



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:37 PM UTC

PDB ID : 8KG3 / pdb_00008kg3
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

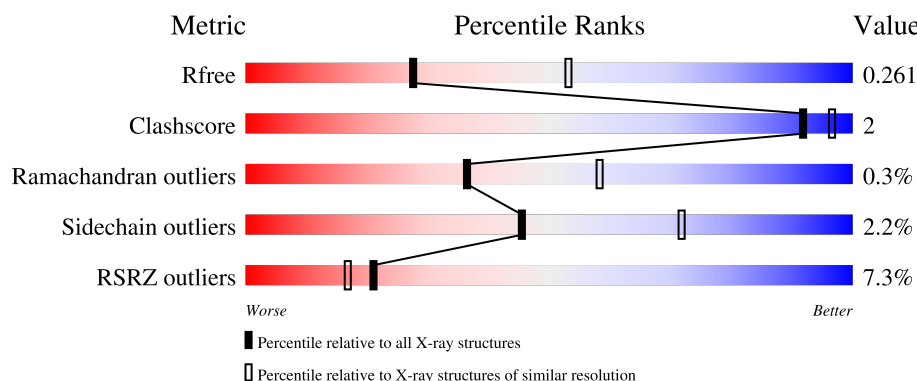
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	6% 90% 6% .
1	B	322	5% 91% 5% .
1	C	322	5% 92% 5% .
1	D	322	7% 91% 5% .
1	E	322	10% 88% 8% .

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Mol	Chain	Length	Quality of chain
1	F	322	6% 91% 5%
1	G	322	4% 89% 7%
1	H	322	6% 91% 6%
1	I	322	8% 91% 6%
1	J	322	9% 89% 8%
1	K	322	11% 90% 7%
1	L	322	10% 89% 7%

2 Entry composition

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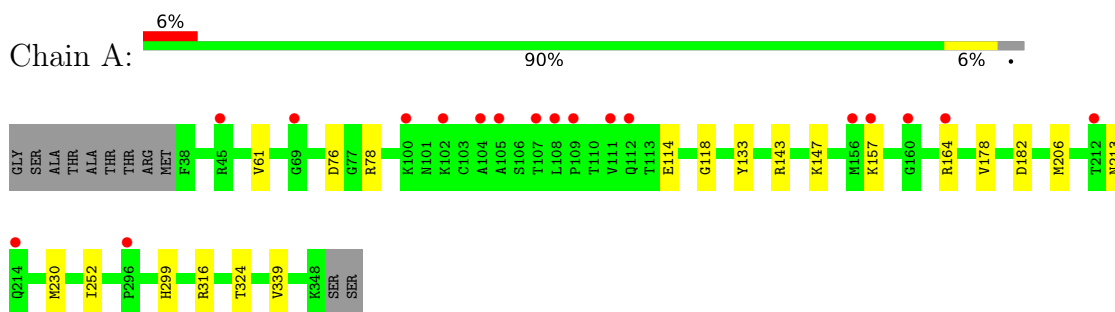
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	13	Total	O	0	0
			13	13		
2	L	15	Total	O	0	0
			15	15		

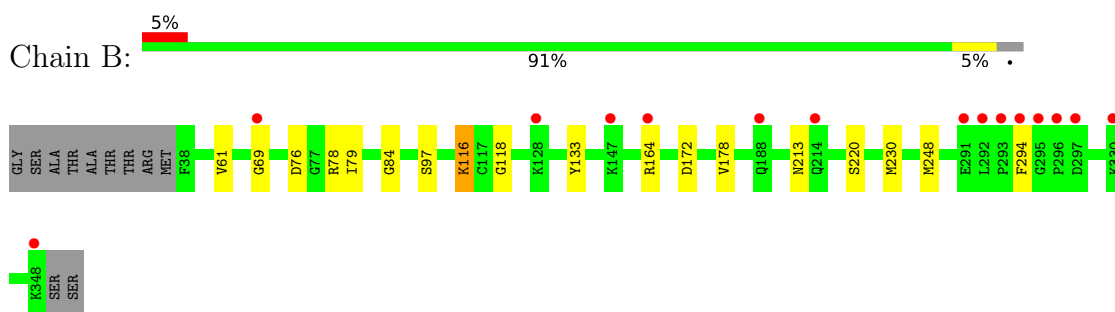
3 Residue-property plots [i](#)

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.

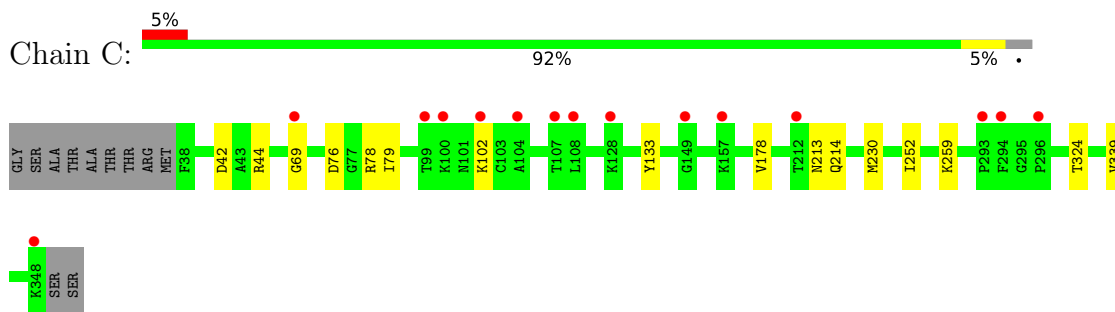
- Molecule 1: Os06g0623700 protein



- Molecule 1: Os06g0623700 protein

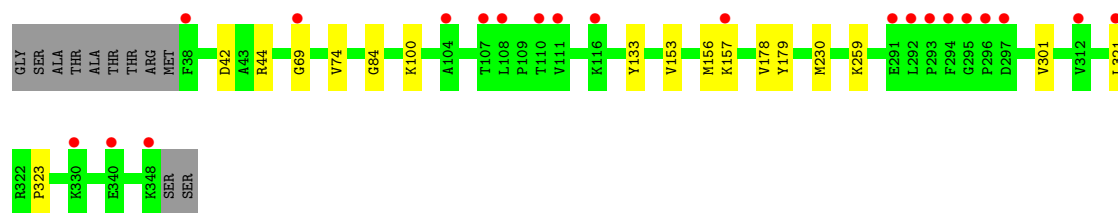


- Molecule 1: Os06g0623700 protein

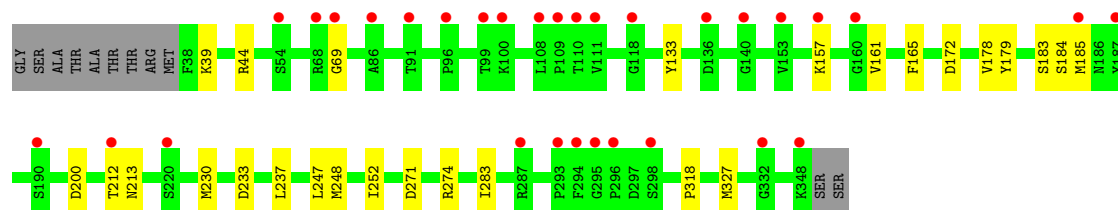
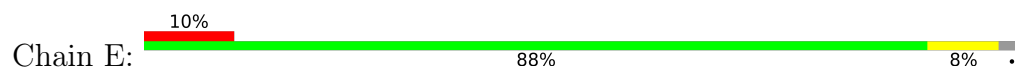


- Molecule 1: Os06g0623700 protein

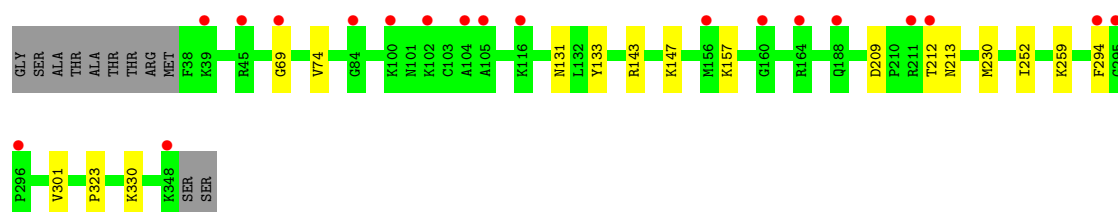




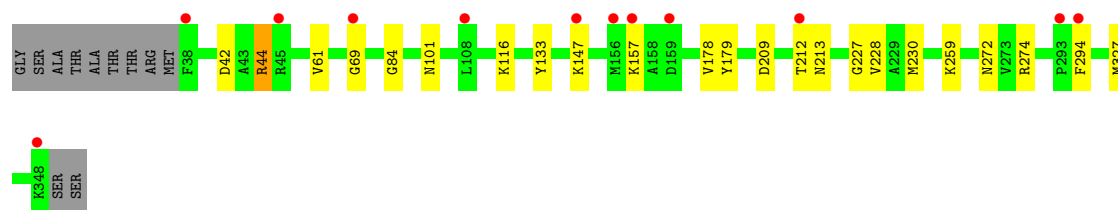
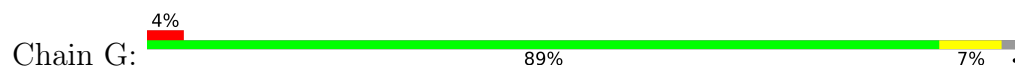
- Molecule 1: Os06g0623700 protein



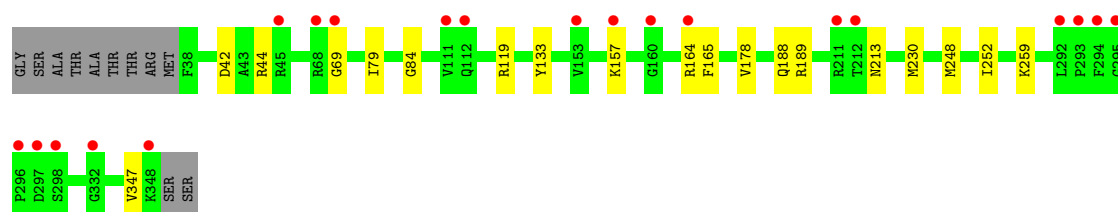
- Molecule 1: Os06g0623700 protein



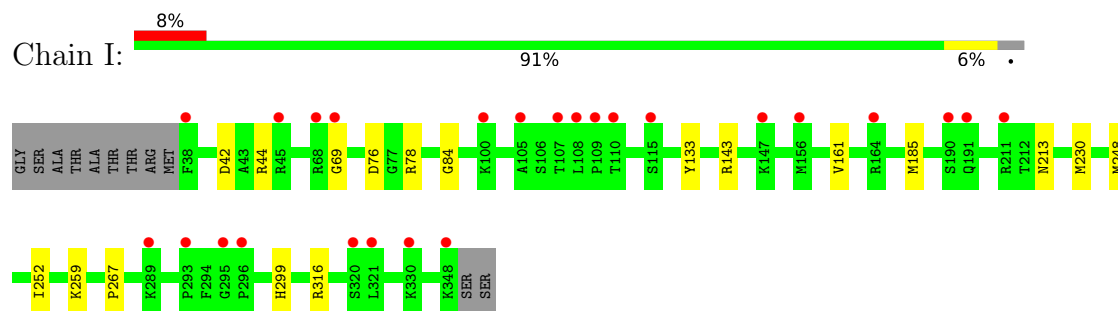
- Molecule 1: Os06g0623700 protein



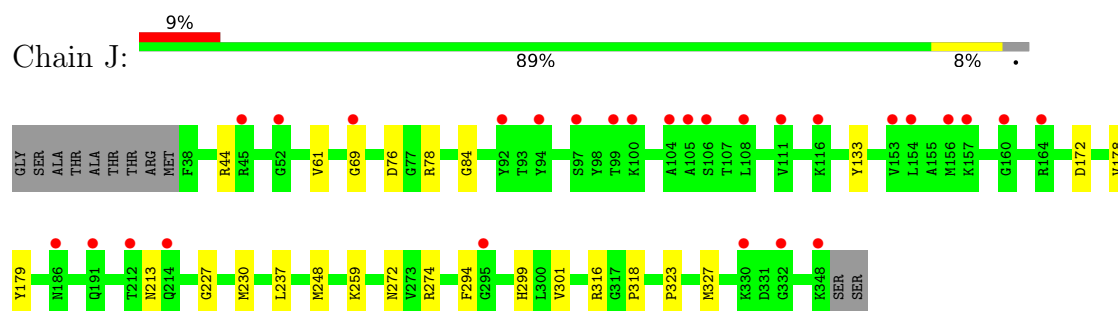
- Molecule 1: Os06g0623700 protein



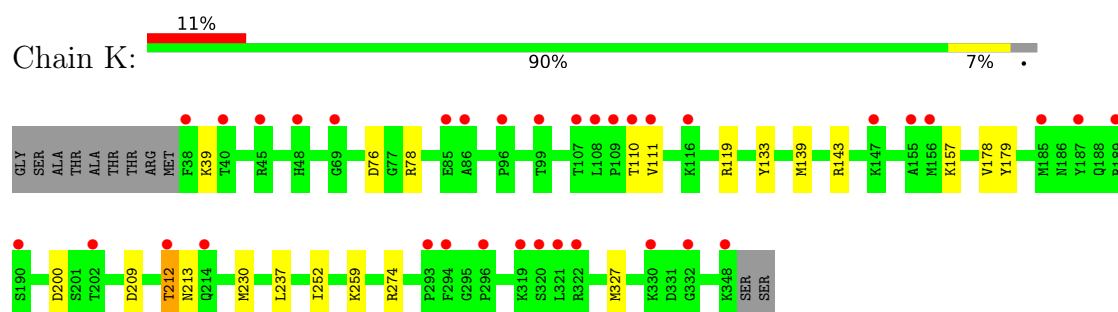
- Molecule 1: Os06g0623700 protein



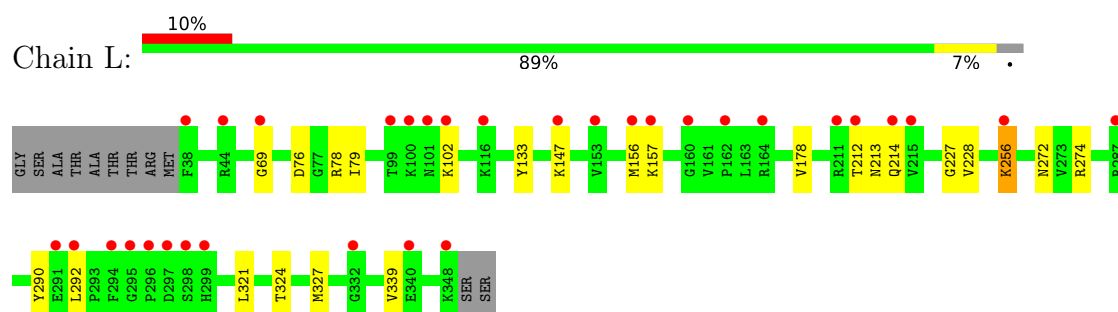
- Molecule 1: Os06g0623700 protein



- Molecule 1: Os06g0623700 protein



- Molecule 1: Os06g0623700 protein



4 Data and refinement statistics

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 48.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.99-2.60) 98.3 (48.99-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.78%)	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 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.01	0/2461	1.32	0/3329
1	B	1.01	0/2458	1.33	2/3326 (0.1%)
1	C	1.02	0/2451	1.34	0/3318
1	D	1.01	0/2453	1.33	3/3321 (0.1%)
1	E	1.02	0/2440	1.33	0/3307
1	F	1.02	0/2453	1.33	2/3321 (0.1%)
1	G	1.02	0/2457	1.34	1/3325 (0.0%)
1	H	1.02	0/2449	1.34	1/3317 (0.0%)
1	I	1.03	0/2439	1.34	1/3306 (0.0%)
1	J	1.02	0/2447	1.34	1/3314 (0.0%)
1	K	1.03	0/2433	1.35	0/3299
1	L	1.04	0/2447	1.34	0/3313
All	All	1.02	0/29388	1.34	11/39796 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	GLY	CA-C-O	-5.67	118.04	122.52
1	G	84	GLY	CA-C-O	-5.47	118.20	122.52
1	H	84	GLY	CA-C-O	-5.41	118.24	122.52
1	J	84	GLY	CA-C-O	-5.41	118.25	122.52
1	B	84	GLY	CA-C-O	-5.34	118.30	122.52
1	D	74	VAL	CA-C-N	5.27	127.34	120.28
1	D	74	VAL	C-N-CA	5.27	127.34	120.28
1	B	118	GLY	CA-C-O	-5.27	118.59	122.23
1	I	84	GLY	CA-C-O	-5.08	118.17	122.29
1	F	74	VAL	CA-C-N	5.03	127.27	120.38
1	F	74	VAL	C-N-CA	5.03	127.27	120.38

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	9	0
1	B	2401	0	2378	6	0
1	C	2394	0	2363	6	0
1	D	2396	0	2363	5	0
1	E	2383	0	2334	13	0
1	F	2396	0	2363	6	0
1	G	2400	0	2374	8	0
1	H	2392	0	2352	7	0
1	I	2382	0	2330	7	0
1	J	2390	0	2352	10	0
1	K	2376	0	2319	8	0
1	L	2390	0	2359	8	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	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (90) 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:J:172:ASP:HB2	1:J:230:MET:HE1	1.76	0.66
1:G:42:ASP:OD1	1:G:44:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ASP:HB2	1:E:230:MET:HE1	1.84	0.59
1:D:133:TYR:CE2	1:D:178:VAL:HG21	2.38	0.58
1:E:274:ARG:HD2	1:E:327:MET:HE1	1.86	0.57
1:L:274:ARG:HD2	1:L:327:MET:HE1	1.86	0.57
1:D:153:VAL:HG11	1:D:156:MET:HE2	1.86	0.56
1:K:133:TYR:CE2	1:K:178:VAL:HG21	2.43	0.53
1:I:230:MET:HE2	1:I:252:ILE:CD1	2.38	0.53
1:E:161:VAL:HG11	1:E:185:MET:HE2	1.92	0.52
1:E:230:MET:HE2	1:E:252:ILE:CD1	2.39	0.51
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:I:161:VAL:HG11	1:I:185:MET:HE2	1.94	0.48
1:A:230:MET:HE2	1:A:252:ILE:CD1	2.44	0.48
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:K:274:ARG:HD2	1:K:327:MET:HE1	1.96	0.47
1:F:230:MET:HE2	1:F:252:ILE:HD13	1.97	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
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:K:139:MET:HA	1:K:139:MET:HE2	1.96	0.46
1:C:230:MET:HE2	1:C:252:ILE:CD1	2.46	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:A:182:ASP:HB2	1:A:206:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:MET:HE2	1:E:252:ILE:HD13	1.99	0.43
1:G:133:TYR:CE2	1:G:178:VAL:HG21	2.53	0.43
1:G:179:TYR:CE1	1:G:230:MET:HE1	2.52	0.43
1:I:299:HIS:O	1:I:316:ARG:HA	2.19	0.43
1:H:230:MET:HE2	1:H:252:ILE:CD1	2.49	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:H:230:MET:HE2	1:H:252:ILE:HD13	2.00	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:G:274:ARG:HD2	1:G:327:MET:HE1	2.00	0.42
1:I:267:PRO:HG3	1:L:292:LEU:HD21	2.01	0.42
1:E:233:ASP:OD1	1:E:233:ASP:C	2.62	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:J:274:ARG:HD2	1:J:327:MET:HE1	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
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:D:179:TYR:CE1	1:D:230:MET:HE1	2.56	0.41
1:E:184:SER:OG	1:E:200:ASP:OD2	2.33	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:B:172:ASP:HB2	1:B:230:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:230:MET:HE2	1:K:252:ILE:CD1	2.51	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%)	36	58
1	C	309/322 (96%)	292 (94%)	16 (5%)	1 (0%)	36	58
1	D	309/322 (96%)	291 (94%)	17 (6%)	1 (0%)	36	58
1	E	309/322 (96%)	289 (94%)	19 (6%)	1 (0%)	36	58
1	F	309/322 (96%)	291 (94%)	17 (6%)	1 (0%)	36	58
1	G	309/322 (96%)	290 (94%)	18 (6%)	1 (0%)	36	58
1	H	309/322 (96%)	290 (94%)	18 (6%)	1 (0%)	36	58
1	I	309/322 (96%)	293 (95%)	15 (5%)	1 (0%)	36	58
1	J	309/322 (96%)	288 (93%)	20 (6%)	1 (0%)	36	58
1	K	309/322 (96%)	289 (94%)	20 (6%)	0	100	100
1	L	309/322 (96%)	288 (93%)	20 (6%)	1 (0%)	36	58
All	All	3708/3864 (96%)	3482 (94%)	216 (6%)	10 (0%)	36	58

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%)	253 (98%)	4 (2%)	55	79
1	B	256/265 (97%)	250 (98%)	6 (2%)	44	71
1	C	255/265 (96%)	251 (98%)	4 (2%)	55	79
1	D	255/265 (96%)	251 (98%)	4 (2%)	55	79
1	E	252/265 (95%)	247 (98%)	5 (2%)	48	74
1	F	255/265 (96%)	250 (98%)	5 (2%)	48	74
1	G	256/265 (97%)	249 (97%)	7 (3%)	39	67
1	H	254/265 (96%)	248 (98%)	6 (2%)	43	70
1	I	252/265 (95%)	249 (99%)	3 (1%)	63	83
1	J	254/265 (96%)	250 (98%)	4 (2%)	55	79
1	K	251/265 (95%)	242 (96%)	9 (4%)	31	58
1	L	254/265 (96%)	243 (96%)	11 (4%)	26	51
All	All	3051/3180 (96%)	2983 (98%)	68 (2%)	45	72

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL

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Mol	Chain	Res	Type
1	A	147	LYS
1	A	157	LYS
1	A	164	ARG
1	B	61	VAL
1	B	116	LYS
1	B	164	ARG
1	B	213	ASN
1	B	220	SER
1	B	248	MET
1	C	102	LYS
1	C	213	ASN
1	C	214	GLN
1	C	259	LYS
1	D	100	LYS
1	D	157	LYS
1	D	259	LYS
1	D	321	LEU
1	E	39	LYS
1	E	157	LYS
1	E	212	THR
1	E	248	MET
1	E	271	ASP
1	F	147	LYS
1	F	157	LYS
1	F	213	ASN
1	F	259	LYS
1	F	330	LYS
1	G	44	ARG
1	G	61	VAL
1	G	147	LYS
1	G	157	LYS
1	G	213	ASN
1	G	228	VAL
1	G	259	LYS
1	H	119	ARG
1	H	157	LYS
1	H	213	ASN
1	H	248	MET
1	H	259	LYS
1	H	347	VAL
1	I	213	ASN
1	I	248	MET

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Mol	Chain	Res	Type
1	I	259	LYS
1	J	61	VAL
1	J	213	ASN
1	J	248	MET
1	J	259	LYS
1	K	39	LYS
1	K	110	THR
1	K	111	VAL
1	K	119	ARG
1	K	157	LYS
1	K	200	ASP
1	K	212	THR
1	K	213	ASN
1	K	259	LYS
1	L	102	LYS
1	L	147	LYS
1	L	156	MET
1	L	157	LYS
1	L	212	THR
1	L	213	ASN
1	L	214	GLN
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. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	HIS
1	B	250	HIS
1	C	221	ASN
1	C	250	HIS
1	D	214	GLN
1	D	250	HIS
1	D	314	GLN
1	F	131	ASN
1	F	250	HIS
1	G	101	ASN
1	G	221	ASN
1	H	250	HIS
1	I	188	GLN

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Mol	Chain	Res	Type
1	I	214	GLN
1	I	250	HIS
1	J	250	HIS
1	K	250	HIS
1	L	250	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	311/322 (96%)	0.27	18 (5%) 29 23	30, 42, 69, 85	0
1	B	311/322 (96%)	0.09	15 (4%) 35 30	31, 40, 59, 80	0
1	C	311/322 (96%)	0.37	15 (4%) 35 30	35, 48, 71, 87	0
1	D	311/322 (96%)	0.38	21 (6%) 23 19	33, 45, 74, 104	0
1	E	311/322 (96%)	0.69	31 (9%) 12 9	34, 54, 76, 83	0
1	F	311/322 (96%)	0.38	19 (6%) 27 22	33, 48, 69, 79	0
1	G	311/322 (96%)	0.38	12 (3%) 43 38	34, 49, 67, 76	0
1	H	311/322 (96%)	0.48	20 (6%) 25 20	35, 49, 72, 95	0
1	I	311/322 (96%)	0.47	25 (8%) 18 14	34, 49, 74, 85	0
1	J	311/322 (96%)	0.70	28 (9%) 15 11	34, 53, 75, 85	0
1	K	311/322 (96%)	0.90	35 (11%) 10 8	37, 61, 84, 95	0
1	L	311/322 (96%)	0.96	32 (10%) 12 9	42, 61, 86, 109	0
All	All	3732/3864 (96%)	0.51	271 (7%) 21 17	30, 50, 77, 109	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	296	PRO	5.6
1	H	69	GLY	5.6
1	C	69	GLY	5.2
1	L	69	GLY	4.9
1	L	212	THR	4.8
1	A	69	GLY	4.7
1	I	156	MET	4.7
1	G	69	GLY	4.6
1	J	212	THR	4.6
1	H	160	GLY	4.5
1	D	38	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	I	109	PRO	4.4
1	J	100	LYS	4.3
1	F	164	ARG	4.3
1	L	295	GLY	4.2
1	D	292	LEU	4.2
1	I	320	SER	4.1
1	K	69	GLY	4.1
1	K	110	THR	4.0
1	L	156	MET	4.0
1	A	108	LEU	3.9
1	H	164	ARG	3.9
1	F	212	THR	3.8
1	H	212	THR	3.8
1	J	105	ALA	3.8
1	L	297	ASP	3.7
1	A	112	GLN	3.7
1	K	321	LEU	3.7
1	A	156	MET	3.7
1	J	99	THR	3.6
1	F	156	MET	3.6
1	H	298	SER	3.6
1	L	299	HIS	3.6
1	A	111	VAL	3.6
1	C	104	ALA	3.5
1	G	212	THR	3.5
1	H	211	ARG	3.5
1	K	212	THR	3.5
1	L	99	THR	3.5
1	A	102	LYS	3.5
1	D	110	THR	3.4
1	L	102	LYS	3.4
1	D	294	PHE	3.4
1	K	147	LYS	3.4
1	K	99	THR	3.4
1	L	38	PHE	3.4
1	E	157	LYS	3.3
1	E	69	GLY	3.3
1	D	157	LYS	3.3
1	D	293	PRO	3.3
1	F	160	GLY	3.3
1	A	107	THR	3.2
1	D	348	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	187	TYR	3.2
1	B	330	LYS	3.2
1	K	330	LYS	3.2
1	L	298	SER	3.2
1	L	348	LYS	3.2
1	F	295	GLY	3.2
1	J	295	GLY	3.2
1	I	110	THR	3.1
1	K	320	SER	3.1
1	E	96	PRO	3.0
1	K	332	GLY	3.0
1	J	156	MET	3.0
1	L	211	ARG	3.0
1	E	296	PRO	3.0
1	F	104	ALA	3.0
1	K	38	PHE	3.0
1	F	102	LYS	2.9
1	K	109	PRO	2.9
1	L	147	LYS	2.9
1	B	164	ARG	2.9
1	C	348	LYS	2.9
1	J	69	GLY	2.9
1	E	111	VAL	2.9
1	K	45	ARG	2.9
1	I	289	LYS	2.9
1	F	100	LYS	2.9
1	B	188	GLN	2.8
1	B	295	GLY	2.8
1	A	109	PRO	2.8
1	L	162	PRO	2.8
1	H	297	ASP	2.8
1	J	154	LEU	2.8
1	C	212	THR	2.8
1	K	156	MET	2.8
1	A	296	PRO	2.8
1	E	190	SER	2.8
1	K	348	LYS	2.8
1	D	296	PRO	2.8
1	J	330	LYS	2.8
1	A	105	ALA	2.8
1	D	340	GLU	2.8
1	E	348	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	147	LYS	2.7
1	I	321	LEU	2.7
1	C	99	THR	2.7
1	F	45	ARG	2.7
1	H	111	VAL	2.7
1	F	69	GLY	2.7
1	L	294	PHE	2.7
1	H	293	PRO	2.7
1	C	100	LYS	2.7
1	B	292	LEU	2.7
1	D	108	LEU	2.7
1	E	185	MET	2.7
1	D	69	GLY	2.7
1	I	115	SER	2.7
1	A	157	LYS	2.7
1	H	296	PRO	2.7
1	E	68	ARG	2.7
1	L	160	GLY	2.7
1	H	294	PHE	2.6
1	K	202	THR	2.6
1	G	45	ARG	2.6
1	K	322	ARG	2.6
1	I	100	LYS	2.6
1	I	295	GLY	2.6
1	L	153	VAL	2.6
1	K	108	LEU	2.6
1	I	45	ARG	2.6
1	C	128	LYS	2.6
1	L	256	LYS	2.6
1	I	69	GLY	2.6
1	E	212	THR	2.5
1	D	107	THR	2.5
1	B	147	LYS	2.5
1	B	348	LYS	2.5
1	H	68	ARG	2.5
1	H	295	GLY	2.5
1	K	293	PRO	2.5
1	E	294	PHE	2.5
1	E	136	ASP	2.5
1	F	211	ARG	2.5
1	B	69	GLY	2.5
1	E	110	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	348	LYS	2.5
1	B	293	PRO	2.5
1	K	155	ALA	2.5
1	G	157	LYS	2.4
1	H	157	LYS	2.4
1	E	298	SER	2.4
1	K	85	GLU	2.4
1	A	160	GLY	2.4
1	K	294	PHE	2.4
1	K	319	LYS	2.4
1	E	140	GLY	2.4
1	F	296	PRO	2.4
1	H	332	GLY	2.4
1	J	157	LYS	2.4
1	L	214	GLN	2.4
1	I	38	PHE	2.4
1	I	105	ALA	2.4
1	C	296	PRO	2.4
1	A	214	GLN	2.4
1	J	191	GLN	2.4
1	F	105	ALA	2.4
1	I	68	ARG	2.4
1	J	106	SER	2.4
1	L	291	GLU	2.4
1	G	147	LYS	2.4
1	C	293	PRO	2.4
1	G	293	PRO	2.4
1	E	118	GLY	2.4
1	F	188	GLN	2.4
1	I	108	LEU	2.3
1	E	295	GLY	2.3
1	C	294	PHE	2.3
1	K	107	THR	2.3
1	D	295	GLY	2.3
1	H	112	GLN	2.3
1	C	107	THR	2.3
1	I	107	THR	2.3
1	I	330	LYS	2.3
1	K	190	SER	2.3
1	K	96	PRO	2.3
1	C	149	GLY	2.3
1	J	108	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	99	THR	2.3
1	E	109	PRO	2.3
1	C	108	LEU	2.3
1	B	128	LYS	2.2
1	K	185	MET	2.2
1	L	157	LYS	2.2
1	K	40	THR	2.2
1	J	52	GLY	2.2
1	E	108	LEU	2.2
1	E	153	VAL	2.2
1	H	153	VAL	2.2
1	J	153	VAL	2.2
1	L	215	VAL	2.2
1	J	104	ALA	2.2
1	K	116	LYS	2.2
1	G	156	MET	2.2
1	E	187	TYR	2.2
1	A	45	ARG	2.2
1	K	189	ARG	2.2
1	L	44	ARG	2.2
1	K	296	PRO	2.2
1	B	297	ASP	2.2
1	E	332	GLY	2.2
1	J	160	GLY	2.2
1	C	102	LYS	2.2
1	I	348	LYS	2.2
1	K	111	VAL	2.2
1	A	104	ALA	2.2
1	A	212	THR	2.2
1	E	91	THR	2.2
1	J	94	TYR	2.2
1	E	293	PRO	2.2
1	A	100	LYS	2.2
1	E	54	SER	2.2
1	J	97	SER	2.2
1	J	116	LYS	2.2
1	L	116	LYS	2.2
1	F	294	PHE	2.2
1	J	164	ARG	2.2
1	I	296	PRO	2.2
1	E	100	LYS	2.2
1	F	116	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	111	VAL	2.2
1	E	220	SER	2.2
1	D	291	GLU	2.1
1	I	211	ARG	2.1
1	L	164	ARG	2.1
1	F	348	LYS	2.1
1	H	348	LYS	2.1
1	G	108	LEU	2.1
1	L	292	LEU	2.1
1	G	159	ASP	2.1
1	J	111	VAL	2.1
1	G	38	PHE	2.1
1	A	164	ARG	2.1
1	L	101	ASN	2.1
1	H	45	ARG	2.1
1	I	191	GLN	2.1
1	E	160	GLY	2.1
1	L	332	GLY	2.1
1	G	294	PHE	2.1
1	I	190	SER	2.1
1	E	287	ARG	2.1
1	J	45	ARG	2.1
1	K	86	ALA	2.1
1	L	340	GLU	2.1
1	L	100	LYS	2.1
1	J	214	GLN	2.1
1	K	214	GLN	2.1
1	J	332	GLY	2.1
1	K	48	HIS	2.1
1	D	312	VAL	2.1
1	B	291	GLU	2.0
1	D	104	ALA	2.0
1	E	86	ALA	2.0
1	C	157	LYS	2.0
1	D	330	LYS	2.0
1	G	348	LYS	2.0
1	B	296	PRO	2.0
1	D	321	LEU	2.0
1	H	292	LEU	2.0
1	F	84	GLY	2.0
1	J	92	TYR	2.0
1	B	294	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	164	ARG	2.0
1	L	287	ARG	2.0
1	D	297	ASP	2.0
1	D	116	LYS	2.0
1	F	39	LYS	2.0
1	I	293	PRO	2.0
1	B	214	GLN	2.0
1	J	186	ASN	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 oligosaccharides 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.