



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2022 – 02:05 PM EST

PDB ID : 7LO0
Title : Structure of human ASF1a in complex with a TLK2 peptide
Authors : Simon, B.; Calderwood, D.; Turk, B.E.; Boggon, T.J.
Deposited on : 2021-02-08
Resolution : 2.71 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	:	2.26
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)	:	2.26

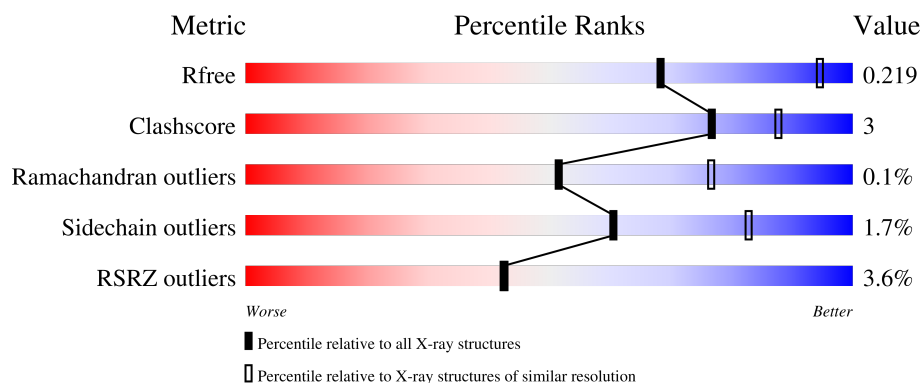
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	157	<div> <div>4%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	157	<div> <div>%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	C	157	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	D	157	<div> <div>3%</div> <div>84%</div> <div>11%</div> <div>.</div> </div>
1	E	157	<div> <div>2%</div> <div>92%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	157	 % 89% 8%
1	G	157	 3% 90% 8%
1	H	157	 6% 89% 8%
2	I	21	 5% 48% 24% 29%
2	J	21	 62% 10% 29%
2	K	21	 5% 67% 5% 29%
2	L	21	 67% 10% 24%
2	M	21	 67% 10% 24%
2	N	21	 57% 29% 14%
2	O	21	 19% 57% 10% 33%
2	P	21	 5% 43% 24% 33%
2	Q	21	 5% 33% 67%
2	R	21	 10% 29% 10% 62%
2	T	21	 29% 5% 67%
2	U	21	 10% 19% 10% 5% 67%
2	V	21	 5% 33% 67%
2	W	21	 5% 29% 5% 67%
2	X	21	 5% 29% 5% 67%
2	Y	21	 29% 5% 67%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22462 atoms, of which 10914 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 Histone chaperone ASF1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	154	Total	C	H	N	O	S	0	0	0
			2431	796	1191	202	238	4			
1	B	153	Total	C	H	N	O	S	0	0	0
			2413	791	1181	201	237	3			
1	C	153	Total	C	H	N	O	S	0	0	0
			2403	791	1171	201	237	3			
1	D	151	Total	C	H	N	O	S	0	0	0
			2368	783	1150	199	233	3			
1	E	152	Total	C	H	N	O	S	0	0	0
			2399	786	1176	200	234	3			
1	F	152	Total	C	H	N	O	S	0	0	0
			2386	786	1163	200	234	3			
1	G	154	Total	C	H	N	O	S	0	0	0
			2427	796	1187	202	238	4			
1	H	152	Total	C	H	N	O	S	0	0	0
			2399	786	1176	200	234	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9Y294
A	0	SER	-	expression tag	UNP Q9Y294
B	-1	GLY	-	expression tag	UNP Q9Y294
B	0	SER	-	expression tag	UNP Q9Y294
C	-1	GLY	-	expression tag	UNP Q9Y294
C	0	SER	-	expression tag	UNP Q9Y294
D	-1	GLY	-	expression tag	UNP Q9Y294
D	0	SER	-	expression tag	UNP Q9Y294
E	-1	GLY	-	expression tag	UNP Q9Y294
E	0	SER	-	expression tag	UNP Q9Y294
F	-1	GLY	-	expression tag	UNP Q9Y294
F	0	SER	-	expression tag	UNP Q9Y294
G	-1	GLY	-	expression tag	UNP Q9Y294

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP Q9Y294
H	-1	GLY	-	expression tag	UNP Q9Y294
H	0	SER	-	expression tag	UNP Q9Y294

- Molecule 2 is a protein called Serine/threonine-protein kinase tousled-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	15	Total	C	H	N	O	0	0	0
			249	77	124	25	23			
2	J	15	Total	C	H	N	O	0	0	0
			249	77	124	25	23			
2	K	15	Total	C	H	N	O	0	0	0
			249	77	124	25	23			
2	L	16	Total	C	H	N	O	0	0	0
			268	83	135	26	24			
2	M	16	Total	C	H	N	O	0	0	0
			268	83	135	26	24			
2	N	18	Total	C	H	N	O	0	0	0
			284	92	135	30	27			
2	O	14	Total	C	H	N	O	0	0	0
			233	72	115	24	22			
2	P	14	Total	C	H	N	O	0	0	0
			209	72	91	24	22			
2	Q	7	Total	C	H	N	O	0	0	0
			132	39	67	14	12			
2	R	8	Total	C	H	N	O	0	0	0
			137	42	67	15	13			
2	T	7	Total	C	H	N	O	0	0	0
			132	39	67	14	12			
2	U	7	Total	C	H	N	O	0	0	0
			132	39	67	14	12			
2	V	7	Total	C	H	N	O	0	0	0
			132	39	67	14	12			
2	W	7	Total	C	H	N	O	0	0	0
			132	39	67	14	12			
2	X	7	Total	C	H	N	O	0	0	0
			132	39	67	14	12			
2	Y	7	Total	C	H	N	O	0	0	0
			132	39	67	14	12			

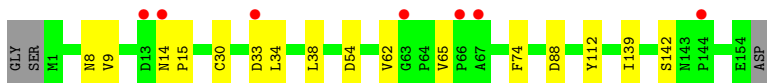
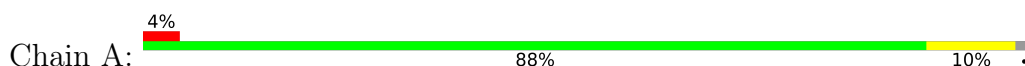
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	29	Total 29	O 29	0	0
3	C	23	Total 23	O 23	0	0
3	D	10	Total 10	O 10	0	0
3	E	28	Total 28	O 28	0	0
3	F	13	Total 13	O 13	0	0
3	G	17	Total 17	O 17	0	0
3	H	6	Total 6	O 6	0	0
3	I	1	Total 1	O 1	0	0
3	J	2	Total 2	O 2	0	0
3	K	2	Total 2	O 2	0	0
3	L	4	Total 4	O 4	0	0
3	M	3	Total 3	O 3	0	0
3	N	2	Total 2	O 2	0	0
3	P	1	Total 1	O 1	0	0
3	T	1	Total 1	O 1	0	0
3	U	2	Total 2	O 2	0	0

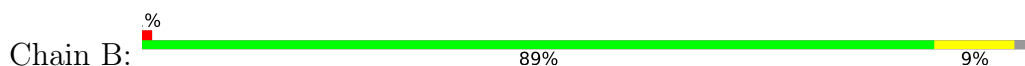
3 Residue-property plots [i](#)

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: Histone chaperone ASF1A



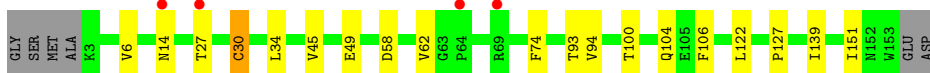
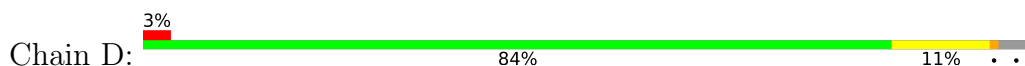
- Molecule 1: Histone chaperone ASF1A



- Molecule 1: Histone chaperone ASF1A



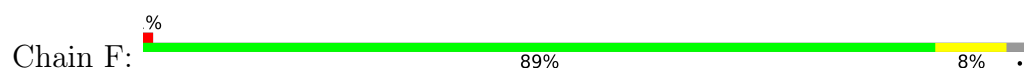
- Molecule 1: Histone chaperone ASF1A



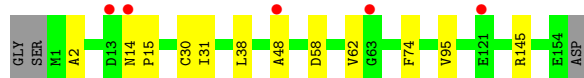
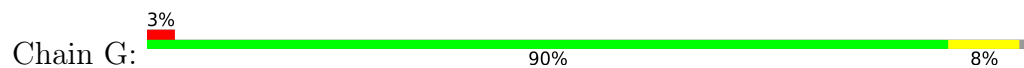
- Molecule 1: Histone chaperone ASF1A



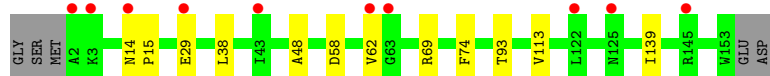
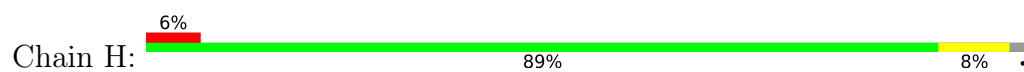
- Molecule 1: Histone chaperone ASF1A



- Molecule 1: Histone chaperone ASF1A



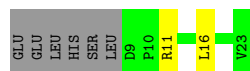
- Molecule 1: Histone chaperone ASF1A



- Molecule 2: Serine/threonine-protein kinase tousled-like 2



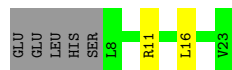
- Molecule 2: Serine/threonine-protein kinase tousled-like 2



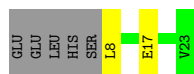
- Molecule 2: Serine/threonine-protein kinase tousled-like 2



- Molecule 2: Serine/threonine-protein kinase tousled-like 2



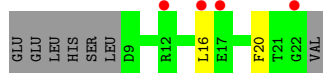
● Molecule 2: Serine/threonine-protein kinase tousled-like 2

Chain M:  67% 10% 24%

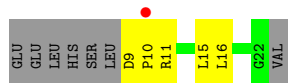
● Molecule 2: Serine/threonine-protein kinase tousled-like 2

Chain N:  57% 29% 14%

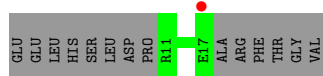
● Molecule 2: Serine/threonine-protein kinase tousled-like 2

Chain O:  19% 57% 10% 33%

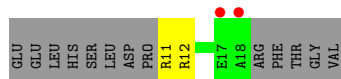
● Molecule 2: Serine/threonine-protein kinase tousled-like 2

Chain P:  5% 43% 24% 33%

● Molecule 2: Serine/threonine-protein kinase tousled-like 2

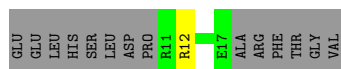
Chain Q:  5% 33% 67%

● Molecule 2: Serine/threonine-protein kinase tousled-like 2

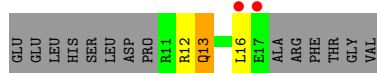
Chain R:  10% 29% 10% 62%

● Molecule 2: Serine/threonine-protein kinase tousled-like 2

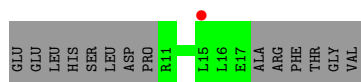
Chain T:  29% 5% 67%



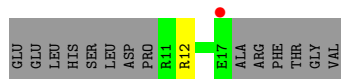
- Molecule 2: Serine/threonine-protein kinase tousled-like 2



- Molecule 2: Serine/threonine-protein kinase tousled-like 2



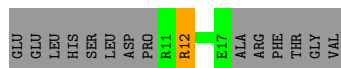
- Molecule 2: Serine/threonine-protein kinase tousled-like 2



- Molecule 2: Serine/threonine-protein kinase tousled-like 2



- Molecule 2: Serine/threonine-protein kinase tousled-like 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.02Å 136.68Å 101.32Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	98.63 – 2.71 98.63 – 2.71	Depositor EDS
% Data completeness (in resolution range)	94.8 (98.63-2.71) 89.0 (98.63-2.71)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.213 , 0.226 0.207 , 0.219	Depositor DCC
R_{free} test set	3080 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22462	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/1273	0.50	0/1741
1	B	0.26	0/1265	0.50	0/1731
1	C	0.26	0/1265	0.49	0/1731
1	D	0.28	0/1251	0.49	0/1712
1	E	0.25	0/1256	0.48	0/1719
1	F	0.37	0/1256	0.50	0/1719
1	G	0.25	0/1273	0.49	0/1741
1	H	0.25	0/1256	0.48	0/1719
2	I	0.54	0/126	0.66	0/168
2	J	0.24	0/126	0.60	0/168
2	K	0.23	0/126	0.60	0/168
2	L	0.23	0/134	0.57	0/179
2	M	0.23	0/134	0.59	0/179
2	N	0.72	0/151	0.64	0/202
2	O	0.24	0/119	0.66	0/158
2	P	0.23	0/119	0.59	0/158
2	Q	0.24	0/64	0.64	0/83
2	R	0.25	0/69	0.47	0/90
2	T	0.27	0/64	0.71	0/83
2	U	0.41	0/64	0.46	0/83
2	V	0.26	0/64	0.70	0/83
2	W	0.26	0/64	0.66	0/83
2	X	0.25	0/64	0.66	0/83
2	Y	0.26	0/64	0.67	0/83
All	All	0.29	0/11647	0.51	0/15864

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	1240	1191	1194	9	0
1	B	1232	1181	1182	7	0
1	C	1232	1171	1182	7	0
1	D	1218	1150	1171	12	0
1	E	1223	1176	1176	5	0
1	F	1223	1163	1176	9	0
1	G	1240	1187	1194	6	0
1	H	1223	1176	1176	7	0
2	I	125	124	124	4	0
2	J	125	124	124	2	0
2	K	125	124	124	1	0
2	L	133	135	135	2	0
2	M	133	135	135	1	0
2	N	149	135	147	5	0
2	O	118	115	115	2	0
2	P	118	91	115	3	0
2	Q	65	67	67	0	0
2	R	70	67	72	2	0
2	T	65	67	67	2	0
2	U	65	67	67	5	0
2	V	65	67	67	0	0
2	W	65	67	67	1	0
2	X	65	67	67	1	0
2	Y	65	67	67	1	0
3	A	22	0	0	0	0
3	B	29	0	0	0	0
3	C	23	0	0	0	0
3	D	10	0	0	0	0
3	E	28	0	0	0	0
3	F	13	0	0	0	0
3	G	17	0	0	0	0
3	H	6	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	4	0	0	0	0
3	M	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	2	0	0	0	0
3	P	1	0	0	0	0
3	T	1	0	0	0	0
3	U	2	0	0	1	0
All	All	11548	10914	11011	68	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 3.

All (68) 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:58:ASP:OD2	2:Y:12:ARG:NH1	2.20	0.75
1:F:88:ASP:OD1	2:N:12:ARG:NH2	2.21	0.72
1:F:58:ASP:OD2	2:W:12:ARG:NH1	2.21	0.72
1:A:88:ASP:OD1	2:I:12:ARG:NH2	2.24	0.71
1:F:14:ASN:HB3	1:F:15:PRO:HD3	1.74	0.70
2:P:9:ASP:HB3	2:P:10:PRO:HD3	1.74	0.70
1:D:62:VAL:HB	2:U:16:LEU:HD21	1.75	0.69
1:B:36:GLU:OE2	1:B:102:ARG:NH1	2.26	0.67
1:D:58:ASP:OD2	2:U:12:ARG:NH1	2.27	0.67
1:G:14:ASN:HB3	1:G:15:PRO:HD3	1.84	0.60
1:A:8:ASN:OD1	1:A:9:VAL:N	2.35	0.59
2:I:18:ALA:O	2:I:22:GLY:N	2.35	0.59
1:A:54:ASP:OD2	2:I:19:ARG:NH2	2.32	0.57
1:F:94:VAL:HG13	2:N:16:LEU:HD22	1.86	0.57
2:N:8:LEU:HD11	2:N:13:GLN:HB2	1.88	0.55
1:B:49:GLU:OE1	2:J:11:ARG:NH2	2.37	0.55
1:D:62:VAL:CB	2:U:16:LEU:HD21	2.37	0.54
2:R:11:ARG:O	2:R:11:ARG:HG2	2.08	0.54
1:G:48:ALA:HB2	2:O:16:LEU:HD21	1.90	0.53
1:B:58:ASP:OD2	2:R:12:ARG:NH1	2.42	0.52
1:B:106:PHE:HB3	1:B:151:ILE:HD13	1.91	0.52
1:G:2:ALA:O	1:G:31:ILE:HD12	2.09	0.51
1:H:48:ALA:HB2	2:P:16:LEU:HD21	1.92	0.51
1:G:38:LEU:HB2	1:G:62:VAL:HG22	1.93	0.51
1:C:14:ASN:HB3	1:C:15:PRO:HD3	1.95	0.49
1:A:14:ASN:ND2	1:A:139:ILE:O	2.46	0.48
1:D:14:ASN:OD1	1:D:139:ILE:N	2.47	0.48
1:F:4:VAL:HG21	1:F:38:LEU:HD21	1.96	0.48
1:F:151:ILE:HD11	1:F:153:TRP:CZ2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:ASN:HB3	1:H:15:PRO:HD3	1.97	0.47
1:D:30:CYS:SG	1:D:34:LEU:HD12	2.54	0.47
1:C:58:ASP:OD2	2:T:12:ARG:NH1	2.48	0.47
1:E:14:ASN:ND2	1:E:139:ILE:O	2.48	0.46
1:E:14:ASN:OD1	1:E:139:ILE:N	2.45	0.46
1:D:45:VAL:O	1:D:93:THR:OG1	2.30	0.46
2:U:13:GLN:NE2	3:U:101:HOH:O	2.49	0.46
1:G:58:ASP:OD2	2:X:12:ARG:NH1	2.49	0.46
1:E:14:ASN:HB3	1:E:15:PRO:HD3	1.98	0.45
1:F:106:PHE:HB3	1:F:151:ILE:HD13	1.99	0.45
1:C:38:LEU:HB2	1:C:62:VAL:HG22	1.97	0.45
1:A:112:TYR:OH	2:I:17:GLU:OE2	2.34	0.44
1:D:94:VAL:HG13	2:L:16:LEU:HD22	1.99	0.43
1:H:93:THR:O	1:H:113:VAL:N	2.44	0.43
1:B:48:ALA:HB2	2:J:16:LEU:HD21	1.99	0.43
1:C:4:VAL:CG2	1:C:34:LEU:HD11	2.48	0.43
1:D:106:PHE:HB3	1:D:151:ILE:HD13	1.99	0.43
1:A:38:LEU:HB2	1:A:62:VAL:HG22	2.00	0.43
1:C:48:ALA:HB2	2:K:16:LEU:HD21	2.00	0.43
1:E:100:THR:HG23	1:E:104:GLN:C	2.38	0.43
1:A:14:ASN:HB3	1:A:15:PRO:HD3	2.00	0.43
1:D:62:VAL:CG1	2:U:16:LEU:HD21	2.49	0.42
1:B:45:VAL:HG21	1:B:94:VAL:CG2	2.49	0.42
1:A:30:CYS:SG	1:A:34:LEU:HG	2.59	0.42
1:F:92:VAL:O	2:N:12:ARG:NH1	2.50	0.42
1:G:145:ARG:HG3	2:O:20:PHE:CD2	2.55	0.42
1:A:142:SER:OG	2:M:17:GLU:OE2	2.32	0.41
2:P:11:ARG:O	2:P:15:LEU:HD23	2.21	0.41
1:C:38:LEU:HB2	1:C:62:VAL:CG2	2.50	0.41
1:C:60:VAL:HA	2:T:12:ARG:O	2.21	0.41
1:D:49:GLU:OE1	2:L:11:ARG:NH2	2.51	0.41
1:H:14:ASN:OD1	1:H:139:ILE:N	2.53	0.41
1:H:29:GLU:HG2	1:H:69:ARG:HG2	2.02	0.41
1:H:38:LEU:HB2	1:H:62:VAL:HG22	2.02	0.41
1:D:100:THR:HG23	1:D:104:GLN:C	2.41	0.40
1:E:140:LEU:N	1:E:140:LEU:HD12	2.36	0.40
1:F:151:ILE:HD11	1:F:153:TRP:CE2	2.56	0.40
1:B:92:VAL:HG11	2:N:10:PRO:HG3	2.04	0.40
1:D:122:LEU:HD12	1:D:127:PRO:HD3	2.04	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	152/157 (97%)	151 (99%)	1 (1%)	0	100	100
1	B	151/157 (96%)	147 (97%)	3 (2%)	1 (1%)	22	45
1	C	151/157 (96%)	147 (97%)	4 (3%)	0	100	100
1	D	149/157 (95%)	147 (99%)	2 (1%)	0	100	100
1	E	150/157 (96%)	147 (98%)	3 (2%)	0	100	100
1	F	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
1	G	152/157 (97%)	152 (100%)	0	0	100	100
1	H	150/157 (96%)	147 (98%)	3 (2%)	0	100	100
2	I	13/21 (62%)	12 (92%)	1 (8%)	0	100	100
2	J	13/21 (62%)	13 (100%)	0	0	100	100
2	K	13/21 (62%)	13 (100%)	0	0	100	100
2	L	14/21 (67%)	14 (100%)	0	0	100	100
2	M	14/21 (67%)	14 (100%)	0	0	100	100
2	N	16/21 (76%)	16 (100%)	0	0	100	100
2	O	12/21 (57%)	12 (100%)	0	0	100	100
2	P	12/21 (57%)	12 (100%)	0	0	100	100
2	Q	5/21 (24%)	5 (100%)	0	0	100	100
2	R	6/21 (29%)	6 (100%)	0	0	100	100
2	T	5/21 (24%)	5 (100%)	0	0	100	100
2	U	5/21 (24%)	5 (100%)	0	0	100	100
2	V	5/21 (24%)	5 (100%)	0	0	100	100
2	W	5/21 (24%)	5 (100%)	0	0	100	100
2	X	5/21 (24%)	5 (100%)	0	0	100	100
2	Y	5/21 (24%)	5 (100%)	0	0	100	100
All	All	1353/1592 (85%)	1334 (99%)	18 (1%)	1 (0%)	51	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	PRO

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	139/141 (99%)	136 (98%)	3 (2%)	52	78
1	B	138/141 (98%)	135 (98%)	3 (2%)	52	78
1	C	138/141 (98%)	137 (99%)	1 (1%)	84	93
1	D	137/141 (97%)	133 (97%)	4 (3%)	42	70
1	E	137/141 (97%)	136 (99%)	1 (1%)	84	93
1	F	137/141 (97%)	136 (99%)	1 (1%)	84	93
1	G	139/141 (99%)	136 (98%)	3 (2%)	52	78
1	H	137/141 (97%)	136 (99%)	1 (1%)	84	93
2	I	13/19 (68%)	13 (100%)	0	100	100
2	J	13/19 (68%)	13 (100%)	0	100	100
2	K	13/19 (68%)	13 (100%)	0	100	100
2	L	14/19 (74%)	14 (100%)	0	100	100
2	M	14/19 (74%)	13 (93%)	1 (7%)	14	33
2	N	16/19 (84%)	15 (94%)	1 (6%)	18	38
2	O	12/19 (63%)	12 (100%)	0	100	100
2	P	12/19 (63%)	12 (100%)	0	100	100
2	Q	7/19 (37%)	7 (100%)	0	100	100
2	R	7/19 (37%)	7 (100%)	0	100	100
2	T	7/19 (37%)	7 (100%)	0	100	100
2	U	7/19 (37%)	6 (86%)	1 (14%)	3	7
2	V	7/19 (37%)	7 (100%)	0	100	100
2	W	7/19 (37%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	7/19 (37%)	7 (100%)	0	100	100
2	Y	7/19 (37%)	6 (86%)	1 (14%)	3	7
All	All	1265/1432 (88%)	1244 (98%)	21 (2%)	60	83

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	65	VAL
1	A	74	PHE
1	B	13	ASP
1	B	74	PHE
1	B	140	LEU
1	C	74	PHE
1	D	6	VAL
1	D	27	THR
1	D	30	CYS
1	D	74	PHE
1	E	74	PHE
1	F	74	PHE
1	G	30	CYS
1	G	74	PHE
1	G	95	VAL
1	H	74	PHE
2	M	8	LEU
2	N	9	ASP
2	U	13	GLN
2	Y	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	23	GLN
2	U	13	GLN

5.3.3 RNA ⓘ

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 monosaccharides 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	154/157 (98%)	0.52	7 (4%) 33 32	30, 46, 78, 111	0
1	B	153/157 (97%)	0.50	1 (0%) 87 89	30, 47, 84, 102	0
1	C	153/157 (97%)	0.50	3 (1%) 65 67	33, 49, 79, 106	0
1	D	151/157 (96%)	0.61	4 (2%) 56 57	30, 58, 95, 132	0
1	E	152/157 (96%)	0.63	3 (1%) 65 67	32, 53, 97, 120	0
1	F	152/157 (96%)	0.58	2 (1%) 77 78	38, 56, 107, 123	0
1	G	154/157 (98%)	0.63	5 (3%) 47 48	38, 56, 84, 109	0
1	H	152/157 (96%)	0.73	10 (6%) 18 17	42, 58, 95, 112	0
2	I	15/21 (71%)	0.58	1 (6%) 17 16	53, 77, 93, 94	0
2	J	15/21 (71%)	0.49	0 100 100	38, 56, 73, 78	0
2	K	15/21 (71%)	0.43	1 (6%) 17 16	50, 66, 89, 96	0
2	L	16/21 (76%)	0.27	0 100 100	40, 50, 59, 62	0
2	M	16/21 (76%)	0.34	0 100 100	40, 49, 62, 78	0
2	N	18/21 (85%)	0.44	0 100 100	41, 47, 83, 85	0
2	O	14/21 (66%)	1.37	4 (28%) 0 0	71, 93, 126, 126	0
2	P	14/21 (66%)	0.94	1 (7%) 16 14	63, 90, 105, 117	0
2	Q	7/21 (33%)	1.10	1 (14%) 2 1	62, 72, 102, 116	0
2	R	8/21 (38%)	1.24	2 (25%) 0 0	58, 62, 94, 111	0
2	T	7/21 (33%)	0.75	0 100 100	52, 61, 81, 91	0
2	U	7/21 (33%)	1.53	2 (28%) 0 0	67, 76, 92, 95	0
2	V	7/21 (33%)	0.83	1 (14%) 2 1	59, 67, 92, 104	0
2	W	7/21 (33%)	0.91	1 (14%) 2 1	69, 76, 103, 104	0
2	X	7/21 (33%)	0.88	1 (14%) 2 1	57, 61, 92, 94	0
2	Y	7/21 (33%)	0.45	0 100 100	53, 61, 87, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	1401/1592 (88%)	0.60	50 (3%)	42 42	30, 54, 95, 132	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	31	ILE	6.4
1	A	33	ASP	4.1
1	D	69	ARG	4.0
2	U	16	LEU	3.9
1	A	63	GLY	3.5
1	G	14	ASN	3.3
1	G	63	GLY	3.3
2	W	17	GLU	3.3
1	B	14	ASN	3.1
1	H	125	ASN	3.1
2	O	12	ARG	3.1
2	R	17	GLU	3.0
1	A	14	ASN	3.0
1	C	2	ALA	3.0
1	E	124	GLU	2.9
2	Q	17	GLU	2.9
1	C	63	GLY	2.9
1	F	14	ASN	2.8
1	D	64	PRO	2.7
1	D	14	ASN	2.7
2	X	16	LEU	2.7
2	U	17	GLU	2.7
2	K	23	VAL	2.6
1	H	122	LEU	2.6
1	H	14	ASN	2.5
1	D	27	THR	2.5
1	H	145	ARG	2.5
2	O	17	GLU	2.4
2	P	10	PRO	2.3
1	G	13	ASP	2.3
1	H	29	GLU	2.3
1	G	48	ALA	2.3
1	A	66	PRO	2.3
2	O	16	LEU	2.3
1	E	7	ASN	2.2
1	A	13	ASP	2.2
1	E	14	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	3	LYS	2.1
2	V	15	LEU	2.1
1	H	43	ILE	2.1
2	I	23	VAL	2.1
1	G	121	GLU	2.1
1	H	63	GLY	2.1
1	A	144	PRO	2.1
2	R	18	ALA	2.1
1	H	2	ALA	2.0
1	A	67	ALA	2.0
1	C	14	ASN	2.0
2	O	22	GLY	2.0
1	H	62	VAL	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.