



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:45 AM EDT

PDB ID : 5MSJ / pdb_00005msj
Title : Mouse PA28alpha
Authors : Huber, E.M.; Groll, M.
Deposited on : 2017-01-05
Resolution : 3.50 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

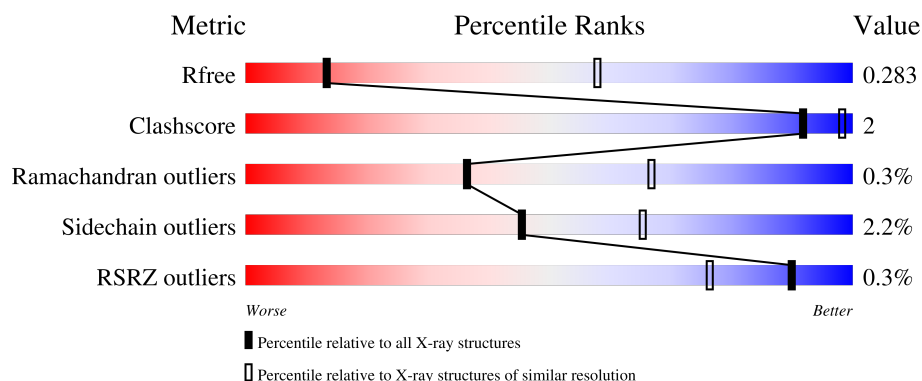
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



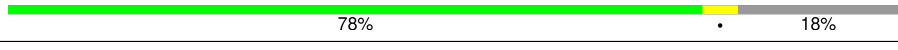
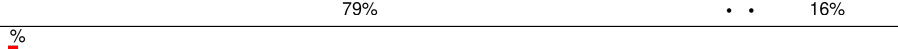
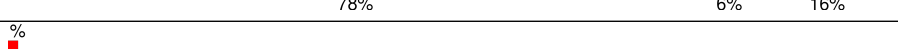
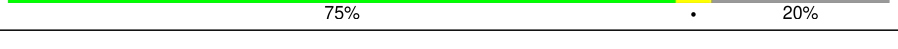
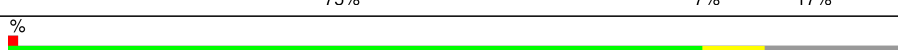
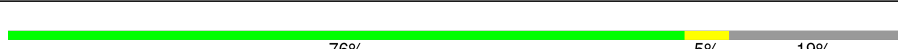
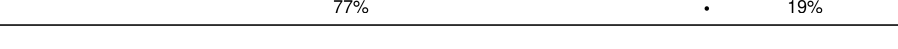
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	249	% 80% 16%
1	B	249	77% 18%
1	C	249	75% 7% 18%
1	D	249	80% 18%
1	E	249	77% 6% 16%

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Mol	Chain	Length	Quality of chain
1	F	249	% 
1	G	249	
1	H	249	
1	I	249	% 
1	J	249	
1	K	249	
1	L	249	
1	M	249	
1	N	249	
1	O	249	% 
1	P	249	
1	Q	249	
1	R	249	
1	S	249	
1	T	249	
1	U	249	% 
1	V	249	
1	W	249	
1	X	249	
1	Y	249	
1	Z	249	
1	a	249	
1	b	249	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 46128 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 Proteasome activator complex subunit 1.

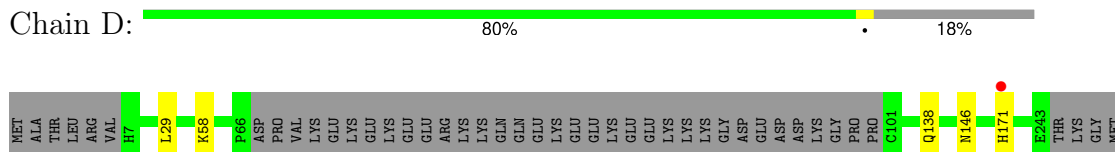
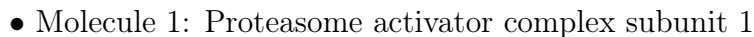
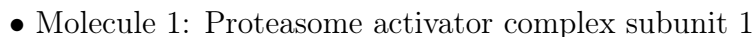
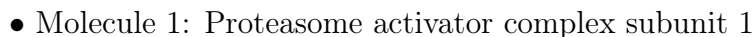
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1690	1081	288	315	6			
1	B	204	Total	C	N	O	S	0	0	0
			1646	1051	282	307	6			
1	C	205	Total	C	N	O	S	0	0	0
			1653	1056	283	308	6			
1	D	203	Total	C	N	O	S	0	0	0
			1635	1045	278	306	6			
1	E	208	Total	C	N	O	S	0	0	0
			1675	1070	286	313	6			
1	F	201	Total	C	N	O	S	0	0	0
			1619	1037	274	302	6			
1	G	205	Total	C	N	O	S	0	0	0
			1649	1054	280	309	6			
1	H	208	Total	C	N	O	S	0	0	0
			1676	1071	286	313	6			
1	I	195	Total	C	N	O	S	0	0	0
			1577	1006	269	297	5			
1	J	202	Total	C	N	O	S	0	0	0
			1635	1047	280	303	5			
1	K	207	Total	C	N	O	S	0	0	0
			1667	1066	285	310	6			
1	L	209	Total	C	N	O	S	0	0	0
			1682	1075	287	314	6			
1	M	201	Total	C	N	O	S	0	0	0
			1622	1038	276	302	6			
1	N	208	Total	C	N	O	S	0	0	0
			1675	1071	286	312	6			
1	O	203	Total	C	N	O	S	0	0	0
			1632	1044	276	306	6			
1	P	208	Total	C	N	O	S	0	0	0
			1675	1071	286	312	6			

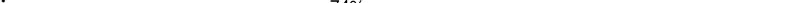
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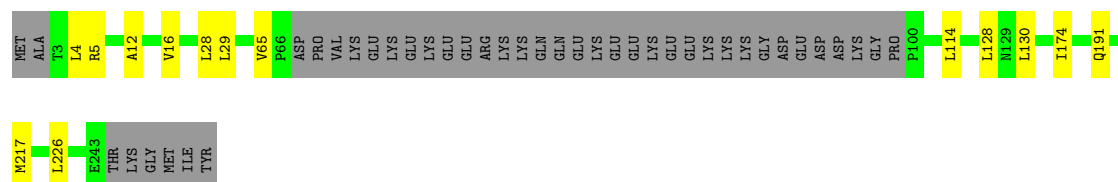
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	203	Total	C	N	O	S	0	0	0
			1635	1045	278	306	6			
1	R	200	Total	C	N	O	S	0	0	0
			1612	1032	273	301	6			
1	S	199	Total	C	N	O	S	0	0	0
			1602	1024	272	300	6			
1	T	206	Total	C	N	O	S	0	0	0
			1661	1062	284	309	6			
1	U	212	Total	C	N	O	S	0	0	0
			1711	1092	290	323	6			
1	V	202	Total	C	N	O	S	0	0	0
			1625	1039	275	305	6			
1	W	204	Total	C	N	O	S	0	0	0
			1647	1053	282	307	5			
1	X	200	Total	C	N	O	S	0	0	0
			1612	1031	273	303	5			
1	Y	201	Total	C	N	O	S	0	0	0
			1622	1037	276	304	5			
1	Z	204	Total	C	N	O	S	0	0	0
			1651	1057	282	307	5			
1	a	209	Total	C	N	O	S	0	0	0
			1683	1076	287	314	6			
1	b	206	Total	C	N	O	S	0	0	0
			1659	1062	284	307	6			

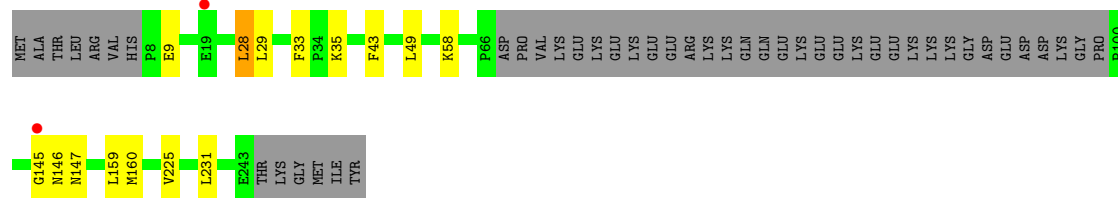
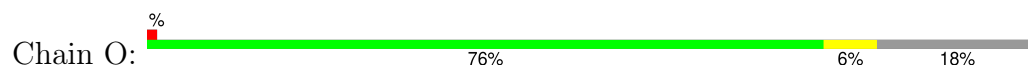
- Molecule 1: Proteasome activator complex subunit 1



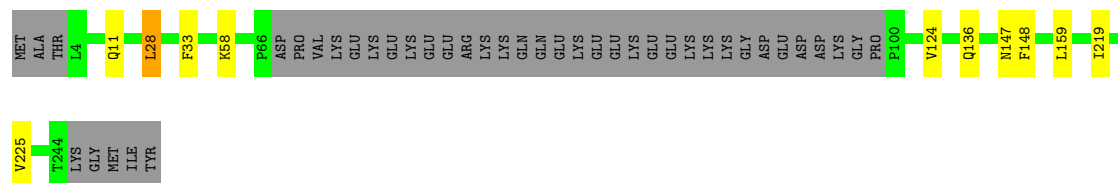
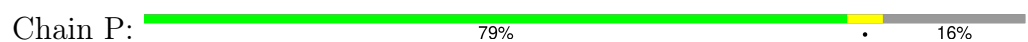
Chain I:  74% 2% 22%



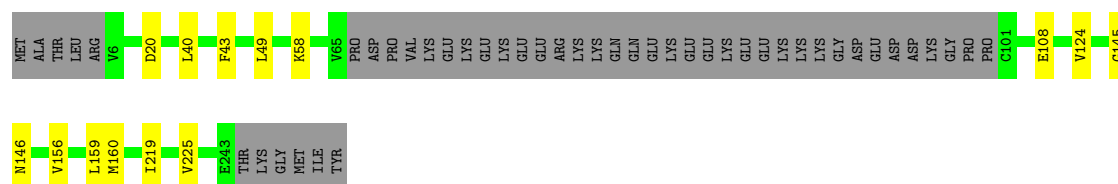
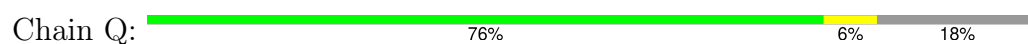
- Molecule 1: Proteasome activator complex subunit 1



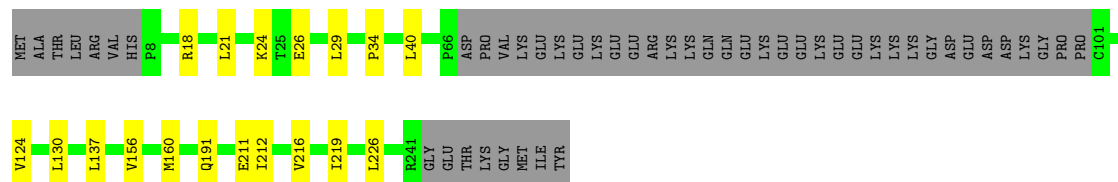
- Molecule 1: Proteasome activator complex subunit 1



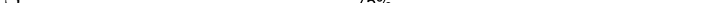
- Molecule 1: Proteasome activator complex subunit 1

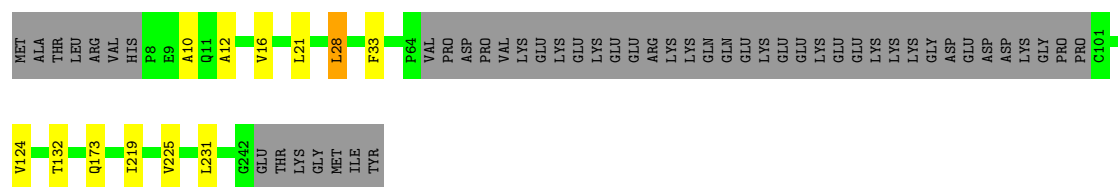


- Molecule 1: Proteasome activator complex subunit 1

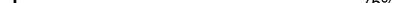


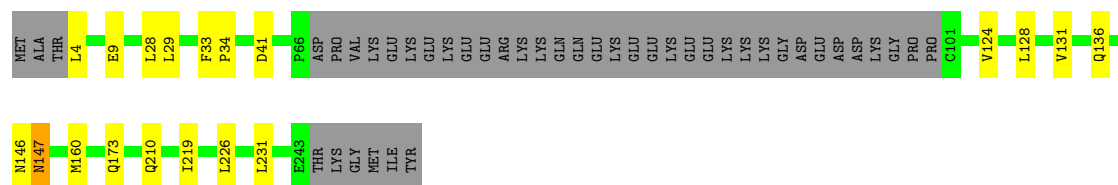
- Molecule 1: Proteasome activator complex subunit 1

Chain S:  75% . 20%

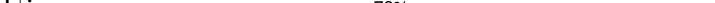


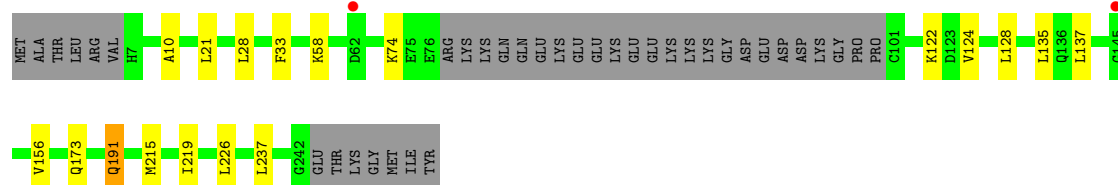
- Molecule 1: Proteasome activator complex subunit 1

Chain T:  75% 7% 17%

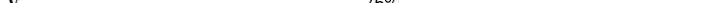


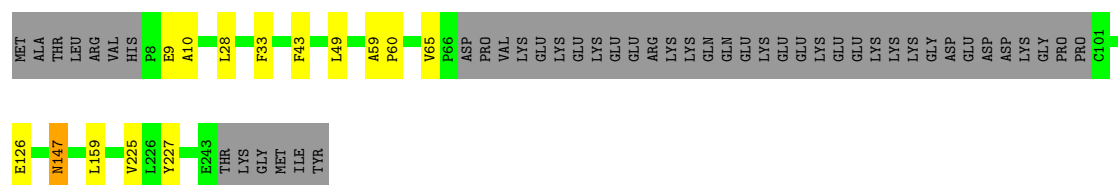
- Molecule 1: Proteasome activator complex subunit 1

Chain U:  78% 7% 15%

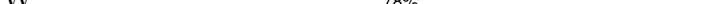


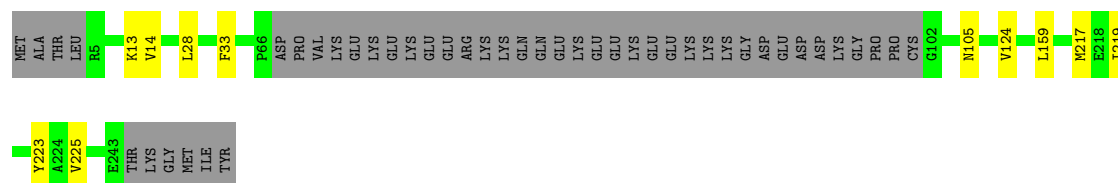
- Molecule 1: Proteasome activator complex subunit 1

Chain V:  76% 5% 19%



- Molecule 1: Proteasome activator complex subunit 1

Chain W:  78% 2% 18%



- Molecule 1: Proteasome activator complex subunit 1

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.79Å 119.80Å 196.67Å 94.21° 98.52° 87.98°	Depositor
Resolution (Å)	29.65 – 3.50 29.65 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.65-3.50) 93.1 (29.65-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.250 , 0.283 0.251 , 0.283	Depositor DCC
R_{free} test set	4638 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	91.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46128	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.50% 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	0.56	0/1722	0.85	0/2329
1	B	0.55	0/1675	0.86	0/2262
1	C	0.55	0/1683	0.86	0/2274
1	D	0.55	0/1665	0.85	0/2250
1	E	0.54	0/1705	0.85	0/2304
1	F	0.54	0/1649	0.87	0/2228
1	G	0.55	0/1679	0.83	0/2270
1	H	0.56	0/1707	0.85	0/2307
1	I	0.55	0/1604	0.86	0/2165
1	J	0.55	0/1664	0.85	0/2248
1	K	0.54	0/1698	0.84	0/2296
1	L	0.56	0/1715	0.85	0/2320
1	M	0.55	0/1652	0.84	0/2232
1	N	0.54	0/1706	0.83	0/2306
1	O	0.54	0/1662	0.84	0/2245
1	P	0.55	0/1706	0.86	0/2306
1	Q	0.55	0/1664	0.86	0/2248
1	R	0.55	0/1641	0.84	0/2217
1	S	0.54	0/1630	0.87	0/2200
1	T	0.54	0/1691	0.85	0/2285
1	U	0.54	0/1742	0.84	0/2352
1	V	0.55	0/1654	0.84	0/2234
1	W	0.54	0/1677	0.84	0/2266
1	X	0.53	0/1640	0.86	0/2214
1	Y	0.55	0/1651	0.84	0/2230
1	Z	0.54	0/1681	0.86	0/2271
1	a	0.55	0/1714	0.85	0/2318
1	b	0.54	0/1690	0.84	0/2284
All	All	0.55	0/46967	0.85	0/63461

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	1690	0	1718	4	0
1	B	1646	0	1672	5	0
1	C	1653	0	1679	7	0
1	D	1635	0	1657	0	0
1	E	1675	0	1705	8	0
1	F	1619	0	1650	9	0
1	G	1649	0	1673	4	0
1	H	1676	0	1702	8	0
1	I	1577	0	1594	6	0
1	J	1635	0	1669	6	0
1	K	1667	0	1695	4	0
1	L	1682	0	1705	13	0
1	M	1622	0	1649	3	0
1	N	1675	0	1705	6	0
1	O	1632	0	1659	7	0
1	P	1675	0	1705	5	0
1	Q	1635	0	1659	7	0
1	R	1612	0	1642	8	0
1	S	1602	0	1629	6	0
1	T	1661	0	1690	10	0
1	U	1711	0	1734	11	0
1	V	1625	0	1651	8	0
1	W	1647	0	1674	6	0
1	X	1612	0	1639	6	0
1	Y	1622	0	1645	4	0
1	Z	1651	0	1683	4	0
1	a	1683	0	1710	3	0
1	b	1659	0	1692	7	0
All	All	46128	0	46885	153	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 (153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:VAL:HG21	1:H:219:ILE:HG23	1.63	0.78
1:E:135:LEU:HD11	1:E:237:LEU:HD22	1.66	0.78
1:F:124:VAL:HG21	1:F:219:ILE:HG23	1.69	0.75
1:L:124:VAL:HG21	1:L:219:ILE:HG23	1.69	0.73
1:U:135:LEU:HD11	1:U:237:LEU:HD22	1.76	0.65
1:Q:124:VAL:HG11	1:Q:219:ILE:HG23	1.77	0.65
1:T:128:LEU:HD13	1:T:226:LEU:HD11	1.80	0.62
1:N:128:LEU:HD12	1:N:226:LEU:HD11	1.84	0.60
1:E:117:LEU:HD21	1:E:215:MET:CE	2.32	0.60
1:R:124:VAL:HG11	1:R:219:ILE:HG23	1.84	0.59
1:V:147:ASN:H	1:V:147:ASN:ND2	2.01	0.58
1:N:28:LEU:HD21	1:N:130:LEU:HD22	1.84	0.58
1:R:24:LYS:HD3	1:R:130:LEU:HD11	1.86	0.58
1:N:12:ALA:O	1:N:16:VAL:HG23	2.05	0.57
1:J:128:LEU:HD13	1:J:226:LEU:HD11	1.86	0.56
1:K:159:LEU:HD21	1:K:225:VAL:HG12	1.87	0.56
1:E:117:LEU:HD21	1:E:215:MET:HE3	1.89	0.55
1:U:124:VAL:HG11	1:U:219:ILE:HG23	1.88	0.55
1:H:124:VAL:HG21	1:H:219:ILE:CG2	2.36	0.55
1:U:124:VAL:CG1	1:U:219:ILE:HG23	2.37	0.55
1:Y:128:LEU:HD12	1:Y:226:LEU:HD11	1.89	0.54
1:C:124:VAL:HG11	1:C:219:ILE:HG23	1.89	0.54
1:I:21:LEU:HD23	1:I:137:LEU:HD12	1.90	0.54
1:S:28:LEU:HD21	1:S:33:PHE:CE1	2.43	0.54
1:R:40:LEU:HD13	1:R:219:ILE:HG22	1.91	0.53
1:T:124:VAL:HG11	1:T:219:ILE:HG23	1.89	0.53
1:X:159:LEU:HD21	1:X:225:VAL:HG12	1.91	0.53
1:F:124:VAL:HG22	1:F:223:TYR:CE2	2.44	0.53
1:L:124:VAL:HG22	1:L:223:TYR:CZ	2.44	0.52
1:a:12:ALA:O	1:a:16:VAL:HG23	2.08	0.52
1:S:12:ALA:O	1:S:16:VAL:HG23	2.09	0.52
1:K:12:ALA:O	1:K:16:VAL:HG23	2.09	0.52
1:b:159:LEU:HD21	1:b:225:VAL:HG12	1.92	0.52
1:U:28:LEU:HD21	1:U:33:PHE:CE1	2.44	0.52
1:V:227:TYR:CE2	1:W:14:VAL:HG21	2.45	0.52
1:R:156:VAL:HG12	1:R:160:MET:HE3	1.92	0.52
1:B:128:LEU:HD12	1:B:226:LEU:HD11	1.91	0.51
1:Z:159:LEU:HD21	1:Z:225:VAL:HG12	1.93	0.51
1:P:124:VAL:HG11	1:P:219:ILE:HG23	1.92	0.51
1:Q:124:VAL:CG1	1:Q:219:ILE:HG23	2.41	0.51
1:W:124:VAL:HG21	1:W:219:ILE:HG23	1.93	0.50
1:A:159:LEU:HD21	1:A:225:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:217:MET:HE2	1:X:129:ASN:HD22	1.77	0.50
1:B:34:PRO:HG2	1:C:10:ALA:HB1	1.93	0.50
1:H:124:VAL:HG22	1:H:223:TYR:CE2	2.47	0.50
1:H:124:VAL:HG22	1:H:223:TYR:CZ	2.47	0.50
1:V:147:ASN:ND2	1:V:147:ASN:N	2.59	0.50
1:X:12:ALA:O	1:X:16:VAL:HG23	2.11	0.50
1:F:159:LEU:HD21	1:F:225:VAL:HG12	1.93	0.49
1:G:28:LEU:HD21	1:G:33:PHE:CE1	2.47	0.49
1:A:48:ALA:HB1	1:A:113:LEU:HD21	1.93	0.49
1:L:48:ALA:HB1	1:L:113:LEU:HD21	1.93	0.49
1:L:12:ALA:O	1:L:16:VAL:HG23	2.13	0.49
1:P:159:LEU:HD21	1:P:225:VAL:HG12	1.94	0.49
1:V:28:LEU:HD21	1:V:33:PHE:CE1	2.47	0.49
1:H:120:GLU:O	1:H:124:VAL:HG23	2.13	0.49
1:U:128:LEU:HD12	1:U:226:LEU:HD11	1.95	0.49
1:V:10:ALA:HB1	1:b:34:PRO:HG2	1.95	0.49
1:X:210:GLN:HE22	1:Y:122:LYS:HD2	1.78	0.49
1:F:124:VAL:HG22	1:F:223:TYR:CZ	2.48	0.49
1:M:28:LEU:HD21	1:M:33:PHE:CE1	2.48	0.48
1:G:211:GLU:HG3	1:G:215:MET:HE2	1.95	0.48
1:R:34:PRO:HG2	1:S:10:ALA:HB1	1.94	0.48
1:R:124:VAL:CG1	1:R:219:ILE:HG23	2.43	0.48
1:T:124:VAL:CG1	1:T:219:ILE:HG23	2.44	0.48
1:Y:159:LEU:HD21	1:Y:225:VAL:HG12	1.96	0.47
1:E:44:LEU:HD21	1:E:217:MET:HG2	1.96	0.47
1:C:211:GLU:HG3	1:C:215:MET:HE3	1.96	0.47
1:S:124:VAL:HG11	1:S:219:ILE:HG23	1.97	0.47
1:Z:28:LEU:HD21	1:Z:33:PHE:CE1	2.50	0.47
1:O:225:VAL:HG21	1:P:136:GLN:NE2	2.30	0.47
1:T:210:GLN:HE22	1:U:122:LYS:HD2	1.80	0.46
1:X:28:LEU:HD21	1:X:33:PHE:CE1	2.50	0.46
1:Q:156:VAL:HG12	1:Q:160:MET:HE3	1.97	0.46
1:J:124:VAL:HG11	1:J:219:ILE:HG23	1.98	0.46
1:J:12:ALA:O	1:J:16:VAL:HG23	2.15	0.46
1:I:124:VAL:HG11	1:I:219:ILE:HG23	1.97	0.46
1:L:128:LEU:HD12	1:L:226:LEU:HD11	1.96	0.46
1:T:28:LEU:HD21	1:T:33:PHE:CE1	2.51	0.46
1:Q:159:LEU:HD21	1:Q:225:VAL:HG12	1.98	0.46
1:B:159:LEU:HD21	1:B:225:VAL:HG12	1.97	0.45
1:L:144:ASP:O	1:O:146:ASN:N	2.48	0.45
1:W:159:LEU:HD21	1:W:225:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ASP:O	1:b:146:ASN:N	2.50	0.45
1:b:28:LEU:HD21	1:b:33:PHE:CE1	2.52	0.45
1:J:147:ASN:HD22	1:Q:145:GLY:HA3	1.82	0.45
1:L:28:LEU:CD1	1:L:33:PHE:CE1	2.99	0.45
1:A:18:ARG:NH2	1:G:228:ASP:OD1	2.50	0.44
1:J:28:LEU:HD12	1:J:29:LEU:N	2.32	0.44
1:K:191:GLN:HE21	1:K:191:GLN:HA	1.82	0.44
1:R:212:ILE:O	1:R:216:VAL:HG23	2.17	0.44
1:T:146:ASN:C	1:T:147:ASN:HD22	2.25	0.44
1:L:120:GLU:O	1:L:124:VAL:HG23	2.18	0.44
1:P:28:LEU:HD21	1:P:33:PHE:CE1	2.53	0.44
1:C:21:LEU:HD23	1:C:137:LEU:HD12	1.99	0.44
1:V:59:ALA:HB1	1:V:60:PRO:HD2	2.00	0.44
1:W:28:LEU:HD21	1:W:33:PHE:CE1	2.53	0.44
1:X:173:GLN:NE2	1:X:215:MET:HE1	2.33	0.44
1:Z:124:VAL:HG21	1:Z:219:ILE:HG12	2.00	0.44
1:O:28:LEU:HD23	1:O:29:LEU:N	2.33	0.44
1:E:210:GLN:HE22	1:F:122:LYS:HD2	1.83	0.43
1:T:131:VAL:HG12	1:T:160:MET:HE2	2.00	0.43
1:H:126:GLU:HA	1:N:217:MET:HE1	2.00	0.43
1:U:21:LEU:HD23	1:U:137:LEU:HD12	1.99	0.43
1:F:120:GLU:O	1:F:124:VAL:HG23	2.18	0.43
1:I:159:LEU:HD21	1:I:225:VAL:CG1	2.48	0.43
1:J:144:ASP:O	1:Q:146:ASN:N	2.46	0.43
1:O:159:LEU:HD21	1:O:225:VAL:HG12	1.99	0.43
1:L:159:LEU:HD21	1:L:225:VAL:HG12	2.00	0.43
1:M:28:LEU:HD21	1:M:33:PHE:CZ	2.54	0.43
1:U:191:GLN:HE21	1:U:191:GLN:HA	1.83	0.43
1:a:210:GLN:HE22	1:b:122:LYS:HD2	1.83	0.43
1:E:159:LEU:HD21	1:E:225:VAL:HG12	2.00	0.43
1:H:135:LEU:HD11	1:H:237:LEU:HD22	2.00	0.43
1:L:34:PRO:HG2	1:M:10:ALA:HB1	2.00	0.43
1:V:159:LEU:HD21	1:V:225:VAL:HG12	2.00	0.43
1:I:173:GLN:NE2	1:I:208:GLU:OE1	2.52	0.43
1:B:107:ASN:O	1:B:111:VAL:HG23	2.19	0.42
1:I:191:GLN:HE21	1:I:191:GLN:HA	1.84	0.42
1:S:124:VAL:CG1	1:S:219:ILE:HG23	2.49	0.42
1:W:124:VAL:HG22	1:W:223:TYR:CZ	2.54	0.42
1:C:159:LEU:HD21	1:C:225:VAL:HG12	2.01	0.42
1:C:29:LEU:HD11	1:C:231:LEU:HD12	2.01	0.42
1:U:156:VAL:HG21	1:U:237:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:LEU:HD11	1:F:33:PHE:CE1	2.55	0.42
1:Y:29:LEU:HD22	1:Z:4:LEU:HD21	2.01	0.42
1:L:63:ILE:HG21	1:L:198:ARG:HD3	2.02	0.42
1:S:225:VAL:HG21	1:T:136:GLN:OE1	2.20	0.42
1:b:43:PHE:CZ	1:b:49:LEU:HD11	2.55	0.42
1:K:29:LEU:HD11	1:K:230:ILE:HG21	2.01	0.41
1:T:147:ASN:HD22	1:T:147:ASN:N	2.19	0.41
1:N:114:LEU:HD13	1:N:174:ILE:HG23	2.03	0.41
1:O:28:LEU:HD21	1:O:33:PHE:CE1	2.55	0.41
1:A:159:LEU:HD21	1:A:225:VAL:CG1	2.51	0.41
1:H:191:GLN:HE21	1:H:191:GLN:HA	1.86	0.41
1:P:124:VAL:CG1	1:P:219:ILE:HG23	2.49	0.41
1:C:128:LEU:HD13	1:C:226:LEU:HD11	2.03	0.41
1:E:53:ASN:O	1:E:53:ASN:ND2	2.54	0.41
1:L:147:ASN:HD22	1:O:145:GLY:HA2	1.85	0.41
1:B:21:LEU:HD23	1:B:137:LEU:HD12	2.02	0.41
1:E:156:VAL:HG21	1:E:237:LEU:HD21	2.02	0.41
1:N:65:VAL:HG13	1:N:65:VAL:O	2.21	0.41
1:T:34:PRO:HG2	1:U:10:ALA:HB1	2.03	0.41
1:O:43:PHE:CZ	1:O:49:LEU:HD11	2.55	0.40
1:V:43:PHE:CZ	1:V:49:LEU:HD11	2.56	0.40
1:F:124:VAL:CG2	1:F:219:ILE:HG23	2.44	0.40
1:Q:43:PHE:CZ	1:Q:49:LEU:HD11	2.56	0.40
1:R:21:LEU:CD2	1:R:137:LEU:HD12	2.52	0.40
1:U:173:GLN:NE2	1:U:215:MET:HE1	2.36	0.40
1:I:124:VAL:CG1	1:I:219:ILE:HG23	2.50	0.40
1:L:49:LEU:CD1	1:L:113:LEU:HD22	2.51	0.40
1:G:192:PRO:O	1:G:198:ARG:NH2	2.55	0.40
1:a:231:LEU:HD21	1:b:11:GLN:HE22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/249 (83%)	201 (98%)	4 (2%)	1 (0%)	24	57
1	B	200/249 (80%)	194 (97%)	6 (3%)	0	100	100
1	C	201/249 (81%)	197 (98%)	3 (2%)	1 (0%)	24	57
1	D	199/249 (80%)	195 (98%)	3 (2%)	1 (0%)	24	57
1	E	204/249 (82%)	199 (98%)	3 (2%)	2 (1%)	12	44
1	F	197/249 (79%)	190 (96%)	7 (4%)	0	100	100
1	G	201/249 (81%)	199 (99%)	1 (0%)	1 (0%)	24	57
1	H	204/249 (82%)	199 (98%)	3 (2%)	2 (1%)	12	44
1	I	191/249 (77%)	189 (99%)	2 (1%)	0	100	100
1	J	198/249 (80%)	194 (98%)	4 (2%)	0	100	100
1	K	203/249 (82%)	200 (98%)	3 (2%)	0	100	100
1	L	205/249 (82%)	200 (98%)	5 (2%)	0	100	100
1	M	197/249 (79%)	194 (98%)	3 (2%)	0	100	100
1	N	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	O	199/249 (80%)	195 (98%)	3 (2%)	1 (0%)	24	57
1	P	204/249 (82%)	200 (98%)	3 (2%)	1 (0%)	24	57
1	Q	199/249 (80%)	195 (98%)	3 (2%)	1 (0%)	24	57
1	R	196/249 (79%)	192 (98%)	4 (2%)	0	100	100
1	S	195/249 (78%)	190 (97%)	5 (3%)	0	100	100
1	T	202/249 (81%)	198 (98%)	4 (2%)	0	100	100
1	U	208/249 (84%)	203 (98%)	4 (2%)	1 (0%)	24	57
1	V	198/249 (80%)	193 (98%)	5 (2%)	0	100	100
1	W	200/249 (80%)	196 (98%)	4 (2%)	0	100	100
1	X	196/249 (79%)	192 (98%)	2 (1%)	2 (1%)	12	44
1	Y	197/249 (79%)	192 (98%)	4 (2%)	1 (0%)	24	57
1	Z	200/249 (80%)	199 (100%)	1 (0%)	0	100	100
1	a	205/249 (82%)	196 (96%)	8 (4%)	1 (0%)	24	57
1	b	202/249 (81%)	198 (98%)	3 (2%)	1 (0%)	24	57
All	All	5611/6972 (80%)	5491 (98%)	103 (2%)	17 (0%)	36	67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	146	ASN
1	D	58	LYS
1	H	58	LYS
1	Y	147	ASN
1	b	146	ASN
1	A	6	VAL
1	C	58	LYS
1	P	58	LYS
1	U	58	LYS
1	E	58	LYS
1	O	58	LYS
1	Q	58	LYS
1	X	58	LYS
1	a	8	PRO
1	G	8	PRO
1	E	60	PRO
1	H	6	VAL

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	188/223 (84%)	182 (97%)	6 (3%)	34	59
1	B	182/223 (82%)	178 (98%)	4 (2%)	45	65
1	C	183/223 (82%)	179 (98%)	4 (2%)	45	65
1	D	181/223 (81%)	177 (98%)	4 (2%)	45	65
1	E	186/223 (83%)	181 (97%)	5 (3%)	39	62
1	F	180/223 (81%)	177 (98%)	3 (2%)	53	70
1	G	183/223 (82%)	181 (99%)	2 (1%)	65	74
1	H	186/223 (83%)	182 (98%)	4 (2%)	45	65
1	I	174/223 (78%)	170 (98%)	4 (2%)	44	64
1	J	181/223 (81%)	174 (96%)	7 (4%)	28	54
1	K	185/223 (83%)	181 (98%)	4 (2%)	45	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	187/223 (84%)	182 (97%)	5 (3%)	39	62
1	M	180/223 (81%)	174 (97%)	6 (3%)	33	58
1	N	186/223 (83%)	182 (98%)	4 (2%)	45	65
1	O	181/223 (81%)	175 (97%)	6 (3%)	33	58
1	P	186/223 (83%)	182 (98%)	4 (2%)	45	65
1	Q	181/223 (81%)	178 (98%)	3 (2%)	53	70
1	R	179/223 (80%)	173 (97%)	6 (3%)	32	57
1	S	177/223 (79%)	172 (97%)	5 (3%)	38	61
1	T	184/223 (82%)	177 (96%)	7 (4%)	29	55
1	U	190/223 (85%)	188 (99%)	2 (1%)	65	74
1	V	180/223 (81%)	176 (98%)	4 (2%)	45	65
1	W	182/223 (82%)	180 (99%)	2 (1%)	65	74
1	X	178/223 (80%)	178 (100%)	0	100	100
1	Y	179/223 (80%)	176 (98%)	3 (2%)	53	70
1	Z	183/223 (82%)	178 (97%)	5 (3%)	39	62
1	a	187/223 (84%)	186 (100%)	1 (0%)	81	80
1	b	184/223 (82%)	181 (98%)	3 (2%)	55	70
All	All	5113/6244 (82%)	5000 (98%)	113 (2%)	45	65

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	18	ARG
1	A	56	ASN
1	A	138	GLN
1	A	171	HIS
1	A	187	LYS
1	B	115	GLN
1	B	128	LEU
1	B	138	GLN
1	B	173	GLN
1	C	19	GLU
1	C	28	LEU
1	C	138	GLN
1	C	171	HIS

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Mol	Chain	Res	Type
1	D	29	LEU
1	D	138	GLN
1	D	146	ASN
1	D	171	HIS
1	E	13	LYS
1	E	18	ARG
1	E	53	ASN
1	E	56	ASN
1	E	138	GLN
1	F	16	VAL
1	F	138	GLN
1	F	173	GLN
1	G	127	GLN
1	G	147	ASN
1	H	6	VAL
1	H	40	LEU
1	H	53	ASN
1	H	191	GLN
1	I	21	LEU
1	I	130	LEU
1	I	138	GLN
1	I	191	GLN
1	J	4	LEU
1	J	28	LEU
1	J	29	LEU
1	J	53	ASN
1	J	146	ASN
1	J	147	ASN
1	J	212	ILE
1	K	4	LEU
1	K	57	LEU
1	K	138	GLN
1	K	191	GLN
1	L	28	LEU
1	L	57	LEU
1	L	63	ILE
1	L	161	THR
1	L	174	ILE
1	M	28	LEU
1	M	108	GLU
1	M	137	LEU
1	M	138	GLN

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Mol	Chain	Res	Type
1	M	147	ASN
1	M	159	LEU
1	N	4	LEU
1	N	5	ARG
1	N	29	LEU
1	N	191	GLN
1	O	9	GLU
1	O	28	LEU
1	O	35	LYS
1	O	147	ASN
1	O	160	MET
1	O	231	LEU
1	P	11	GLN
1	P	28	LEU
1	P	147	ASN
1	P	148	PHE
1	Q	20	ASP
1	Q	40	LEU
1	Q	108	GLU
1	R	18	ARG
1	R	26	GLU
1	R	29	LEU
1	R	191	GLN
1	R	211	GLU
1	R	226	LEU
1	S	21	LEU
1	S	28	LEU
1	S	132	THR
1	S	173	GLN
1	S	231	LEU
1	T	4	LEU
1	T	9	GLU
1	T	29	LEU
1	T	41	ASP
1	T	147	ASN
1	T	173	GLN
1	T	231	LEU
1	U	74	LYS
1	U	191	GLN
1	V	9	GLU
1	V	65	VAL
1	V	126	GLU

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Mol	Chain	Res	Type
1	V	147	ASN
1	W	13	LYS
1	W	105	ASN
1	Y	128	LEU
1	Y	130	LEU
1	Y	146	ASN
1	Z	19	GLU
1	Z	53	ASN
1	Z	124	VAL
1	Z	146	ASN
1	Z	167	LEU
1	a	173	GLN
1	b	4	LEU
1	b	54	LEU
1	b	56	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	146	ASN
1	A	193	HIS
1	A	210	GLN
1	B	115	GLN
1	B	138	GLN
1	B	162	ASN
1	B	164	HIS
1	B	171	HIS
1	B	173	GLN
1	B	193	HIS
1	B	210	GLN
1	C	191	GLN
1	D	27	ASN
1	D	146	ASN
1	D	147	ASN
1	D	210	GLN
1	E	53	ASN
1	E	56	ASN
1	E	162	ASN
1	E	210	GLN
1	F	105	ASN
1	F	138	GLN

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Mol	Chain	Res	Type
1	F	146	ASN
1	F	173	GLN
1	F	193	HIS
1	F	202	HIS
1	G	11	GLN
1	H	53	ASN
1	H	105	ASN
1	H	127	GLN
1	H	147	ASN
1	H	164	HIS
1	H	171	HIS
1	H	191	GLN
1	H	221	ASN
1	I	53	ASN
1	I	129	ASN
1	I	138	GLN
1	I	191	GLN
1	J	146	ASN
1	J	221	ASN
1	K	11	GLN
1	K	105	ASN
1	K	191	GLN
1	L	129	ASN
1	L	147	ASN
1	L	199	GLN
1	L	202	HIS
1	M	53	ASN
1	M	136	GLN
1	M	138	GLN
1	M	162	ASN
1	N	105	ASN
1	N	136	GLN
1	N	138	GLN
1	N	146	ASN
1	N	147	ASN
1	N	191	GLN
1	O	146	ASN
1	O	173	GLN
1	O	210	GLN
1	P	11	GLN
1	P	105	ASN
1	P	136	GLN

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Mol	Chain	Res	Type
1	Q	146	ASN
1	Q	147	ASN
1	Q	199	GLN
1	R	53	ASN
1	R	191	GLN
1	S	136	GLN
1	T	147	ASN
1	T	210	GLN
1	U	147	ASN
1	U	173	GLN
1	U	191	GLN
1	U	193	HIS
1	V	146	ASN
1	V	147	ASN
1	W	11	GLN
1	W	105	ASN
1	W	115	GLN
1	W	153	GLN
1	X	129	ASN
1	X	138	GLN
1	X	147	ASN
1	Y	105	ASN
1	Y	127	GLN
1	Y	191	GLN
1	Z	115	GLN
1	Z	173	GLN
1	a	50	ASN
1	b	56	ASN
1	b	173	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	210/249 (84%)	0.01	2 (0%) 79 56	66, 89, 122, 152	0
1	B	204/249 (81%)	0.02	1 (0%) 87 68	70, 95, 136, 141	0
1	C	205/249 (82%)	0.04	0 100 100	71, 97, 133, 149	0
1	D	203/249 (81%)	0.09	1 (0%) 87 68	76, 100, 148, 160	0
1	E	208/249 (83%)	0.17	1 (0%) 87 68	82, 105, 135, 148	0
1	F	201/249 (80%)	0.02	3 (1%) 72 47	73, 95, 137, 152	0
1	G	205/249 (82%)	-0.02	1 (0%) 87 68	71, 88, 122, 138	0
1	H	208/249 (83%)	0.03	1 (0%) 87 68	79, 100, 134, 162	0
1	I	195/249 (78%)	0.10	2 (1%) 79 56	79, 105, 143, 158	0
1	J	202/249 (81%)	0.02	0 100 100	75, 98, 143, 154	0
1	K	207/249 (83%)	0.03	0 100 100	75, 101, 144, 157	0
1	L	209/249 (83%)	0.04	1 (0%) 87 68	76, 106, 137, 165	0
1	M	201/249 (80%)	0.05	0 100 100	75, 107, 145, 157	0
1	N	208/249 (83%)	0.03	0 100 100	73, 98, 137, 147	0
1	O	203/249 (81%)	0.04	2 (0%) 79 56	71, 93, 125, 147	0
1	P	208/249 (83%)	-0.01	0 100 100	72, 95, 132, 144	0
1	Q	203/249 (81%)	-0.04	0 100 100	76, 100, 129, 135	0
1	R	200/249 (80%)	0.00	0 100 100	81, 100, 140, 171	0
1	S	199/249 (79%)	0.02	0 100 100	69, 94, 137, 159	0
1	T	206/249 (82%)	0.08	0 100 100	70, 93, 131, 139	0
1	U	212/249 (85%)	-0.02	2 (0%) 81 58	69, 92, 144, 174	0
1	V	202/249 (81%)	0.02	0 100 100	76, 95, 134, 161	0
1	W	204/249 (81%)	-0.03	0 100 100	73, 95, 137, 150	0
1	X	200/249 (80%)	-0.02	0 100 100	69, 94, 128, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	201/249 (80%)	-0.00	0 100 100	67, 96, 136, 162	0
1	Z	204/249 (81%)	-0.03	0 100 100	68, 95, 134, 159	0
1	a	209/249 (83%)	0.05	0 100 100	71, 98, 133, 155	0
1	b	206/249 (82%)	0.02	1 (0%) 87 68	71, 97, 133, 148	0
All	All	5723/6972 (82%)	0.03	18 (0%) 90 76	66, 97, 137, 174	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	145	GLY	4.0
1	b	62	ASP	2.6
1	L	144	ASP	2.5
1	D	171	HIS	2.4
1	A	171	HIS	2.4
1	B	145	GLY	2.4
1	E	203	GLU	2.4
1	G	6	VAL	2.3
1	U	62	ASP	2.3
1	H	206	GLU	2.2
1	I	203	GLU	2.2
1	A	228	ASP	2.2
1	F	106	CYS	2.2
1	I	145	GLY	2.2
1	O	19	GLU	2.1
1	F	149	GLY	2.1
1	U	145	GLY	2.1
1	F	8	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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.