



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:19 PM UTC

PDB ID : 5MFD / pdb_00005mfd
Title : Designed armadillo repeat protein YIIIM⁷6AII in complex with pD₋(KR)₅
Authors : Hansen, S.; Kiefer, J.; Madhurantakam, C.; Mittl, P.; Plueckthun, A.
Deposited on : 2016-11-18
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

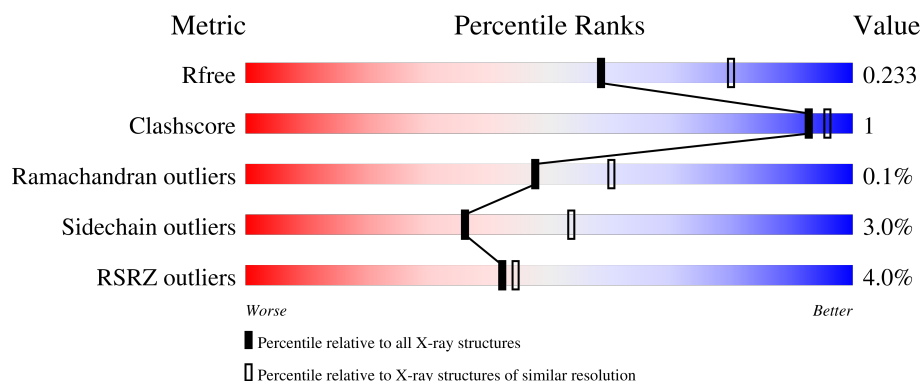
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	328	2% 90% 9% .
1	C	328	% 94% 5% .
1	E	328	2% 93% 5% ..
1	G	328	2% 91% 6% .
1	I	328	2% 96% . ..

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Mol	Chain	Length	Quality of chain
1	J	328	2% 95% 3%
1	K	328	2% 93% 5%
1	L	328	2% 90% 8%
2	B	109	9% 84% 8%
2	D	109	16% 92% 6%
2	F	109	13% 88% 8%
2	H	109	30% 87% 6% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22833 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 YIIIM"6AII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2386	1489	406	490	1			
1	C	323	Total	C	N	O	S	0	0	0
			2386	1489	406	490	1			
1	E	323	Total	C	N	O	S	0	2	0
			2414	1511	410	492	1			
1	G	322	Total	C	N	O	S	0	1	0
			2394	1497	407	489	1			
1	I	323	Total	C	N	O	S	0	0	0
			2386	1489	406	490	1			
1	J	324	Total	C	N	O	S	0	1	0
			2410	1506	411	492	1			
1	K	323	Total	C	N	O	S	0	1	0
			2400	1500	408	491	1			
1	L	323	Total	C	N	O	S	0	2	0
			2409	1506	410	492	1			

- Molecule 2 is a protein called Capsid decoration protein,pD_(KR)5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O	S	0	0	0
			777	487	139	149	2			
2	D	107	Total	C	N	O	S	0	0	0
			792	495	144	151	2			
2	F	105	Total	C	N	O	S	0	0	0
			777	487	139	149	2			
2	H	104	Total	C	N	O	S	0	0	0
			768	481	137	148	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	GLY	-	expression tag	UNP P03712

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	PRO	-	expression tag	UNP P03712
D	18	GLY	-	expression tag	UNP P03712
D	19	PRO	-	expression tag	UNP P03712
F	18	GLY	-	expression tag	UNP P03712
F	19	PRO	-	expression tag	UNP P03712
H	18	GLY	-	expression tag	UNP P03712
H	19	PRO	-	expression tag	UNP P03712

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total Ca 8 8	0	0
3	C	1	Total Ca 1 1	0	0
3	E	9	Total Ca 9 9	0	0
3	F	1	Total Ca 1 1	0	0
3	G	9	Total Ca 9 9	0	0
3	H	1	Total Ca 1 1	0	0
3	I	4	Total Ca 4 4	0	0
3	J	4	Total Ca 4 4	0	0
3	K	10	Total Ca 10 10	0	0
3	L	2	Total Ca 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	19	Total O 19 19	0	0
4	C	58	Total O 58 58	0	0
4	D	16	Total O 16 16	0	0

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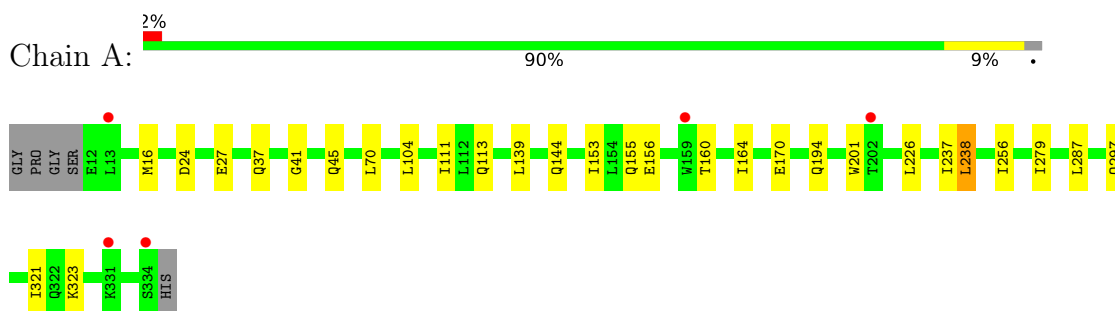
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	60	Total 60	O 60	0	0
4	F	7	Total 7	O 7	0	0
4	G	27	Total 27	O 27	0	0
4	H	2	Total 2	O 2	0	0
4	I	65	Total 65	O 65	0	0
4	J	61	Total 61	O 61	0	0
4	K	98	Total 98	O 98	0	0
4	L	43	Total 43	O 43	0	0

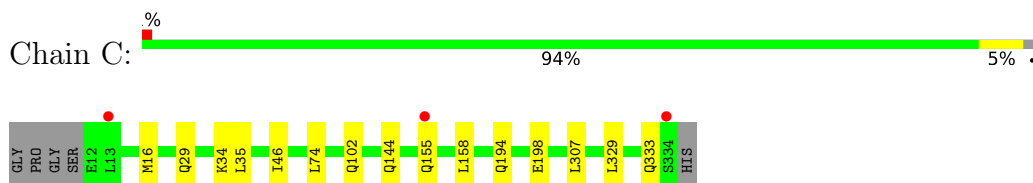
3 Residue-property plots [i](#)

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.

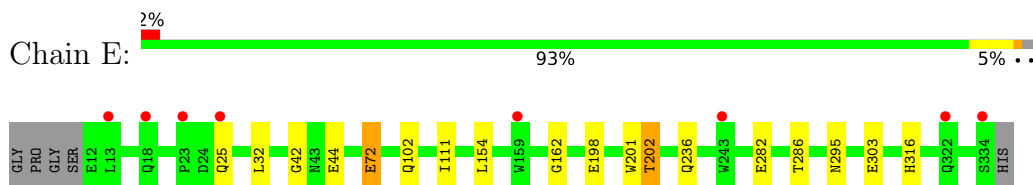
- Molecule 1: YIIIM"6AII



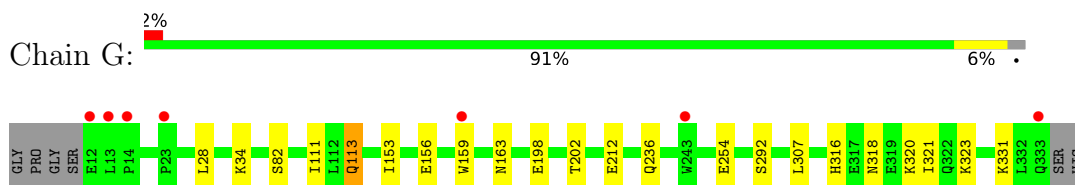
- Molecule 1: YIIIM"6AII



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- Molecule 1: YIIIM"6AII



- Molecule 1: YIIIM"6AII

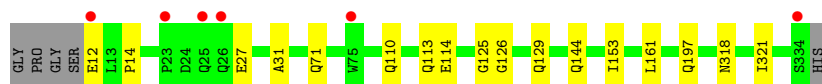




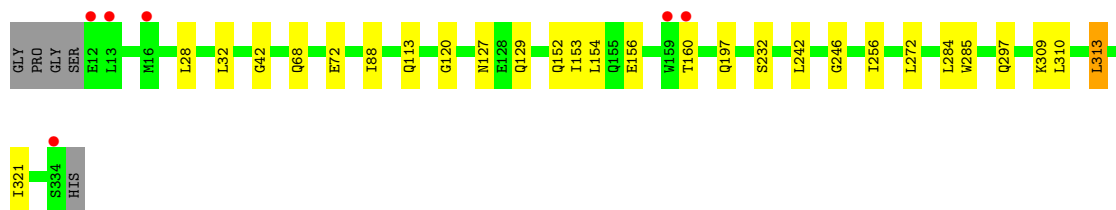
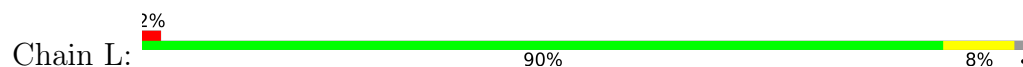
• Molecule 1: YIIIM"6AII



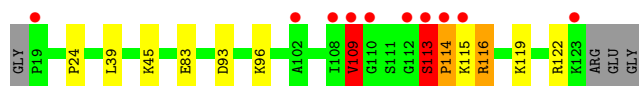
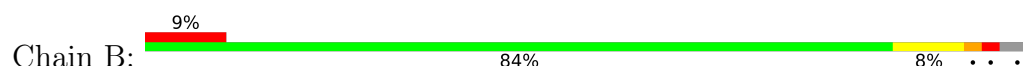
• Molecule 1: YIIIM"6AII



• Molecule 1: YIIIM"6AII



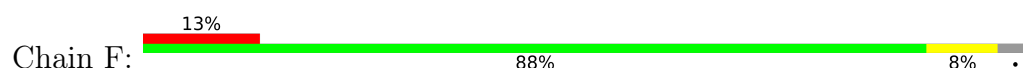
• Molecule 2: Capsid decoration protein,pD_(KR)5



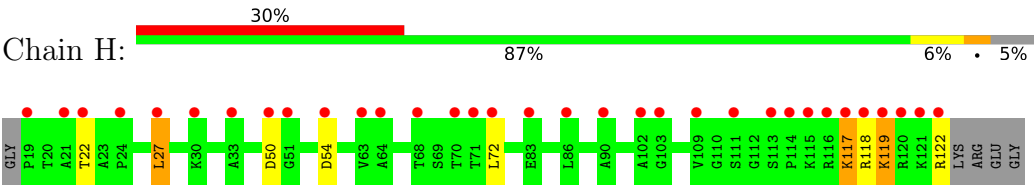
• Molecule 2: Capsid decoration protein,pD_(KR)5



• Molecule 2: Capsid decoration protein,pD_(KR)5



● Molecule 2: Capsid decoration protein,pD_(KR)5



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	194.66Å 194.66Å 241.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 2.30 49.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.12-2.30) 99.8 (49.12-2.30)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.190 , 0.214 0.206 , 0.233	Depositor DCC
R_{free} test set	15176 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22833	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.79	0/2412	1.46	4/3289 (0.1%)
1	C	0.78	0/2412	1.47	0/3289
1	E	0.78	0/2444	1.46	4/3335 (0.1%)
1	G	0.77	0/2422	1.45	4/3304 (0.1%)
1	I	0.79	0/2412	1.45	0/3289
1	J	0.79	0/2439	1.44	8/3327 (0.2%)
1	K	0.79	0/2428	1.45	8/3312 (0.2%)
1	L	0.78	0/2437	1.44	3/3323 (0.1%)
2	B	0.86	2/791 (0.3%)	1.24	3/1069 (0.3%)
2	D	0.75	0/806	1.17	0/1089
2	F	0.85	0/791	1.21	3/1069 (0.3%)
2	H	0.83	0/782	1.18	2/1058 (0.2%)
All	All	0.79	2/22576 (0.0%)	1.42	39/30753 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	109	VAL	CA-C	5.75	1.60	1.52
2	B	113	SER	CA-C	5.49	1.59	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	ARG	CA-C-N	6.56	133.51	121.70
2	B	122	ARG	C-N-CA	6.56	133.51	121.70
1	L	232	SER	N-CA-C	6.16	117.14	109.57
2	B	116	ARG	N-CA-C	5.99	118.10	110.61
1	K	321	ILE	CA-C-N	5.80	127.98	120.44
1	K	321	ILE	C-N-CA	5.80	127.98	120.44
1	K	31	ALA	CA-C-N	5.76	127.92	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	31	ALA	C-N-CA	5.76	127.92	120.44
1	J	321	ILE	CA-C-N	5.62	128.06	120.65
1	J	321	ILE	C-N-CA	5.62	128.06	120.65
2	H	54	ASP	CA-CB-CG	5.56	118.16	112.60
1	L	321	ILE	CA-C-N	5.55	127.72	120.28
1	L	321	ILE	C-N-CA	5.55	127.72	120.28
1	A	321	ILE	CA-C-N	5.50	127.97	120.54
1	A	321	ILE	C-N-CA	5.50	127.97	120.54
1	G	321	ILE	CA-C-N	5.49	127.95	120.54
1	G	321	ILE	C-N-CA	5.49	127.95	120.54
1	K	318	ASN	CA-C-N	5.49	127.90	120.38
1	K	318	ASN	C-N-CA	5.49	127.90	120.38
2	H	50	ASP	CA-CB-CG	5.39	117.99	112.60
1	G	316	HIS	CA-C-N	5.39	127.76	120.38
1	G	316	HIS	C-N-CA	5.39	127.76	120.38
1	J	316	HIS	CA-C-N	5.32	127.67	120.38
1	J	316	HIS	C-N-CA	5.32	127.67	120.38
1	J	132	ALA	CA-C-N	5.23	127.62	120.46
1	J	132	ALA	C-N-CA	5.23	127.62	120.46
2	F	69	SER	CA-C-N	5.21	127.26	120.28
2	F	69	SER	C-N-CA	5.21	127.26	120.28
1	K	27	GLU	CA-C-N	5.19	127.49	120.44
1	K	27	GLU	C-N-CA	5.19	127.49	120.44
2	F	115	LYS	N-CA-C	5.12	115.05	108.34
1	E	316	HIS	CA-C-N	5.10	127.36	120.38
1	E	316	HIS	C-N-CA	5.10	127.36	120.38
1	A	237	ILE	CA-C-N	5.05	127.01	120.44
1	A	237	ILE	C-N-CA	5.05	127.01	120.44
1	J	73	ALA	CA-C-N	5.05	127.46	120.29
1	J	73	ALA	C-N-CA	5.05	127.46	120.29
1	E	42	GLY	CA-C-N	5.03	127.28	120.38
1	E	42	GLY	C-N-CA	5.03	127.28	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2386	0	2399	10	0
1	C	2386	0	2399	6	0
1	E	2414	0	2416	5	0
1	G	2394	0	2403	10	0
1	I	2386	0	2399	3	0
1	J	2410	0	2415	2	0
1	K	2400	0	2407	4	0
1	L	2409	0	2420	12	0
2	B	777	0	801	8	0
2	D	792	0	816	6	0
2	F	777	0	801	2	0
2	H	768	0	788	10	0
3	A	8	0	0	0	0
3	C	1	0	0	0	0
3	E	9	0	0	0	0
3	F	1	0	0	0	0
3	G	9	0	0	0	0
3	H	1	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	10	0	0	0	0
3	L	2	0	0	0	0
4	A	29	0	0	0	0
4	B	19	0	0	0	0
4	C	58	0	0	0	0
4	D	16	0	0	0	0
4	E	60	0	0	0	0
4	F	7	0	0	0	0
4	G	27	0	0	0	0
4	H	2	0	0	0	0
4	I	65	0	0	0	0
4	J	61	0	0	0	0
4	K	98	0	0	0	0
4	L	43	0	0	0	0
All	All	22833	0	22464	65	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 1.

All (65) 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)
2:B:113:SER:HB2	2:B:114:PRO:HD3	1.65	0.78
2:H:117:LYS:HA	2:H:117:LYS:HE3	1.69	0.74
1:G:163:ASN:HA	2:H:117:LYS:NZ	2.03	0.74
2:D:81:ARG:HG2	2:D:83:GLU:HG2	1.72	0.69
1:G:198:GLU:O	1:G:202:THR:HG23	1.94	0.67
2:H:117:LYS:HA	2:H:117:LYS:CE	2.26	0.66
1:G:163:ASN:HA	2:H:117:LYS:HZ2	1.63	0.61
1:G:113:GLN:HG2	1:G:156:GLU:HG3	1.82	0.61
1:E:198:GLU:O	1:E:202:THR:HG23	2.02	0.60
1:C:16:MET:HE2	1:C:35:LEU:HG	1.83	0.59
2:B:119:LYS:HB2	2:D:123:LYS:HB2	1.85	0.58
2:H:27:LEU:HD11	2:H:72:LEU:HD21	1.85	0.58
1:E:282:GLU:O	1:E:286:THR:HG23	2.03	0.57
1:I:113:GLN:HG3	1:I:156:GLU:HG3	1.87	0.56
1:L:113:GLN:HG2	1:L:156:GLU:HG3	1.90	0.54
1:A:113:GLN:HG3	1:A:156:GLU:HG3	1.90	0.53
1:A:156:GLU:O	1:A:160:THR:HG23	2.08	0.53
1:L:120:GLY:HA3	1:L:160:THR:HG22	1.91	0.53
1:G:82:SER:HA	2:H:119:LYS:HE2	1.91	0.53
1:A:41:GLY:HA3	1:A:45:GLN:HE21	1.73	0.53
1:L:284:LEU:HD21	1:L:313:LEU:HD23	1.90	0.52
1:G:159:TRP:CH2	2:H:118:ARG:HB2	2.45	0.52
1:L:256:ILE:HG22	1:L:297:GLN:HG2	1.92	0.52
1:C:329:LEU:O	1:C:333:GLN:HG2	2.09	0.51
2:B:93:ASP:HB3	2:B:96:LYS:HB2	1.93	0.51
1:A:155:GLN:OE1	1:A:194:GLN:HG2	2.12	0.50
2:B:24:PRO:HB2	2:B:45:LYS:HG2	1.94	0.50
1:J:113:GLN:HG2	1:J:156:GLU:HG3	1.94	0.50
1:L:88:ILE:HG22	1:L:129:GLN:HG2	1.94	0.50
1:L:256:ILE:CG2	1:L:297:GLN:HG2	2.42	0.49
1:G:292:SER:HB3	1:G:331:LYS:HD3	1.94	0.49
1:I:13:LEU:HA	1:I:16:MET:HE3	1.95	0.48
1:K:12:GLU:HB3	1:K:14:PRO:HD2	1.95	0.48
1:G:159:TRP:HH2	2:H:118:ARG:HB2	1.78	0.48
1:K:110:GLN:O	1:K:114:GLU:HG2	2.14	0.48
1:E:162:GLY:HA3	1:E:201:TRP:CZ3	2.48	0.48
2:F:122:ARG:HH11	2:F:123:LYS:HE2	1.79	0.48
1:L:246:GLY:HA3	1:L:285:TRP:CZ3	2.49	0.47
1:L:120:GLY:CA	1:L:160:THR:HG22	2.45	0.47
1:G:163:ASN:HA	2:H:117:LYS:HZ3	1.76	0.46
1:L:156:GLU:O	1:L:160:THR:HG23	2.16	0.46
1:E:32:LEU:HG	1:E:72:GLU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TRP:CZ2	2:B:116:ARG:HG2	2.51	0.45
2:D:25:GLY:HA3	2:D:72:LEU:HG	1.98	0.44
1:A:70:LEU:HD22	1:A:111:ILE:HG12	2.00	0.44
2:H:22:THR:HG21	1:L:127:ASN:H	1.81	0.44
1:E:236:GLN:HE21	1:I:110:GLN:HG3	1.83	0.44
2:B:115:LYS:HB2	2:D:124:ARG:NH2	2.33	0.43
1:C:46:ILE:HD11	2:D:121:LYS:NZ	2.34	0.43
1:G:318:ASN:OD1	1:G:320:LYS:HB2	2.19	0.43
1:A:238:LEU:HD12	1:A:279:ILE:HG12	2.00	0.43
2:B:113:SER:CB	2:B:114:PRO:HD3	2.44	0.43
2:F:25:GLY:HA3	2:F:72:LEU:HG	2.01	0.42
1:C:158:LEU:HB3	1:C:198:GLU:HB3	2.01	0.42
1:K:126:GLY:H	1:K:129:GLN:NE2	2.18	0.42
1:L:32:LEU:HB3	1:L:72:GLU:HB3	2.02	0.42
1:L:272:LEU:HB3	1:L:309[A]:LYS:HG2	2.02	0.42
1:C:155:GLN:CD	1:C:194:GLN:HG2	2.44	0.42
1:A:139:LEU:HD21	1:A:164:ILE:HG21	2.02	0.41
1:A:24:ASP:HB3	1:A:27:GLU:HB2	2.02	0.41
1:C:16:MET:HE3	1:C:34:LYS:HB3	2.01	0.41
1:J:16:MET:HE3	1:J:34:LYS:HB3	2.03	0.41
1:A:256:ILE:HG22	1:A:297:GLN:HG2	2.02	0.40
1:K:125:GLY:HA3	1:K:129:GLN:HE21	1.86	0.40
2:B:115:LYS:HB2	2:D:124:ARG:HH21	1.86	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	321/328 (98%)	320 (100%)	1 (0%)	0	100	100
1	C	321/328 (98%)	321 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	323/328 (98%)	321 (99%)	2 (1%)	0	100	100
1	G	321/328 (98%)	320 (100%)	1 (0%)	0	100	100
1	I	321/328 (98%)	319 (99%)	2 (1%)	0	100	100
1	J	323/328 (98%)	321 (99%)	2 (1%)	0	100	100
1	K	322/328 (98%)	321 (100%)	1 (0%)	0	100	100
1	L	323/328 (98%)	322 (100%)	0	1 (0%)	36	46
2	B	103/109 (94%)	95 (92%)	5 (5%)	3 (3%)	3	2
2	D	105/109 (96%)	101 (96%)	4 (4%)	0	100	100
2	F	103/109 (94%)	99 (96%)	4 (4%)	0	100	100
2	H	102/109 (94%)	97 (95%)	5 (5%)	0	100	100
All	All	2988/3060 (98%)	2957 (99%)	27 (1%)	4 (0%)	48	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	113	SER
2	B	109	VAL
2	B	114	PRO
1	L	42	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	253/256 (99%)	243 (96%)	10 (4%)	28	42
1	C	253/256 (99%)	248 (98%)	5 (2%)	48	67
1	E	255/256 (100%)	246 (96%)	9 (4%)	32	48
1	G	253/256 (99%)	243 (96%)	10 (4%)	28	42
1	I	253/256 (99%)	249 (98%)	4 (2%)	55	73
1	J	255/256 (100%)	248 (97%)	7 (3%)	39	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	254/256 (99%)	248 (98%)	6 (2%)	43	62
1	L	255/256 (100%)	246 (96%)	9 (4%)	32	48
2	B	80/82 (98%)	77 (96%)	3 (4%)	29	44
2	D	81/82 (99%)	81 (100%)	0	100	100
2	F	80/82 (98%)	77 (96%)	3 (4%)	29	44
2	H	79/82 (96%)	75 (95%)	4 (5%)	21	32
All	All	2351/2376 (99%)	2281 (97%)	70 (3%)	36	53

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	37	GLN
1	A	104	LEU
1	A	144	GLN
1	A	153	ILE
1	A	170	GLU
1	A	226	LEU
1	A	238	LEU
1	A	287	LEU
1	A	323	LYS
2	B	39	LEU
2	B	83	GLU
2	B	109	VAL
1	C	29	GLN
1	C	74	LEU
1	C	102	GLN
1	C	144	GLN
1	C	307	LEU
1	E	25	GLN
1	E	44	GLU
1	E	72	GLU
1	E	102	GLN
1	E	111	ILE
1	E	154	LEU
1	E	202	THR
1	E	295	ASN
1	E	303	GLU
2	F	39	LEU
2	F	71	THR

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Mol	Chain	Res	Type
2	F	116	ARG
1	G	28	LEU
1	G	34	LYS
1	G	111	ILE
1	G	113	GLN
1	G	153	ILE
1	G	212	GLU
1	G	236	GLN
1	G	254	GLU
1	G	307	LEU
1	G	323	LYS
2	H	27	LEU
2	H	117	LYS
2	H	119	LYS
2	H	122	ARG
1	I	13	LEU
1	I	153	ILE
1	I	242	LEU
1	I	296	GLU
1	J	12	GLU
1	J	15	GLN
1	J	33	ARG
1	J	72	GLU
1	J	113	GLN
1	J	153	ILE
1	J	322	GLN
1	K	71	GLN
1	K	113	GLN
1	K	144	GLN
1	K	153	ILE
1	K	161	LEU
1	K	197	GLN
1	L	28	LEU
1	L	68	GLN
1	L	152	GLN
1	L	153	ILE
1	L	154	LEU
1	L	197	GLN
1	L	242	LEU
1	L	310	LEU
1	L	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	60	GLN
1	A	215	GLN
1	A	234	ASN
1	A	314	GLN
1	A	333	GLN
1	C	29	GLN
1	C	43	ASN
1	C	155	GLN
1	C	194	GLN
1	C	270	GLN
2	D	67	GLN
1	E	29	GLN
1	E	127	ASN
1	E	152	GLN
1	E	169	ASN
1	E	211	ASN
1	E	236	GLN
1	E	270	GLN
1	E	322	GLN
1	G	21	ASN
1	G	37	GLN
1	G	110	GLN
1	G	113	GLN
1	G	152	GLN
1	G	253	ASN
1	G	255	GLN
1	G	281	GLN
1	I	15	GLN
1	I	21	ASN
1	I	25	GLN
1	I	37	GLN
1	I	47	GLN
1	I	110	GLN
1	I	152	GLN
1	I	197	GLN
1	J	43	ASN
1	J	68	GLN
1	J	152	GLN
1	J	197	GLN
1	J	278	GLN
1	K	19	GLN

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Mol	Chain	Res	Type
1	K	21	ASN
1	K	25	GLN
1	K	60	GLN
1	K	68	GLN
1	K	71	GLN
1	K	85	ASN
1	K	110	GLN
1	K	113	GLN
1	K	129	GLN
1	K	152	GLN
1	K	194	GLN
1	K	197	GLN
1	K	205	ASN
1	K	213	GLN
1	K	318	ASN
1	L	19	GLN
1	L	25	GLN
1	L	26	GLN
1	L	43	ASN
1	L	45	GLN
1	L	110	GLN
1	L	152	GLN
1	L	197	GLN
1	L	278	GLN
1	L	281	GLN
1	L	318	ASN
1	L	326	GLN
1	L	333	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

Of 49 ligands modelled in this entry, 49 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	323/328 (98%)	0.32	5 (1%) 72 73	61, 83, 112, 137	0
1	C	323/328 (98%)	0.04	3 (0%) 81 82	50, 65, 112, 134	0
1	E	323/328 (98%)	0.10	8 (2%) 58 60	31, 67, 93, 121	2 (0%)
1	G	322/328 (98%)	0.27	7 (2%) 62 64	33, 77, 112, 138	1 (0%)
1	I	323/328 (98%)	-0.02	5 (1%) 72 73	52, 64, 103, 128	0
1	J	324/328 (98%)	0.07	7 (2%) 62 64	31, 64, 97, 125	1 (0%)
1	K	323/328 (98%)	-0.04	6 (1%) 66 68	29, 59, 90, 107	1 (0%)
1	L	323/328 (98%)	0.19	6 (1%) 66 68	30, 73, 102, 129	2 (0%)
2	B	105/109 (96%)	0.76	10 (9%) 14 15	57, 81, 119, 129	0
2	D	107/109 (98%)	1.02	17 (15%) 5 5	60, 88, 116, 140	0
2	F	105/109 (96%)	0.89	14 (13%) 7 8	60, 88, 123, 136	0
2	H	104/109 (95%)	1.81	33 (31%) 1 1	75, 112, 146, 156	0
All	All	3005/3060 (98%)	0.26	121 (4%) 42 44	29, 71, 113, 156	7 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	123	LYS	7.2
2	B	109	VAL	7.2
2	H	122	ARG	6.6
2	H	114	PRO	6.4
2	H	118	ARG	6.2
2	H	19	PRO	5.7
1	E	243[A]	TRP	5.4
2	B	114	PRO	5.4
2	B	123	LYS	5.3
2	H	121	LYS	5.2
2	H	119	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	L	159[A]	TRP	5.1
2	F	19	PRO	5.0
2	F	119	LYS	4.8
1	E	159[A]	TRP	4.8
2	B	115	LYS	4.7
1	E	334	SER	4.6
2	H	117	LYS	4.5
2	H	109	VAL	4.4
2	D	95	THR	4.4
2	H	24	PRO	4.4
2	D	124	ARG	4.4
1	K	334	SER	4.4
1	A	334	SER	4.2
2	H	115	LYS	4.2
2	H	116	ARG	4.2
2	H	113	SER	4.1
2	B	19	PRO	4.1
2	F	117	LYS	4.1
2	F	118	ARG	3.9
2	F	120	ARG	3.8
1	I	334	SER	3.8
2	F	121	LYS	3.5
2	H	68	THR	3.4
1	C	334	SER	3.4
1	C	13	LEU	3.4
2	F	116	ARG	3.4
2	B	110	GLY	3.4
2	F	114	PRO	3.3
2	H	22	THR	3.3
2	H	120	ARG	3.3
2	B	113	SER	3.3
2	H	21	ALA	3.2
2	H	103	GLY	3.2
2	D	114	PRO	3.2
2	H	63	VAL	3.2
1	G	159	TRP	3.2
2	B	112	GLY	3.1
1	G	12	GLU	3.1
1	L	334	SER	3.1
1	G	333	GLN	3.1
1	G	13	LEU	3.0
2	F	122	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	335	HIS	3.0
2	H	111	SER	3.0
1	L	12	GLU	2.9
1	K	26	GLN	2.9
2	F	85	VAL	2.9
1	G	243[A]	TRP	2.8
2	H	90	ALA	2.8
2	H	102	ALA	2.8
2	D	123	LYS	2.8
2	D	18	GLY	2.8
2	H	64	ALA	2.8
2	D	115	LYS	2.7
2	D	22	THR	2.7
1	E	13	LEU	2.7
2	H	71	THR	2.7
1	J	12	GLU	2.6
2	H	70	THR	2.6
2	H	27	LEU	2.6
1	E	18	GLN	2.6
1	K	25	GLN	2.6
2	F	115	LYS	2.6
1	L	16	MET	2.5
1	J	34	LYS	2.5
2	D	19	PRO	2.5
1	J	13	LEU	2.4
1	E	25	GLN	2.4
1	K	12	GLU	2.4
2	D	109	VAL	2.4
1	I	13	LEU	2.4
2	H	72	LEU	2.4
2	H	86	LEU	2.4
1	A	159	TRP	2.4
1	G	23	PRO	2.3
1	K	23	PRO	2.3
2	F	109	VAL	2.3
1	G	14	PRO	2.3
2	B	102	ALA	2.3
2	D	122	ARG	2.3
2	D	62	ALA	2.3
1	A	202	THR	2.3
2	D	73	THR	2.3
2	B	108	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	12	GLU	2.3
1	A	331	LYS	2.3
2	H	30	LYS	2.3
2	F	95	THR	2.2
1	J	159[A]	TRP	2.2
1	J	23	PRO	2.2
2	H	83	GLU	2.2
1	C	155	GLN	2.2
2	D	102	ALA	2.2
1	K	75	TRP	2.2
1	L	13	LEU	2.2
2	H	51	GLY	2.2
1	L	160	THR	2.2
1	A	13	LEU	2.1
1	E	23	PRO	2.1
2	D	96	LYS	2.1
2	D	97	LYS	2.1
1	I	37	GLN	2.1
2	H	33	ALA	2.1
1	E	322	GLN	2.1
2	H	50	ASP	2.1
1	I	159	TRP	2.1
2	D	113	SER	2.0
1	J	37	GLN	2.0
2	D	54	ASP	2.0
2	H	54	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	406	1/1	0.76	0.31	135,135,135,135	0
3	CA	C	401	1/1	0.82	0.20	118,118,118,118	0
3	CA	G	406	1/1	0.83	0.13	156,156,156,156	0
3	CA	G	405	1/1	0.85	0.10	140,140,140,140	0
3	CA	A	405	1/1	0.86	0.17	119,119,119,119	0
3	CA	I	401	1/1	0.88	0.27	112,112,112,112	0
3	CA	J	404	1/1	0.88	0.13	127,127,127,127	0
3	CA	L	402	1/1	0.88	0.15	115,115,115,115	0
3	CA	J	402	1/1	0.91	0.17	111,111,111,111	0
3	CA	H	201	1/1	0.91	0.20	112,112,112,112	0
3	CA	F	201	1/1	0.91	0.13	108,108,108,108	0
3	CA	E	406	1/1	0.92	0.24	101,101,101,101	0
3	CA	K	406	1/1	0.93	0.24	105,105,105,105	0
3	CA	K	410	1/1	0.93	0.07	102,102,102,102	0
3	CA	J	401	1/1	0.93	0.21	113,113,113,113	0
3	CA	E	405	1/1	0.94	0.10	91,91,91,91	0
3	CA	K	407	1/1	0.94	0.15	100,100,100,100	0
3	CA	A	407	1/1	0.95	0.12	72,72,72,72	0
3	CA	I	402	1/1	0.95	0.19	86,86,86,86	0
3	CA	J	403	1/1	0.95	0.10	81,81,81,81	0
3	CA	L	401	1/1	0.95	0.18	107,107,107,107	0
3	CA	I	403	1/1	0.95	0.09	92,92,92,92	0
3	CA	A	404	1/1	0.96	0.06	65,65,65,65	0
3	CA	A	408	1/1	0.96	0.08	77,77,77,77	0
3	CA	K	409	1/1	0.96	0.09	66,66,66,66	0
3	CA	A	402	1/1	0.96	0.08	77,77,77,77	0
3	CA	A	403	1/1	0.96	0.09	72,72,72,72	0
3	CA	K	402	1/1	0.96	0.09	66,66,66,66	0
3	CA	K	403	1/1	0.97	0.08	74,74,74,74	0
3	CA	K	405	1/1	0.97	0.08	77,77,77,77	0
3	CA	E	403	1/1	0.97	0.11	74,74,74,74	0
3	CA	E	407	1/1	0.97	0.08	73,73,73,73	0
3	CA	G	408	1/1	0.97	0.08	67,67,67,67	0
3	CA	A	401	1/1	0.97	0.07	71,71,71,71	0
3	CA	G	403	1/1	0.97	0.07	71,71,71,71	0
3	CA	G	404	1/1	0.97	0.09	76,76,76,76	0
3	CA	G	402	1/1	0.98	0.04	61,61,61,61	0
3	CA	E	409	1/1	0.98	0.04	102,102,102,102	0
3	CA	G	407	1/1	0.98	0.06	72,72,72,72	0
3	CA	K	408	1/1	0.98	0.05	63,63,63,63	0
3	CA	K	401	1/1	0.98	0.07	67,67,67,67	0
3	CA	E	404	1/1	0.98	0.05	67,67,67,67	0
3	CA	G	409	1/1	0.98	0.04	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	K	404	1/1	0.98	0.04	77,77,77,77	0
3	CA	E	402	1/1	0.99	0.04	62,62,62,62	0
3	CA	E	401	1/1	0.99	0.02	66,66,66,66	0
3	CA	G	401	1/1	0.99	0.03	72,72,72,72	0
3	CA	I	404	1/1	0.99	0.03	60,60,60,60	0
3	CA	E	408	1/1	0.99	0.04	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.