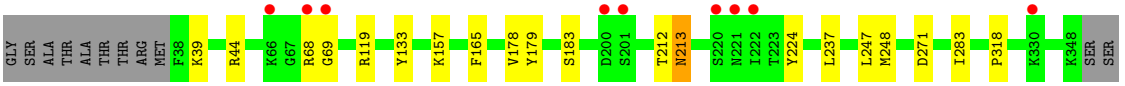
Chain D:



- Molecule 1: Os06g0623700 protein

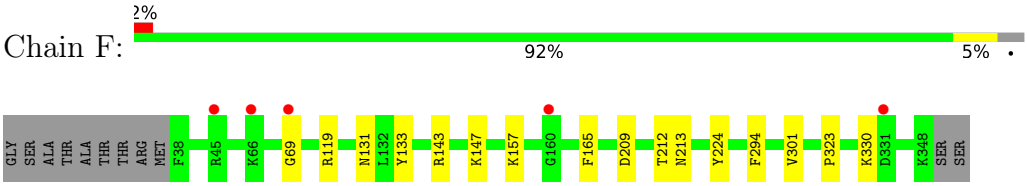
Chain E:





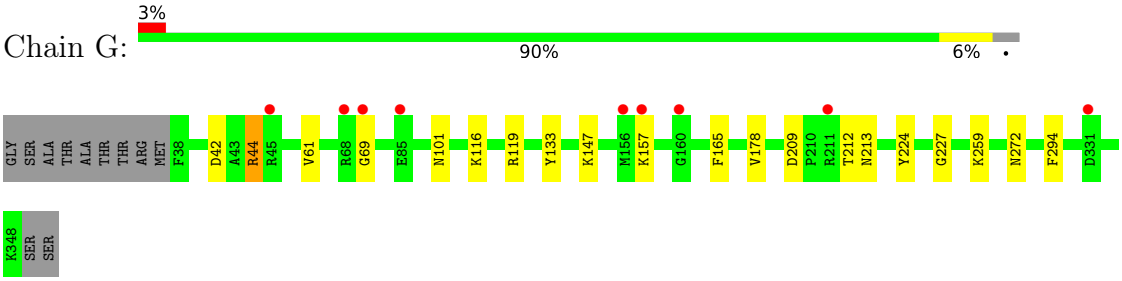
- Molecule 1: Os06g0623700 protein

Chain F:



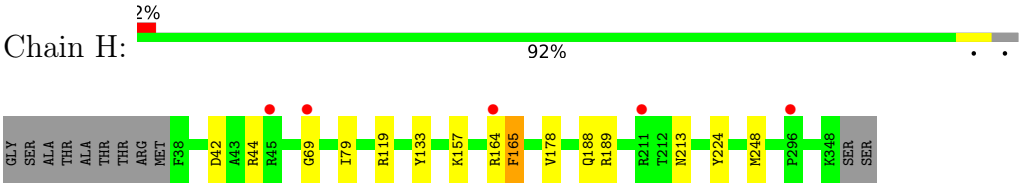
• Molecule 1: Os06g0623700 protein

Chain G:



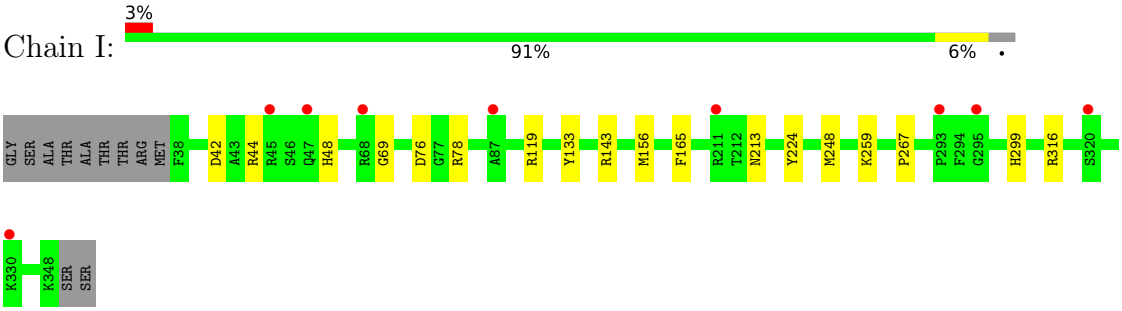
• Molecule 1: Os06g0623700 protein

Chain H:



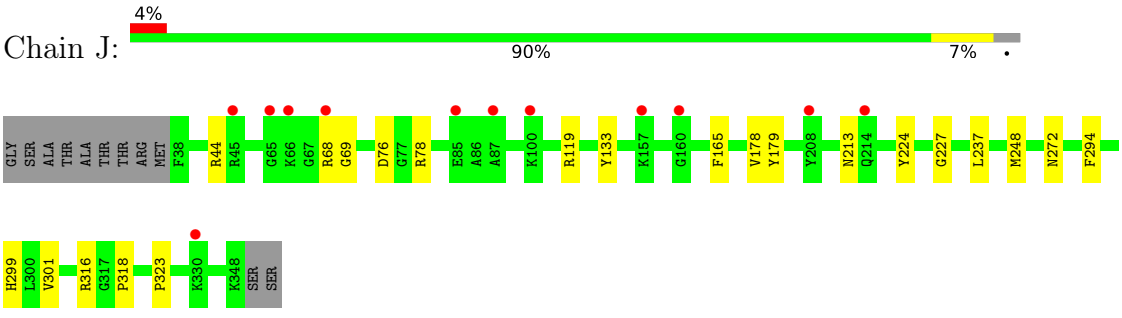
• Molecule 1: Os06g0623700 protein

Chain I:



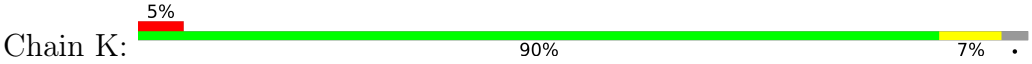
• Molecule 1: Os06g0623700 protein

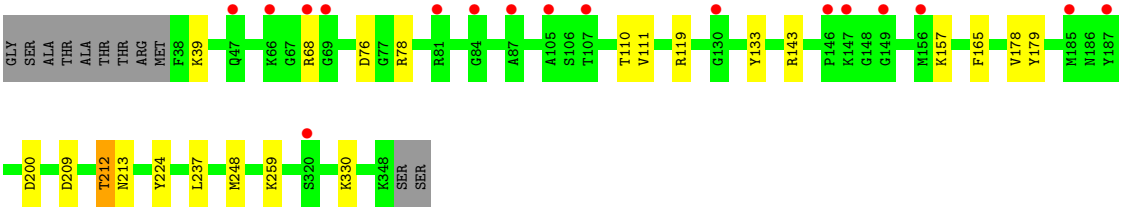
Chain J:



• Molecule 1: Os06g0623700 protein

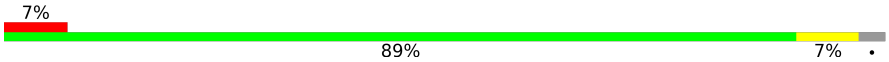
Chain K:

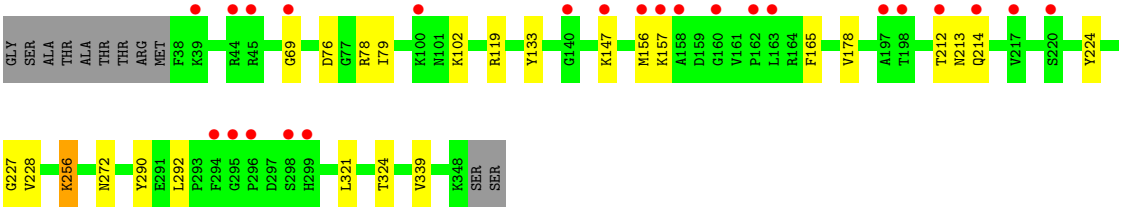




• Molecule 1: Os06g0623700 protein

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	105.98Å 108.52Å 123.07Å 94.14° 98.74° 97.23°	Depositor
Resolution (Å)	48.99 – 2.60 48.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.99-2.60) 98.3 (48.94-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.225 , 0.260 0.228 , 0.261	Depositor DCC
R_{free} test set	7877 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28949	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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

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	0/2461	0.73	0/3329
1	B	0.64	0/2458	0.73	0/3326
1	C	0.65	0/2451	0.72	0/3318
1	D	0.65	0/2453	0.73	0/3321
1	E	0.65	0/2440	0.73	0/3307
1	F	0.65	0/2453	0.73	0/3321
1	G	0.65	0/2457	0.73	0/3325
1	H	0.65	0/2449	0.72	0/3317
1	I	0.65	0/2439	0.72	0/3306
1	J	0.65	0/2447	0.73	0/3314
1	K	0.66	0/2433	0.73	0/3299
1	L	0.66	0/2447	0.74	0/3313
All	All	0.65	0/29388	0.73	0/39796

There are no bond length outliers.

There are no bond angle outliers.

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	2404	0	2385	7	0
1	B	2401	0	2378	5	0
1	C	2394	0	2363	5	0
1	D	2396	0	2363	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2383	0	2334	6	0
1	F	2396	0	2363	5	0
1	G	2400	0	2374	6	0
1	H	2392	0	2352	5	0
1	I	2382	0	2330	5	0
1	J	2390	0	2352	8	0
1	K	2376	0	2319	5	0
1	L	2390	0	2359	7	0
2	A	29	0	0	0	0
2	B	34	0	0	0	0
2	C	20	0	0	0	0
2	D	24	0	0	0	0
2	E	20	0	0	0	0
2	F	18	0	0	0	0
2	G	16	0	0	0	0
2	H	18	0	0	0	0
2	I	21	0	0	0	0
2	J	17	0	0	0	0
2	K	13	0	0	0	0
2	L	15	0	0	0	0
All	All	28949	0	28272	64	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 1.

All (64) 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:I:76:ASP:OD2	1:I:78:ARG:NH1	2.25	0.68
1:G:42:ASP:OD1	1:G:44:ARG:HD3	1.97	0.64
1:D:133:TYR:CE2	1:D:178:VAL:HG21	2.38	0.58
1:K:133:TYR:CE2	1:K:178:VAL:HG21	2.43	0.53
1:J:299:HIS:O	1:J:316:ARG:HA	2.12	0.50
1:J:44:ARG:HA	1:J:318:PRO:HD3	1.94	0.50
1:J:133:TYR:CE2	1:J:178:VAL:HG21	2.47	0.50
1:G:209:ASP:HB3	1:G:212:THR:HG22	1.93	0.50
1:L:227:GLY:HA3	1:L:272:ASN:HA	1.95	0.49
1:D:42:ASP:OD1	1:D:44:ARG:HD3	2.14	0.48
1:A:76:ASP:OD2	1:A:78:ARG:NH1	2.47	0.47
1:F:301:VAL:HB	1:F:323:PRO:HG2	1.96	0.47
1:L:133:TYR:CE2	1:L:178:VAL:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:VAL:HB	1:D:323:PRO:HG2	1.97	0.46
1:B:97:SER:HB3	1:B:116:LYS:O	2.16	0.46
1:E:133:TYR:CE2	1:E:178:VAL:HG21	2.50	0.46
1:E:165:PHE:CD2	1:E:183:SER:HB2	2.50	0.46
1:H:133:TYR:CE2	1:H:178:VAL:HG21	2.51	0.46
1:L:324:THR:HG21	1:L:339:VAL:HG13	1.97	0.46
1:C:76:ASP:OD2	1:C:78:ARG:NH1	2.49	0.45
1:I:42:ASP:OD1	1:I:44:ARG:HD3	2.17	0.45
1:A:133:TYR:CE2	1:A:178:VAL:HG21	2.51	0.45
1:B:76:ASP:OD2	1:B:78:ARG:NH1	2.50	0.45
1:L:76:ASP:OD2	1:L:78:ARG:NH1	2.50	0.45
1:C:324:THR:HG21	1:C:339:VAL:HG13	1.98	0.45
1:B:294:PHE:CZ	1:J:294:PHE:CZ	3.05	0.45
1:J:76:ASP:OD2	1:J:78:ARG:NH1	2.50	0.44
1:B:133:TYR:CE2	1:B:178:VAL:HG21	2.52	0.44
1:K:76:ASP:OD2	1:K:78:ARG:NH1	2.50	0.44
1:G:133:TYR:CE2	1:G:178:VAL:HG21	2.53	0.43
1:I:299:HIS:O	1:I:316:ARG:HA	2.19	0.43
1:K:179:TYR:CD2	1:K:237:LEU:HD11	2.54	0.43
1:C:42:ASP:OD1	1:C:44:ARG:HD3	2.18	0.43
1:B:79:ILE:HD12	1:B:79:ILE:N	2.34	0.43
1:F:133:TYR:CZ	1:F:143:ARG:HD3	2.53	0.43
1:J:301:VAL:HB	1:J:323:PRO:HG2	2.00	0.43
1:H:42:ASP:OD1	1:H:44:ARG:HD3	2.19	0.42
1:I:267:PRO:HG3	1:L:292:LEU:HD21	2.01	0.42
1:C:79:ILE:N	1:C:79:ILE:HD12	2.34	0.42
1:E:179:TYR:CD2	1:E:237:LEU:HD11	2.55	0.42
1:F:209:ASP:HB3	1:F:212:THR:HG22	2.02	0.42
1:H:79:ILE:HD12	1:H:79:ILE:N	2.35	0.42
1:A:299:HIS:O	1:A:316:ARG:HA	2.20	0.42
1:F:294:PHE:CZ	1:G:294:PHE:CZ	3.07	0.42
1:J:179:TYR:CD2	1:J:237:LEU:HD11	2.55	0.42
1:E:44:ARG:HA	1:E:318:PRO:HD3	2.01	0.41
1:K:209:ASP:HB3	1:K:212:THR:HG23	2.02	0.41
1:G:101:ASN:HD22	1:G:116:LYS:HB3	1.85	0.41
1:A:133:TYR:CZ	1:A:143:ARG:HD3	2.55	0.41
1:H:164:ARG:HG3	1:H:188:GLN:HG2	2.02	0.41
1:A:324:THR:HG21	1:A:339:VAL:HG13	2.01	0.41
1:E:213:ASN:O	1:E:213:ASN:ND2	2.50	0.41
1:F:131:ASN:HD22	1:F:143:ARG:HD2	1.85	0.41
1:A:213:ASN:O	1:A:213:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TYR:CE2	1:C:178:VAL:HG21	2.55	0.41
1:G:227:GLY:HA3	1:G:272:ASN:HA	2.02	0.41
1:H:165:PHE:CZ	1:H:189:ARG:HA	2.55	0.41
1:I:133:TYR:CZ	1:I:143:ARG:HD3	2.56	0.41
1:K:133:TYR:CZ	1:K:143:ARG:HD3	2.56	0.41
1:A:114:GLU:O	1:A:118:GLY:N	2.48	0.41
1:L:79:ILE:HD12	1:L:79:ILE:N	2.36	0.41
1:L:256:LYS:H	1:L:256:LYS:HE2	1.85	0.40
1:E:247:LEU:HD11	1:E:283:ILE:HG13	2.02	0.40
1:J:227:GLY:HA3	1:J:272:ASN:HA	2.03	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	309/322 (96%)	290 (94%)	19 (6%)	0	100	100
1	B	309/322 (96%)	291 (94%)	17 (6%)	1 (0%)	41	64
1	C	309/322 (96%)	292 (94%)	16 (5%)	1 (0%)	41	64
1	D	309/322 (96%)	291 (94%)	17 (6%)	1 (0%)	41	64
1	E	309/322 (96%)	289 (94%)	19 (6%)	1 (0%)	41	64
1	F	309/322 (96%)	291 (94%)	17 (6%)	1 (0%)	41	64
1	G	309/322 (96%)	290 (94%)	18 (6%)	1 (0%)	41	64
1	H	309/322 (96%)	290 (94%)	18 (6%)	1 (0%)	41	64
1	I	309/322 (96%)	293 (95%)	15 (5%)	1 (0%)	41	64
1	J	309/322 (96%)	288 (93%)	20 (6%)	1 (0%)	41	64
1	K	309/322 (96%)	289 (94%)	20 (6%)	0	100	100
1	L	309/322 (96%)	288 (93%)	20 (6%)	1 (0%)	41	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3708/3864 (96%)	3482 (94%)	216 (6%)	10 (0%)	41 64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	GLY
1	C	69	GLY
1	E	69	GLY
1	F	69	GLY
1	G	69	GLY
1	H	69	GLY
1	I	69	GLY
1	J	69	GLY
1	D	69	GLY
1	L	69	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	257/265 (97%)	251 (98%)	6 (2%)	50 75
1	B	256/265 (97%)	247 (96%)	9 (4%)	36 62
1	C	255/265 (96%)	248 (97%)	7 (3%)	44 71
1	D	255/265 (96%)	248 (97%)	7 (3%)	44 71
1	E	252/265 (95%)	243 (96%)	9 (4%)	35 61
1	F	255/265 (96%)	248 (97%)	7 (3%)	44 71
1	G	256/265 (97%)	247 (96%)	9 (4%)	36 62
1	H	254/265 (96%)	248 (98%)	6 (2%)	49 74
1	I	252/265 (95%)	244 (97%)	8 (3%)	39 65
1	J	254/265 (96%)	248 (98%)	6 (2%)	49 74
1	K	251/265 (95%)	237 (94%)	14 (6%)	21 42
1	L	254/265 (96%)	240 (94%)	14 (6%)	21 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3051/3180 (96%)	2949 (97%)	102 (3%)	38 64

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ARG
1	A	147	LYS
1	A	157	LYS
1	A	164	ARG
1	A	165	PHE
1	A	224	TYR
1	B	68	ARG
1	B	119	ARG
1	B	147	LYS
1	B	164	ARG
1	B	165	PHE
1	B	213	ASN
1	B	220	SER
1	B	224	TYR
1	B	248	MET
1	C	119	ARG
1	C	165	PHE
1	C	213	ASN
1	C	214	GLN
1	C	224	TYR
1	C	259	LYS
1	C	271	ASP
1	D	100	LYS
1	D	119	ARG
1	D	157	LYS
1	D	165	PHE
1	D	224	TYR
1	D	259	LYS
1	D	321	LEU
1	E	39	LYS
1	E	68	ARG
1	E	119	ARG
1	E	157	LYS
1	E	212	THR
1	E	213	ASN
1	E	224	TYR
1	E	248	MET

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Mol	Chain	Res	Type
1	E	271	ASP
1	F	119	ARG
1	F	147	LYS
1	F	157	LYS
1	F	165	PHE
1	F	213	ASN
1	F	224	TYR
1	F	330	LYS
1	G	44	ARG
1	G	61	VAL
1	G	119	ARG
1	G	147	LYS
1	G	157	LYS
1	G	165	PHE
1	G	213	ASN
1	G	224	TYR
1	G	259	LYS
1	H	119	ARG
1	H	157	LYS
1	H	165	PHE
1	H	213	ASN
1	H	224	TYR
1	H	248	MET
1	I	48	HIS
1	I	119	ARG
1	I	156	MET
1	I	165	PHE
1	I	213	ASN
1	I	224	TYR
1	I	248	MET
1	I	259	LYS
1	J	68	ARG
1	J	119	ARG
1	J	165	PHE
1	J	213	ASN
1	J	224	TYR
1	J	248	MET
1	K	39	LYS
1	K	68	ARG
1	K	110	THR
1	K	111	VAL
1	K	119	ARG

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Mol	Chain	Res	Type
1	K	157	LYS
1	K	165	PHE
1	K	200	ASP
1	K	212	THR
1	K	213	ASN
1	K	224	TYR
1	K	248	MET
1	K	259	LYS
1	K	330	LYS
1	L	102	LYS
1	L	119	ARG
1	L	147	LYS
1	L	156	MET
1	L	157	LYS
1	L	165	PHE
1	L	212	THR
1	L	213	ASN
1	L	214	GLN
1	L	224	TYR
1	L	228	VAL
1	L	256	LYS
1	L	290	TYR
1	L	321	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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, 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	311/322 (96%)	0.17	5 (1%)	72	68	30, 42, 69, 85	0
1	B	311/322 (96%)	0.02	3 (0%)	82	80	31, 40, 59, 80	0
1	C	311/322 (96%)	0.25	8 (2%)	56	50	35, 48, 71, 87	0
1	D	311/322 (96%)	0.25	8 (2%)	56	50	33, 45, 74, 104	0
1	E	311/322 (96%)	0.31	9 (2%)	51	45	34, 54, 76, 83	0
1	F	311/322 (96%)	0.11	5 (1%)	72	68	33, 48, 69, 79	0
1	G	311/322 (96%)	0.15	9 (2%)	51	45	34, 49, 67, 76	0
1	H	311/322 (96%)	0.21	5 (1%)	72	68	35, 49, 72, 95	0
1	I	311/322 (96%)	0.15	9 (2%)	51	45	34, 49, 74, 85	0
1	J	311/322 (96%)	0.27	12 (3%)	39	32	34, 53, 75, 85	0
1	K	311/322 (96%)	0.51	17 (5%)	25	19	37, 61, 84, 95	0
1	L	311/322 (96%)	0.52	24 (7%)	13	10	42, 61, 86, 109	0
All	All	3732/3864 (96%)	0.24	114 (3%)	49	42	30, 50, 77, 109	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	160	GLY	3.8
1	L	294	PHE	3.8
1	D	107	THR	3.7
1	K	107	THR	3.7
1	D	105	ALA	3.6
1	L	160	GLY	3.5
1	C	107	THR	3.5
1	C	69	GLY	3.4
1	E	220	SER	3.3
1	B	330	LYS	3.2
1	L	147	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	149	GLY	3.2
1	K	87	ALA	3.2
1	A	69	GLY	3.1
1	I	45	ARG	3.1
1	K	68	ARG	3.1
1	F	160	GLY	3.1
1	K	69	GLY	3.1
1	L	156	MET	3.1
1	G	85	GLU	3.0
1	L	295	GLY	3.0
1	A	147	LYS	3.0
1	G	69	GLY	3.0
1	D	294	PHE	2.9
1	L	299	HIS	2.9
1	L	296	PRO	2.8
1	J	66	LYS	2.8
1	K	47	GLN	2.8
1	I	330	LYS	2.7
1	A	66	LYS	2.7
1	G	156	MET	2.7
1	F	45	ARG	2.7
1	D	38	PHE	2.7
1	I	87	ALA	2.7
1	J	330	LYS	2.7
1	C	105	ALA	2.6
1	K	147	LYS	2.6
1	L	214	GLN	2.6
1	L	162	PRO	2.6
1	A	45	ARG	2.6
1	E	330	LYS	2.6
1	K	66	LYS	2.6
1	L	100	LYS	2.6
1	J	100	LYS	2.5
1	C	109	PRO	2.5
1	E	221	ASN	2.5
1	I	295	GLY	2.5
1	L	69	GLY	2.5
1	L	197	ALA	2.5
1	K	105	ALA	2.5
1	L	157	LYS	2.5
1	C	330	LYS	2.4
1	K	320	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	68	ARG	2.4
1	K	156	MET	2.4
1	G	211	ARG	2.4
1	K	84	GLY	2.4
1	K	185	MET	2.4
1	H	164	ARG	2.4
1	H	45	ARG	2.4
1	H	296	PRO	2.4
1	D	87	ALA	2.4
1	E	68	ARG	2.4
1	B	147	LYS	2.4
1	G	157	LYS	2.4
1	C	186	ASN	2.4
1	E	69	GLY	2.3
1	H	69	GLY	2.3
1	G	45	ARG	2.3
1	J	45	ARG	2.3
1	J	208	TYR	2.3
1	L	39	LYS	2.3
1	F	331	ASP	2.3
1	G	160	GLY	2.3
1	D	187	TYR	2.3
1	B	39	LYS	2.3
1	F	69	GLY	2.3
1	J	214	GLN	2.3
1	G	68	ARG	2.3
1	I	211	ARG	2.3
1	L	44	ARG	2.3
1	E	201	SER	2.2
1	K	187	TYR	2.2
1	J	85	GLU	2.2
1	E	200	ASP	2.2
1	G	331	ASP	2.2
1	I	320	SER	2.2
1	D	330	LYS	2.2
1	E	66	LYS	2.2
1	L	158	ALA	2.2
1	L	217	VAL	2.1
1	D	69	GLY	2.1
1	H	211	ARG	2.1
1	J	65	GLY	2.1
1	L	212	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	222	ILE	2.1
1	K	81	ARG	2.1
1	J	87	ALA	2.1
1	A	156	MET	2.1
1	L	163	LEU	2.1
1	F	66	LYS	2.1
1	L	298	SER	2.1
1	I	47	GLN	2.1
1	C	102	LYS	2.1
1	L	140	GLY	2.1
1	J	157	LYS	2.0
1	I	68	ARG	2.0
1	C	106	SER	2.0
1	K	130	GLY	2.0
1	L	220	SER	2.0
1	I	293	PRO	2.0
1	K	146	PRO	2.0
1	L	45	ARG	2.0
1	L	198	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.