



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:36 PM EDT

PDB ID : 6TXZ / pdb_00006txz
Title : FAB PART OF M6903 IN COMPLEX WITH HUMAN TIM3
Authors : Musil, D.; Sood, V.
Deposited on : 2020-01-15
Resolution : 3.06 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

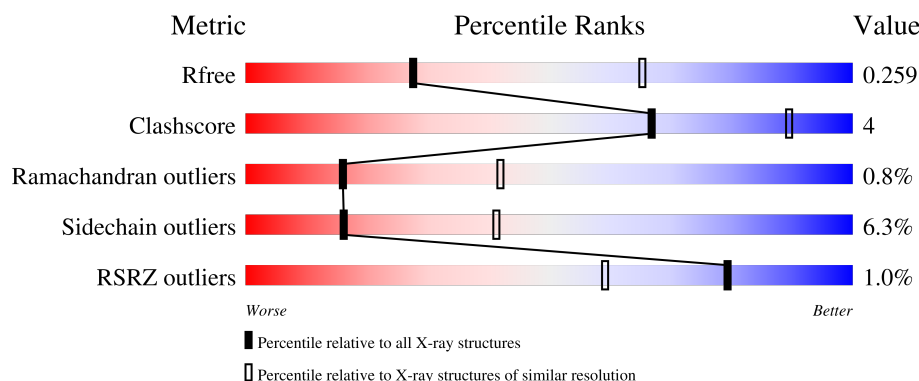
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	110	% 83% 14% ..
1	B	110	 90% 8% ..
1	C	110	 86% 10% ..
1	D	110	 91% 7% ..
2	H	229	% 81% 13% ..

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Mol	Chain	Length	Quality of chain
2	I	229	78%15%6%
2	J	229	73%15%8%
2	K	229	76%15%7%
3	L	214	78%16%.
3	M	214	82%14%.
3	N	214	85%12%.
3	O	214	89%9%.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16053 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 Hepatitis A virus cellular receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	11	0	0
			863	550	145	161	7			
1	B	109	Total	C	N	O	S	12	0	0
			863	550	145	161	7			
1	C	109	Total	C	N	O	S	13	0	0
			863	550	145	161	7			
1	D	109	Total	C	N	O	S	10	0	0
			863	550	145	161	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP Q8TDQ0
B	21	MET	-	initiating methionine	UNP Q8TDQ0
C	21	MET	-	initiating methionine	UNP Q8TDQ0
D	21	MET	-	initiating methionine	UNP Q8TDQ0

- Molecule 2 is a protein called Fab H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	25	0	0
			1624	1027	270	321	6			
2	I	216	Total	C	N	O	S	34	0	0
			1602	1014	266	315	7			
2	J	210	Total	C	N	O	S	27	0	0
			1570	998	260	306	6			
2	K	213	Total	C	N	O	S	31	0	0
			1588	1007	263	311	7			

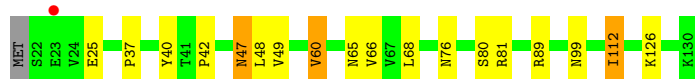
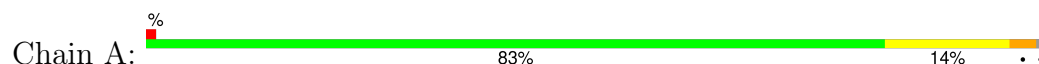
- Molecule 3 is a protein called Fab L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	21	0	0
			1547	967	256	319	5			
3	M	210	Total	C	N	O	S	18	0	0
			1553	970	257	321	5			
3	N	210	Total	C	N	O	S	49	0	0
			1555	971	258	321	5			
3	O	211	Total	C	N	O	S	27	0	0
			1562	975	259	323	5			

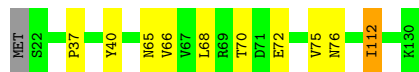
3 Residue-property plots [i](#)

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.

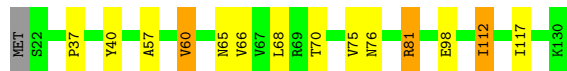
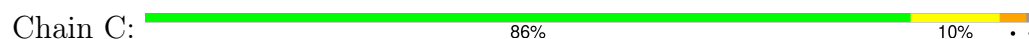
- Molecule 1: Hepatitis A virus cellular receptor 2



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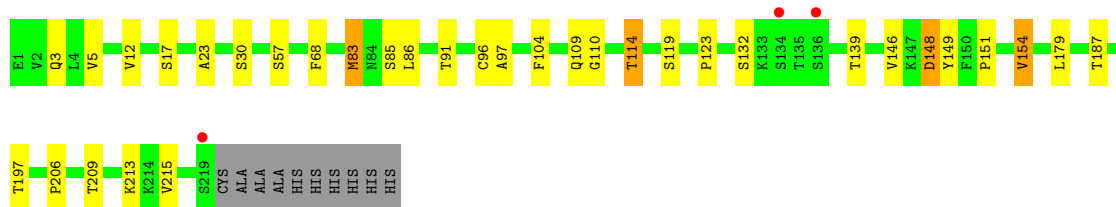
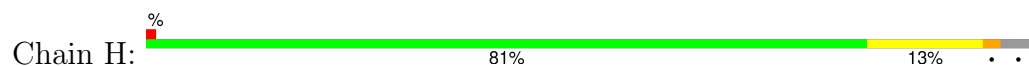
- Molecule 1: Hepatitis A virus cellular receptor 2



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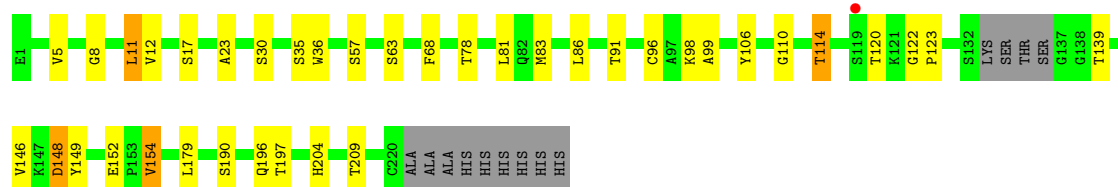


- Molecule 2: Fab H



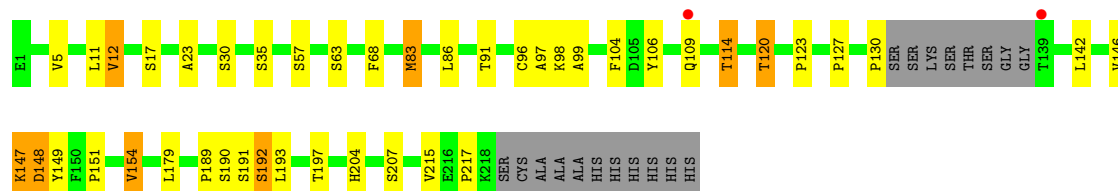
- Molecule 2: Fab H

Chain I:  78% 15% • 6%



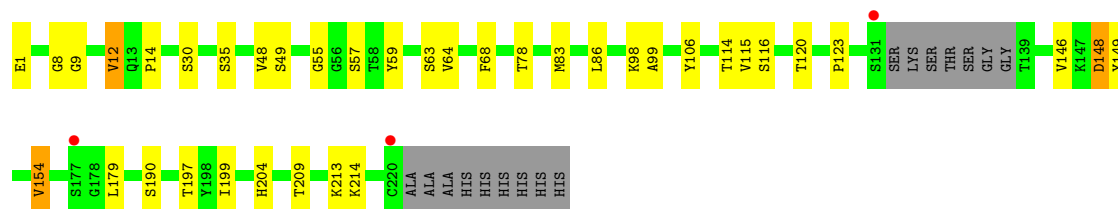
- Molecule 2: Fab H

Chain J:  73% 15% • 8%



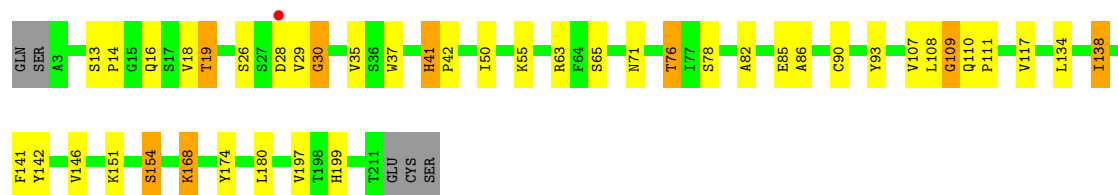
- Molecule 2: Fab H

Chain K:  76% 15% • 7%



- Molecule 3: Fab L

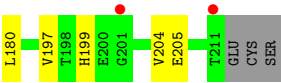
Chain L:  78% 16% • •



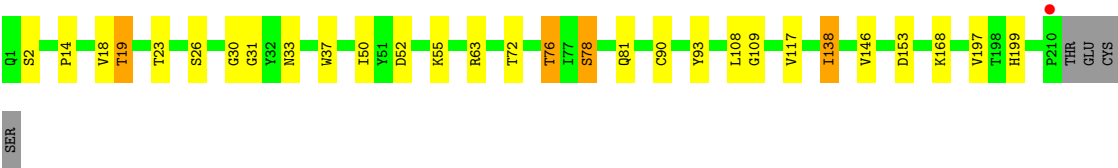
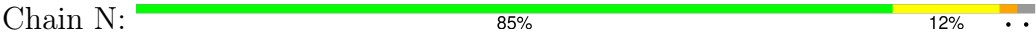
- Molecule 3: Fab L

Chain M:  82% 14% • •

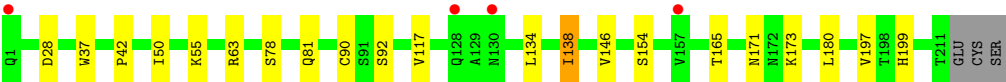
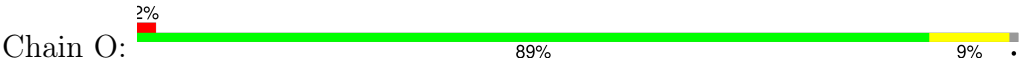




● Molecule 3: Fab L



● Molecule 3: Fab L



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.35Å 270.12Å 197.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 3.06 48.60 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.60-3.06) 99.0 (48.60-3.06)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.197 , 0.253 0.205 , 0.259	Depositor DCC
R_{free} test set	523 reflections (0.86%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16053	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	0.89	0/884	1.20	5/1202 (0.4%)
1	B	0.83	0/884	1.19	3/1202 (0.2%)
1	C	0.87	0/884	1.21	4/1202 (0.3%)
1	D	0.84	0/884	1.17	2/1202 (0.2%)
2	H	0.84	1/1664 (0.1%)	1.25	5/2266 (0.2%)
2	I	0.74	0/1641	1.17	3/2234 (0.1%)
2	J	0.78	1/1609 (0.1%)	1.19	6/2192 (0.3%)
2	K	0.77	0/1627	1.21	6/2216 (0.3%)
3	L	0.83	0/1585	1.27	12/2163 (0.6%)
3	M	0.79	0/1591	1.17	3/2171 (0.1%)
3	N	0.76	0/1593	1.16	2/2173 (0.1%)
3	O	0.82	0/1600	1.16	3/2183 (0.1%)
All	All	0.81	2/16446 (0.0%)	1.20	54/22406 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	83	MET	SD-CE	-7.30	1.61	1.79
2	J	83	MET	SD-CE	-5.29	1.66	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	108	LEU	N-CA-C	7.97	119.60	111.07
3	L	28	ASP	CA-CB-CG	7.12	119.72	112.60
1	B	76	ASN	CA-CB-CG	6.51	119.11	112.60
1	C	60	VAL	N-CA-CB	6.32	117.53	110.51
3	L	82	ALA	CA-C-N	6.28	128.98	120.38
3	L	82	ALA	C-N-CA	6.28	128.98	120.38
2	J	68	PHE	CA-CB-CG	6.19	119.99	113.80
3	L	71	ASN	CA-CB-CG	6.18	118.78	112.60
2	I	68	PHE	CA-CB-CG	6.18	119.98	113.80
2	K	55	GLY	CA-C-N	6.12	126.77	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	55	GLY	C-N-CA	6.12	126.77	119.98
3	L	109	GLY	N-CA-C	6.10	121.39	113.27
3	O	154	SER	CA-C-N	6.06	128.89	120.65
3	O	154	SER	C-N-CA	6.06	128.89	120.65
2	I	8	GLY	N-CA-C	-5.94	102.01	112.77
2	H	68	PHE	CA-CB-CG	5.94	119.74	113.80
2	K	1	GLU	CA-C-N	5.88	131.33	122.98
2	K	1	GLU	C-N-CA	5.88	131.33	122.98
3	M	154	SER	CA-C-N	5.83	128.58	120.65
3	M	154	SER	C-N-CA	5.83	128.58	120.65
3	N	108	LEU	N-CA-C	5.79	117.67	111.36
2	H	132	SER	CA-C-N	5.73	128.24	120.38
2	H	132	SER	C-N-CA	5.73	128.24	120.38
2	K	68	PHE	CA-CB-CG	5.73	119.53	113.80
3	L	41	HIS	CA-CB-CG	5.72	119.52	113.80
1	A	47	ASN	CA-CB-CG	5.71	118.31	112.60
3	O	28	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	65	ASN	CA-C-N	5.60	128.22	120.49
1	A	65	ASN	C-N-CA	5.60	128.22	120.49
2	J	147	LYS	CA-C-N	5.53	132.10	121.54
2	J	147	LYS	C-N-CA	5.53	132.10	121.54
1	A	60	VAL	N-CA-CB	5.49	116.61	110.51
2	H	110	GLY	N-CA-C	5.47	119.58	112.25
2	H	109	GLN	N-CA-C	-5.45	99.64	108.41
2	J	191	SER	CA-C-N	5.36	129.17	120.60
2	J	191	SER	C-N-CA	5.36	129.17	120.60
1	A	76	ASN	CA-CB-CG	5.29	117.89	112.60
3	L	111	PRO	CA-C-N	5.24	128.21	120.82
3	L	111	PRO	C-N-CA	5.24	128.21	120.82
3	L	154	SER	CA-C-N	5.23	127.76	120.65
3	L	154	SER	C-N-CA	5.23	127.76	120.65
2	K	8	GLY	N-CA-C	-5.22	100.80	113.18
1	D	65	ASN	CA-C-N	5.18	127.64	120.49
1	D	65	ASN	C-N-CA	5.18	127.64	120.49
2	J	109	GLN	N-CA-C	-5.14	100.70	108.67
1	B	65	ASN	CA-C-N	5.14	127.58	120.49
1	B	65	ASN	C-N-CA	5.14	127.58	120.49
3	M	173	LYS	N-CA-C	-5.13	102.41	110.36
1	C	65	ASN	CA-C-N	5.06	127.47	120.49
1	C	65	ASN	C-N-CA	5.06	127.47	120.49
1	C	76	ASN	CA-CB-CG	5.06	117.66	112.60
2	I	110	GLY	N-CA-C	5.06	119.03	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	153	ASP	CA-CB-CG	5.03	117.63	112.60
3	L	141	PHE	CA-CB-CG	5.02	118.82	113.80

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	863	0	832	7	0
1	B	863	0	832	3	0
1	C	863	0	832	7	0
1	D	863	0	832	4	0
2	H	1624	0	1587	10	0
2	I	1602	0	1561	13	0
2	J	1570	0	1535	22	0
2	K	1588	0	1550	14	0
3	L	1547	0	1496	16	0
3	M	1553	0	1501	12	0
3	N	1555	0	1505	9	0
3	O	1562	0	1512	6	0
All	All	16053	0	15575	114	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 4.

All (114) 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)
3:M:138:ILE:HG12	3:M:197:VAL:HG11	1.71	0.72
3:L:138:ILE:HG12	3:L:197:VAL:HG11	1.72	0.71
3:N:138:ILE:HG12	3:N:197:VAL:HG11	1.73	0.68
3:O:138:ILE:HG12	3:O:197:VAL:HG11	1.76	0.66
2:J:127:PRO:HB3	2:J:215:VAL:HG12	1.77	0.64
3:N:19:THR:HB	3:N:76:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PRO:HG3	1:B:37:PRO:HG3	1.80	0.64
1:C:37:PRO:HG3	1:D:37:PRO:HG3	1.80	0.61
3:M:110:GLN:HG2	3:M:111:PRO:HD2	1.83	0.60
1:D:118:MET:HG2	2:K:59:TYR:HA	1.84	0.59
2:J:83:MET:HE2	2:J:86:LEU:HD21	1.86	0.58
3:O:171:ASN:OD1	3:O:173:LYS:HB2	2.04	0.58
3:L:134:LEU:HD12	3:L:180:LEU:HD23	1.86	0.57
2:I:83:MET:HE2	2:I:86:LEU:HD21	1.86	0.57
3:M:134:LEU:HD12	3:M:180:LEU:HD23	1.87	0.57
2:J:146:VAL:HG11	2:J:154:VAL:HG11	1.86	0.57
3:O:134:LEU:HD12	3:O:180:LEU:HD23	1.87	0.56
2:K:83:MET:HE2	2:K:86:LEU:HD21	1.88	0.56
2:J:130:PRO:HG2	2:J:193:LEU:HD21	1.87	0.56
2:I:146:VAL:HG11	2:I:154:VAL:HG11	1.89	0.55
2:H:139:THR:HB	2:H:187:THR:HG22	1.89	0.54
2:J:11:LEU:HD22	2:J:120:THR:HG22	1.89	0.54
1:C:81:ARG:HA	1:C:98:GLU:HG2	1.90	0.53
2:I:148:ASP:HB3	2:I:179:LEU:HD13	1.91	0.53
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.90	0.53
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.91	0.53
2:J:123:PRO:HB3	2:J:149:TYR:HB3	1.91	0.52
2:K:146:VAL:HG11	2:K:154:VAL:HG11	1.90	0.52
1:D:80:SER:O	1:D:81:ARG:HB2	2.10	0.52
2:H:146:VAL:HG11	2:H:154:VAL:HG11	1.91	0.52
2:K:12:VAL:HG23	2:K:115:VAL:HG22	1.90	0.52
3:M:171:ASN:OD1	3:M:173:LYS:HB2	2.09	0.52
2:J:151:PRO:O	2:J:204:HIS:HE1	1.93	0.52
2:I:123:PRO:HB3	2:I:149:TYR:HB3	1.92	0.52
1:C:40:TYR:HB3	1:C:112:ILE:HD12	1.91	0.51
2:J:127:PRO:CB	2:J:215:VAL:HG12	2.40	0.51
2:K:123:PRO:HB3	2:K:149:TYR:HB3	1.92	0.51
2:J:204:HIS:HD2	2:J:207:SER:OG	1.92	0.51
2:K:197:THR:HG23	2:K:214:LYS:HE3	1.92	0.51
2:J:193:LEU:HD23	2:J:217:PRO:HG3	1.93	0.50
3:N:33:ASN:O	3:N:52:ASP:HA	2.11	0.50
3:L:85:GLU:HG3	3:L:107:VAL:H	1.76	0.50
2:J:12:VAL:HG21	2:J:86:LEU:HD13	1.94	0.50
2:J:130:PRO:HG3	2:J:142:LEU:HB3	1.92	0.50
2:K:123:PRO:HD2	2:K:209:THR:HG21	1.94	0.50
2:I:122:GLY:HA2	2:I:204:HIS:HD2	1.77	0.49
3:L:146:VAL:HG12	3:L:199:HIS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:35:SER:OG	2:I:99:ALA:HB2	2.13	0.49
2:J:148:ASP:HB3	2:J:179:LEU:HD13	1.95	0.49
3:L:13:SER:O	3:L:16:GLN:HB2	2.13	0.49
2:I:123:PRO:HD2	2:I:209:THR:HG21	1.94	0.48
2:J:35:SER:OG	2:J:99:ALA:HB2	2.13	0.48
2:K:148:ASP:HB3	2:K:179:LEU:HD13	1.94	0.48
3:L:168:LYS:HG2	3:L:174:TYR:CZ	2.48	0.48
3:O:63:ARG:HB2	3:O:78:SER:O	2.13	0.48
1:D:45:PRO:HD3	3:M:157:VAL:HG22	1.95	0.48
2:H:148:ASP:HB3	2:H:179:LEU:HD13	1.94	0.48
2:J:189:PRO:HB2	2:J:192:SER:HB3	1.94	0.48
3:M:63:ARG:HB2	3:M:78:SER:O	2.14	0.48
3:M:26:SER:HA	3:M:30:GLY:HA3	1.96	0.47
3:L:110:GLN:HB2	3:L:142:TYR:CE2	2.49	0.47
1:A:60:VAL:HG23	3:L:93:TYR:O	2.15	0.47
3:N:63:ARG:HB2	3:N:78:SER:O	2.14	0.47
3:N:146:VAL:HG12	3:N:199:HIS:HB2	1.95	0.47
3:L:63:ARG:HB2	3:L:78:SER:O	2.14	0.47
1:C:60:VAL:HG23	3:N:93:TYR:O	2.14	0.46
2:K:35:SER:HB2	2:K:49:SER:O	2.15	0.46
3:L:19:THR:HB	3:L:76:THR:HB	1.96	0.46
2:J:91:THR:HG23	2:J:114:THR:HA	1.96	0.46
2:K:35:SER:OG	2:K:99:ALA:HB2	2.16	0.45
1:A:40:TYR:HB3	1:A:112:ILE:HD12	1.97	0.45
2:K:98:LYS:HD3	2:K:106:TYR:HD2	1.82	0.45
2:J:130:PRO:HD2	2:J:217:PRO:HA	1.98	0.45
3:O:146:VAL:HG12	3:O:199:HIS:HB2	1.98	0.45
3:M:146:VAL:HG12	3:M:199:HIS:HB2	1.98	0.44
1:B:40:TYR:HB3	1:B:112:ILE:HD12	1.99	0.44
3:L:14:PRO:HD3	3:L:109:GLY:H	1.81	0.44
1:C:57:ALA:HB3	3:N:30:GLY:CA	2.47	0.43
3:O:37:TRP:CZ3	3:O:90:CYS:HB3	2.53	0.43
1:A:42:PRO:HB3	1:A:47:ASN:O	2.18	0.43
1:C:117:ILE:HD13	3:M:205:GLU:HB2	2.01	0.43
2:J:98:LYS:HD3	2:J:106:TYR:HD2	1.83	0.43
2:I:36:TRP:NE1	2:I:81:LEU:HB2	2.34	0.43
3:N:14:PRO:HD3	3:N:109:GLY:H	1.83	0.43
2:K:14:PRO:HD3	2:K:116:SER:C	2.43	0.43
3:L:26:SER:HA	3:L:30:GLY:HA3	1.99	0.43
2:J:204:HIS:CD2	2:J:207:SER:OG	2.72	0.42
2:I:36:TRP:CE2	2:I:81:LEU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:97:ALA:HB1	2:J:104:PHE:HB3	2.02	0.42
2:K:204:HIS:HB3	2:K:209:THR:HB	2.01	0.42
3:L:41:HIS:ND1	3:L:86:ALA:HB2	2.35	0.42
2:H:5:VAL:HG23	2:H:23:ALA:HB3	2.02	0.42
1:A:25:GLU:HG2	1:A:126:LYS:HD3	2.02	0.42
1:A:60:VAL:HG23	3:L:93:TYR:HB2	2.02	0.42
2:I:11:LEU:HG	2:I:114:THR:HB	2.02	0.42
3:M:85:GLU:HG3	3:M:106:THR:HA	2.02	0.42
3:L:29:VAL:HG13	3:L:35:VAL:HG21	2.02	0.41
2:I:5:VAL:HG23	2:I:23:ALA:HB3	2.02	0.41
3:N:37:TRP:CZ3	3:N:90:CYS:HB3	2.55	0.41
1:A:48:LEU:HD21	1:A:89:ARG:HA	2.02	0.41
1:C:70:THR:HG22	1:C:75:VAL:HG22	2.02	0.41
2:I:98:LYS:HD3	2:I:106:TYR:HD2	1.85	0.41
2:H:151:PRO:HD2	2:H:206:PRO:CB	2.51	0.41
2:K:48:VAL:HG13	2:K:64:VAL:HG11	2.03	0.41
1:B:70:THR:HG22	1:B:75:VAL:HG22	2.02	0.41
2:H:97:ALA:HB1	2:H:104:PHE:HB3	2.03	0.41
2:H:123:PRO:HD2	2:H:209:THR:HG21	2.02	0.41
2:I:91:THR:HG23	2:I:114:THR:HA	2.01	0.41
3:L:37:TRP:CZ3	3:L:90:CYS:HB3	2.56	0.40
2:J:142:LEU:HD13	2:J:215:VAL:CG2	2.51	0.40
2:H:91:THR:HG23	2:H:114:THR:HA	2.03	0.40
2:J:5:VAL:HG23	2:J:23:ALA:HB3	2.03	0.40
3:M:37:TRP:CZ3	3:M:90:CYS:HB3	2.57	0.40
3:M:168:LYS:HD3	3:M:172:ASN:HA	2.03	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	107/110 (97%)	96 (90%)	9 (8%)	2 (2%)	6	23
1	B	107/110 (97%)	94 (88%)	13 (12%)	0	100	100
1	C	107/110 (97%)	95 (89%)	11 (10%)	1 (1%)	14	39
1	D	107/110 (97%)	96 (90%)	10 (9%)	1 (1%)	14	39
2	H	217/229 (95%)	209 (96%)	7 (3%)	1 (0%)	24	52
2	I	212/229 (93%)	203 (96%)	8 (4%)	1 (0%)	24	52
2	J	206/229 (90%)	199 (97%)	6 (3%)	1 (0%)	24	52
2	K	209/229 (91%)	198 (95%)	9 (4%)	2 (1%)	12	37
3	L	207/214 (97%)	196 (95%)	9 (4%)	2 (1%)	12	37
3	M	208/214 (97%)	197 (95%)	8 (4%)	3 (1%)	9	29
3	N	208/214 (97%)	199 (96%)	7 (3%)	2 (1%)	12	37
3	O	209/214 (98%)	196 (94%)	12 (6%)	1 (0%)	24	52
All	All	2104/2212 (95%)	1978 (94%)	109 (5%)	17 (1%)	16	42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	42	PRO
3	M	3	ALA
3	M	42	PRO
3	O	42	PRO
2	H	148	ASP
2	I	148	ASP
2	J	148	ASP
2	K	9	GLY
2	K	148	ASP
1	C	81	ARG
1	D	81	ARG
3	M	30	GLY
3	N	2	SER
1	A	81	ARG
1	A	99	ASN
3	N	31	GLY
3	L	30	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	94/95 (99%)	89 (95%)	5 (5%)	20	47
1	B	94/95 (99%)	90 (96%)	4 (4%)	26	53
1	C	94/95 (99%)	91 (97%)	3 (3%)	34	60
1	D	94/95 (99%)	90 (96%)	4 (4%)	26	53
2	H	181/188 (96%)	168 (93%)	13 (7%)	13	37
2	I	178/188 (95%)	162 (91%)	16 (9%)	9	29
2	J	174/188 (93%)	161 (92%)	13 (8%)	12	36
2	K	177/188 (94%)	166 (94%)	11 (6%)	16	42
3	L	175/180 (97%)	164 (94%)	11 (6%)	16	41
3	M	176/180 (98%)	163 (93%)	13 (7%)	13	36
3	N	176/180 (98%)	163 (93%)	13 (7%)	13	36
3	O	177/180 (98%)	170 (96%)	7 (4%)	28	56
All	All	1790/1852 (97%)	1677 (94%)	113 (6%)	16	41

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

Mol	Chain	Res	Type
1	A	49	VAL
1	A	66	VAL
1	A	68	LEU
1	A	80	SER
1	A	112	ILE
1	B	66	VAL
1	B	68	LEU
1	B	72	GLU
1	B	112	ILE
1	C	66	VAL
1	C	68	LEU
1	C	112	ILE
1	D	66	VAL
1	D	68	LEU

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Mol	Chain	Res	Type
1	D	81	ARG
1	D	112	ILE
2	H	3	GLN
2	H	12	VAL
2	H	17	SER
2	H	30	SER
2	H	57	SER
2	H	85	SER
2	H	96	CYS
2	H	114	THR
2	H	119	SER
2	H	154	VAL
2	H	197	THR
2	H	213	LYS
2	H	215	VAL
2	I	11	LEU
2	I	12	VAL
2	I	17	SER
2	I	30	SER
2	I	57	SER
2	I	63	SER
2	I	78	THR
2	I	96	CYS
2	I	114	THR
2	I	120	THR
2	I	139	THR
2	I	152	GLU
2	I	154	VAL
2	I	190	SER
2	I	196	GLN
2	I	197	THR
2	J	12	VAL
2	J	17	SER
2	J	30	SER
2	J	57	SER
2	J	63	SER
2	J	96	CYS
2	J	114	THR
2	J	120	THR
2	J	147	LYS
2	J	154	VAL
2	J	190	SER

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Mol	Chain	Res	Type
2	J	192	SER
2	J	197	THR
2	K	12	VAL
2	K	30	SER
2	K	57	SER
2	K	63	SER
2	K	78	THR
2	K	114	THR
2	K	120	THR
2	K	154	VAL
2	K	190	SER
2	K	199	ILE
2	K	213	LYS
3	L	18	VAL
3	L	19	THR
3	L	50	ILE
3	L	55	LYS
3	L	65	SER
3	L	76	THR
3	L	117	VAL
3	L	138	ILE
3	L	151	LYS
3	L	154	SER
3	L	168	LYS
3	M	2	SER
3	M	5	THR
3	M	23	THR
3	M	50	ILE
3	M	55	LYS
3	M	81	GLN
3	M	117	VAL
3	M	138	ILE
3	M	154	SER
3	M	165	THR
3	M	168	LYS
3	M	169	GLN
3	M	204	VAL
3	N	18	VAL
3	N	19	THR
3	N	23	THR
3	N	26	SER
3	N	50	ILE

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Mol	Chain	Res	Type
3	N	55	LYS
3	N	72	THR
3	N	76	THR
3	N	78	SER
3	N	81	GLN
3	N	117	VAL
3	N	138	ILE
3	N	168	LYS
3	O	50	ILE
3	O	55	LYS
3	O	81	GLN
3	O	92	SER
3	O	117	VAL
3	O	138	ILE
3	O	165	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	B	33	ASN
1	B	99	ASN
1	C	47	ASN
1	D	33	ASN
1	D	99	ASN
2	H	39	GLN
2	H	77	ASN
2	H	82	GLN
2	H	84	ASN
2	H	168	HIS
2	I	82	GLN
2	I	84	ASN
2	I	168	HIS
2	I	204	HIS
2	J	13	GLN
2	J	39	GLN
2	J	84	ASN
2	J	168	HIS
2	J	204	HIS
2	K	84	ASN
2	K	196	GLN
3	L	40	GLN

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Mol	Chain	Res	Type
3	L	71	ASN
3	L	169	GLN
3	L	186	GLN
3	L	190	HIS
3	L	196	GLN
3	M	16	GLN
3	M	39	GLN
3	M	81	GLN
3	M	110	GLN
3	M	190	HIS
3	N	16	GLN
3	N	39	GLN
3	N	40	GLN
3	N	81	GLN
3	N	186	GLN
3	O	16	GLN
3	O	33	ASN
3	O	39	GLN
3	O	81	GLN
3	O	172	ASN
3	O	186	GLN
3	O	196	GLN
3	O	199	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	109/110 (99%)	-0.34	1 (0%) 81 61	43, 61, 81, 90	6 (5%)
1	B	109/110 (99%)	-0.06	0 100 100	53, 78, 104, 117	6 (5%)
1	C	109/110 (99%)	-0.12	0 100 100	55, 72, 95, 98	5 (4%)
1	D	109/110 (99%)	-0.25	0 100 100	43, 69, 86, 105	3 (2%)
2	H	219/229 (95%)	-0.27	3 (1%) 73 51	40, 60, 85, 115	12 (5%)
2	I	216/229 (94%)	0.20	1 (0%) 87 72	64, 96, 119, 140	16 (7%)
2	J	210/229 (91%)	-0.15	2 (0%) 79 59	53, 75, 103, 117	12 (5%)
2	K	213/229 (93%)	0.06	3 (1%) 73 51	58, 84, 109, 125	14 (6%)
3	L	209/214 (97%)	-0.13	1 (0%) 87 72	50, 73, 93, 113	10 (4%)
3	M	210/214 (98%)	-0.05	5 (2%) 59 37	55, 76, 98, 131	11 (5%)
3	N	210/214 (98%)	0.08	1 (0%) 87 72	58, 93, 136, 157	20 (9%)
3	O	211/214 (98%)	-0.13	4 (1%) 66 43	40, 69, 94, 121	10 (4%)
All	All	2134/2212 (96%)	-0.08	21 (0%) 79 59	40, 76, 112, 157	125 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	220	CYS	5.0
3	M	211	THR	3.3
2	H	219	SER	3.3
3	N	210	PRO	3.0
2	K	177	SER	2.8
3	L	28	ASP	2.7
3	M	28	ASP	2.6
3	M	27	SER	2.6
3	M	130	ASN	2.5
2	J	139	THR	2.5
2	H	136	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	131	SER	2.5
3	O	130	ASN	2.4
3	O	128	GLN	2.4
2	I	119	SER	2.3
3	M	201	GLY	2.3
3	O	1	GLN	2.2
2	H	134	SER	2.1
2	J	109	GLN	2.1
1	A	23	GLU	2.0
3	O	157	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 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.