



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:08 pm BST

PDB ID : 6TXZ
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 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	:	2.11
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)	:	2.11

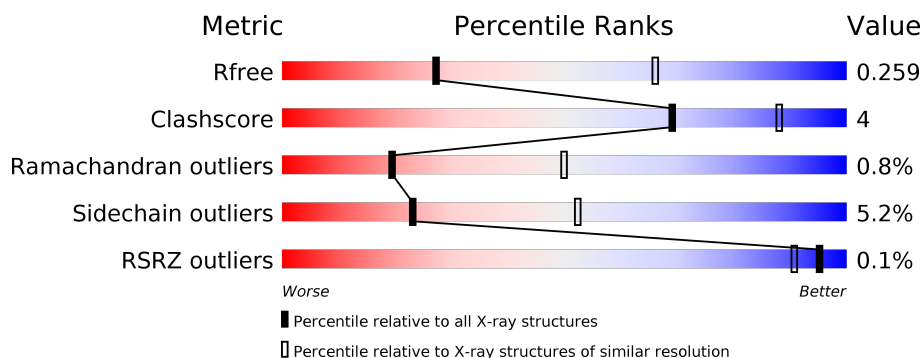
1 Overall quality at a glance

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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (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 on 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	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	B	110	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	C	110	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	D	110	<div> <div>92%</div> <div>6%</div> <div>..</div> </div>
2	H	229	<div> <div>82%</div> <div>13%</div> <div>..</div> </div>
2	I	229	<div> <div>81%</div> <div>12%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	229	 74%15%8%
2	K	229	 79%13%7%
3	L	214	 80%16%..
3	M	214	 82%15%.
3	N	214	 86%11%..
3	O	214	 90%8%.

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.

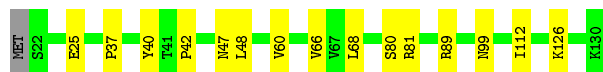
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	21	0	0
			1547	967	256	319	5			
3	M	210	Total	C	N	O	S	18	0	0
			1553	970	257	321	5			
3	N	210	Total	C	N	O	S	49	0	0
			1555	971	258	321	5			
3	O	211	Total	C	N	O	S	27	0	0
			1562	975	259	323	5			

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

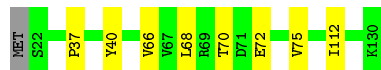
- Molecule 1: Hepatitis A virus cellular receptor 2

Chain A: 




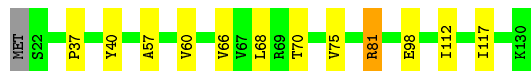
- Molecule 1: Hepatitis A virus cellular receptor 2

Chain B: 



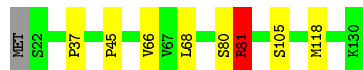
- Molecule 1: Hepatitis A virus cellular receptor 2

Chain C: 




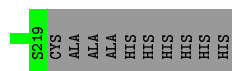
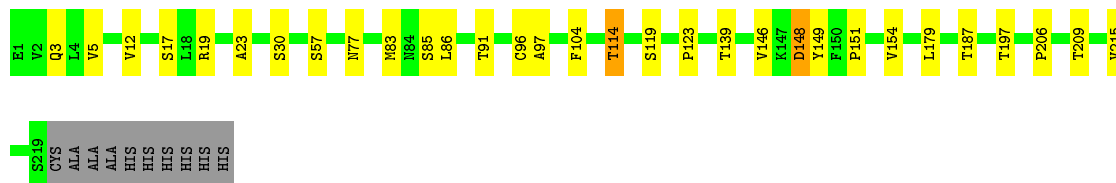
- Molecule 1: Hepatitis A virus cellular receptor 2

Chain D: 


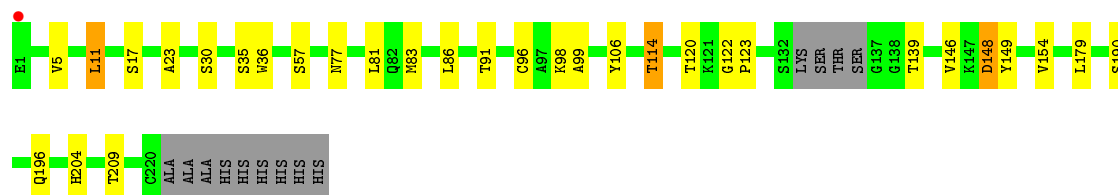


- Molecule 2: Fab H

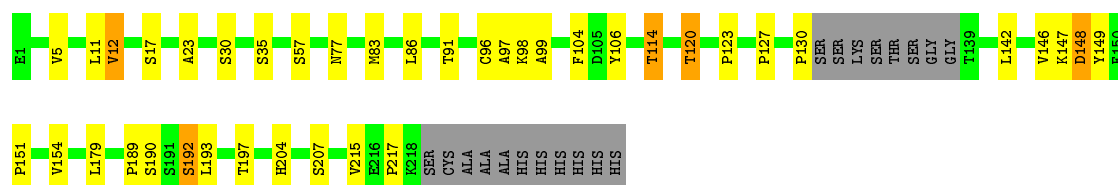
Chain H: 




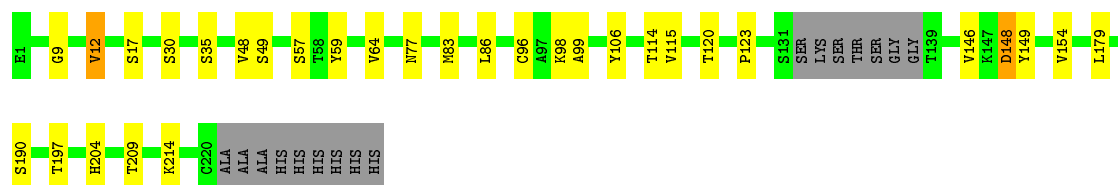
● Molecule 2: Fab H

Chain I:  81% 12% • 6%

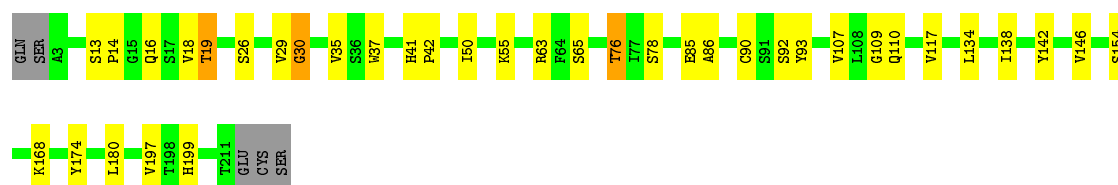
● Molecule 2: Fab H

Chain J:  74% 15% • 8%


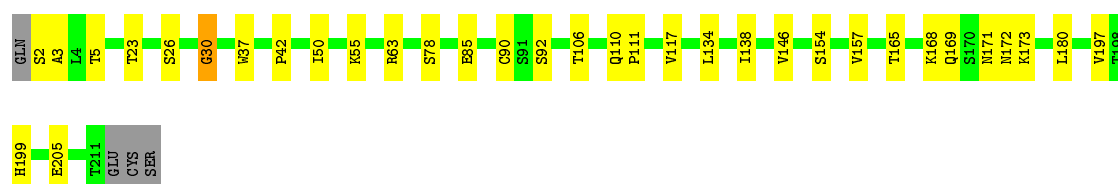
● Molecule 2: Fab H

Chain K:  79% 13% • 7%

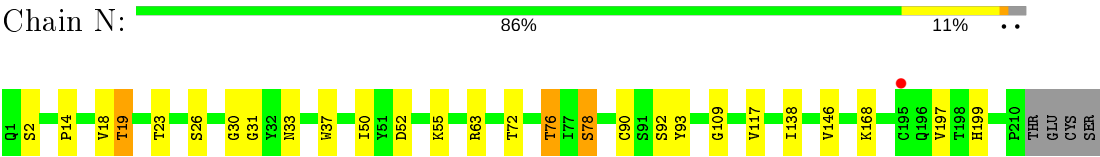
● Molecule 3: Fab L

Chain L:  80% 16% ••

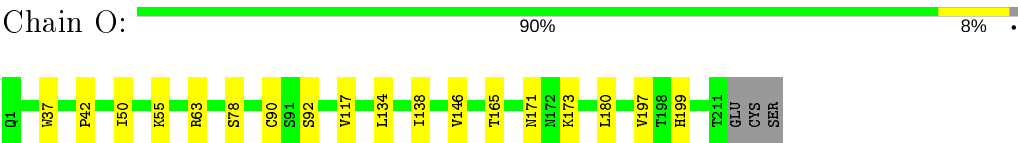
● Molecule 3: Fab L

Chain M:  82% 15% •

● 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 49.22 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.60-3.06) 99.1 (49.22-3.06)	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 (0.87%)	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)	0.29 , 45.2	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 [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	0.53	0/884	0.74	0/1202
1	B	0.50	0/884	0.72	0/1202
1	C	0.52	0/884	0.74	0/1202
1	D	0.50	0/884	0.72	0/1202
2	H	0.50	0/1664	0.75	0/2266
2	I	0.43	0/1641	0.69	0/2234
2	J	0.46	0/1609	0.70	0/2192
2	K	0.46	0/1627	0.72	0/2216
3	L	0.50	0/1585	0.73	0/2163
3	M	0.46	0/1591	0.69	0/2171
3	N	0.44	0/1593	0.66	0/2173
3	O	0.49	0/1600	0.68	0/2183
All	All	0.48	0/16446	0.71	0/22406

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 [i](#)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	13	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	113	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 (113) 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
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
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
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
2:J:83:MET:HE2	2:J:86:LEU:HD21	1.87	0.56
3:O:134:LEU:HD12	3:O:180:LEU:HD23	1.87	0.56
2:J:130:PRO:HG2	2:J:193:LEU:HD21	1.87	0.56
2:I:83:MET:HE2	2:I:86:LEU:HD21	1.87	0.55
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:K:83:MET:HE2	2:K:86:LEU:HD21	1.89	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	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:LYS:HD3	3:M:172:ASN:HA	2.03	0.40
3:M:37:TRP:CZ3	3:M:90:CYS:HB3	2.57	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	107/110 (97%)	96 (90%)	9 (8%)	2 (2%)	8	29
1	B	107/110 (97%)	94 (88%)	13 (12%)	0	100	100
1	C	107/110 (97%)	95 (89%)	11 (10%)	1 (1%)	17	47
1	D	107/110 (97%)	96 (90%)	10 (9%)	1 (1%)	17	47
2	H	217/229 (95%)	209 (96%)	7 (3%)	1 (0%)	29	60
2	I	212/229 (93%)	203 (96%)	8 (4%)	1 (0%)	29	60
2	J	206/229 (90%)	199 (97%)	6 (3%)	1 (0%)	29	60
2	K	209/229 (91%)	198 (95%)	9 (4%)	2 (1%)	15	45
3	L	207/214 (97%)	196 (95%)	9 (4%)	2 (1%)	15	45
3	M	208/214 (97%)	197 (95%)	8 (4%)	3 (1%)	11	36
3	N	208/214 (97%)	199 (96%)	7 (3%)	2 (1%)	15	45
3	O	209/214 (98%)	196 (94%)	12 (6%)	1 (0%)	29	60
All	All	2104/2212 (95%)	1978 (94%)	109 (5%)	17 (1%)	19	50

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%)	91 (97%)	3 (3%)	39	68
1	B	94/95 (99%)	91 (97%)	3 (3%)	39	68
1	C	94/95 (99%)	92 (98%)	2 (2%)	53	77
1	D	94/95 (99%)	90 (96%)	4 (4%)	29	59
2	H	181/188 (96%)	168 (93%)	13 (7%)	14	40
2	I	178/188 (95%)	167 (94%)	11 (6%)	18	46
2	J	174/188 (93%)	162 (93%)	12 (7%)	15	42
2	K	177/188 (94%)	168 (95%)	9 (5%)	24	53
3	L	175/180 (97%)	166 (95%)	9 (5%)	24	53
3	M	176/180 (98%)	166 (94%)	10 (6%)	20	49
3	N	176/180 (98%)	164 (93%)	12 (7%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	O	177/180 (98%)	172 (97%)	5 (3%)	43 71
All	All	1790/1852 (97%)	1697 (95%)	93 (5%)	23 52

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	68	LEU
1	A	80	SER
1	B	66	VAL
1	B	68	LEU
1	B	72	GLU
1	C	66	VAL
1	C	68	LEU
1	D	66	VAL
1	D	68	LEU
1	D	81	ARG
1	D	105	SER
2	H	3	GLN
2	H	12	VAL
2	H	17	SER
2	H	19	ARG
2	H	30	SER
2	H	57	SER
2	H	77	ASN
2	H	85	SER
2	H	96	CYS
2	H	114	THR
2	H	119	SER
2	H	197	THR
2	H	215	VAL
2	I	11	LEU
2	I	17	SER
2	I	30	SER
2	I	57	SER
2	I	77	ASN
2	I	96	CYS
2	I	114	THR
2	I	120	THR
2	I	139	THR
2	I	190	SER
2	I	196	GLN

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Mol	Chain	Res	Type
2	J	12	VAL
2	J	17	SER
2	J	30	SER
2	J	57	SER
2	J	77	ASN
2	J	96	CYS
2	J	114	THR
2	J	120	THR
2	J	147	LYS
2	J	190	SER
2	J	192	SER
2	J	197	THR
2	K	12	VAL
2	K	17	SER
2	K	30	SER
2	K	57	SER
2	K	77	ASN
2	K	96	CYS
2	K	114	THR
2	K	120	THR
2	K	190	SER
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	92	SER
3	L	117	VAL
3	L	154	SER
3	M	2	SER
3	M	5	THR
3	M	23	THR
3	M	50	ILE
3	M	55	LYS
3	M	92	SER
3	M	117	VAL
3	M	154	SER
3	M	165	THR
3	M	169	GLN
3	N	18	VAL
3	N	19	THR

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Mol	Chain	Res	Type
3	N	23	THR
3	N	26	SER
3	N	50	ILE
3	N	55	LYS
3	N	72	THR
3	N	76	THR
3	N	78	SER
3	N	92	SER
3	N	117	VAL
3	N	168	LYS
3	O	50	ILE
3	O	55	LYS
3	O	92	SER
3	O	117	VAL
3	O	165	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	47	ASN
2	H	77	ASN
2	H	84	ASN
2	H	175	GLN
2	I	77	ASN
2	I	175	GLN
2	I	203	ASN
2	I	204	HIS
2	J	13	GLN
2	J	77	ASN
2	J	168	HIS
2	J	175	GLN
2	J	203	ASN
2	J	204	HIS
2	K	77	ASN
2	K	168	HIS
2	K	196	GLN
2	K	203	ASN
3	L	186	GLN
3	L	190	HIS
3	M	16	GLN
3	M	186	GLN
3	M	190	HIS

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Mol	Chain	Res	Type
3	N	16	GLN
3	N	110	GLN
3	N	186	GLN
3	O	16	GLN
3	O	186	GLN
3	O	190	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 carbohydrates 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	109/110 (99%)	-0.42	0	100	100	50, 61, 82, 96	6 (5%)
1	B	109/110 (99%)	-0.40	0	100	100	59, 80, 104, 117	6 (5%)
1	C	109/110 (99%)	-0.46	0	100	100	55, 73, 95, 98	5 (4%)
1	D	109/110 (99%)	-0.47	0	100	100	52, 69, 86, 105	3 (2%)
2	H	219/229 (95%)	-0.43	0	100	100	46, 61, 85, 115	12 (5%)
2	I	216/229 (94%)	-0.21	1 (0%)	91	79	64, 98, 120, 140	16 (7%)
2	J	210/229 (91%)	-0.36	0	100	100	53, 76, 103, 122	12 (5%)
2	K	213/229 (93%)	-0.34	0	100	100	58, 86, 112, 140	14 (6%)
3	L	209/214 (97%)	-0.41	0	100	100	50, 74, 95, 113	10 (4%)
3	M	210/214 (98%)	-0.45	0	100	100	56, 77, 101, 131	11 (5%)
3	N	210/214 (98%)	-0.24	1 (0%)	91	79	60, 96, 141, 157	20 (9%)
3	O	211/214 (98%)	-0.42	0	100	100	51, 70, 96, 121	10 (4%)
All	All	2134/2212 (96%)	-0.37	2 (0%)	95	91	46, 77, 115, 157	125 (5%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1	GLU	2.0
3	N	195	CYS	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 [i](#)

There are no carbohydrates 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.