



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2025 – 10:10 AM EDT

PDB ID : 9DHK / pdb_00009dhk
Title : RMI1-RMI2 bound to cyclic peptide L3
Authors : Bythell-Douglas, R.; Lau, Y.; Alcock, L.J.; Patel, K.; Gao, T.; Deshpande, C.
Deposited on : 2024-09-03
Resolution : 2.35 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

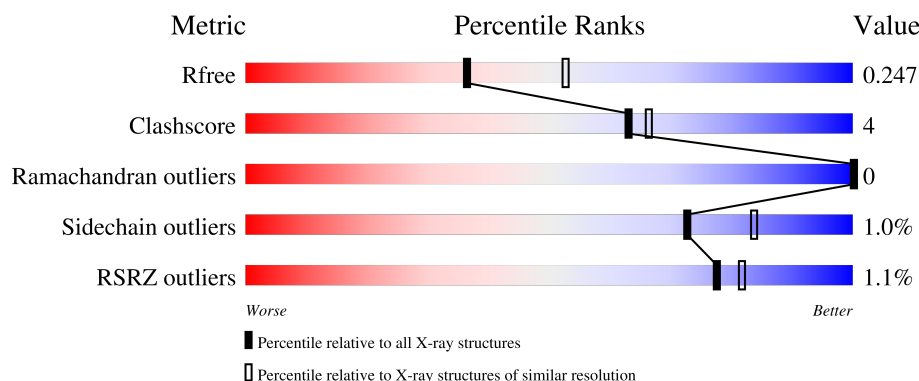
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	152	
1	D	152	
1	J	152	
2	B	147	
2	K	147	

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Mol	Chain	Length	Quality of chain
3	E	135	<div><div>%</div><div><div></div><div>83%</div><div>17%</div></div></div>
4	G	145	<div><div>%</div><div><div></div><div>87%</div><div>12%</div></div><div></div></div>
5	H	139	<div><div></div><div><div></div><div>81%</div><div>16%</div></div><div><div></div><div></div></div></div>
6	C	15	<div><div></div><div><div></div><div>87%</div><div>13%</div></div></div>
6	F	15	<div><div></div><div><div></div><div>80%</div><div>13%</div><div>7%</div></div></div>
6	I	15	<div><div><div>7%</div></div><div><div></div><div>73%</div><div>27%</div></div></div>
6	L	15	<div><div></div><div><div></div><div>93%</div><div>7%</div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18874 atoms, of which 9398 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 RecQ-mediated genome instability protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	H	N	O	S	31	2	0
			2288	722	1169	176	212	9			
1	D	145	Total	C	H	N	O	S	32	2	0
			2330	734	1188	181	218	9			
1	J	142	Total	C	H	N	O	S	31	1	0
			2277	718	1160	177	213	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	MET	-	initiating methionine	UNP Q9H9A7
D	474	MET	-	initiating methionine	UNP Q9H9A7
J	474	MET	-	initiating methionine	UNP Q9H9A7

- Molecule 2 is a protein called RecQ-mediated genome instability protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	135	Total	C	H	N	O	S	16	0	0
			2084	642	1049	199	185	9			
2	K	137	Total	C	H	N	O	S	16	0	0
			2105	649	1059	201	187	9			

- Molecule 3 is a protein called RecQ-mediated genome instability protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	135	Total	C	H	N	O	S	17	0	0
			2083	642	1048	199	185	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	12	UNK	-	expression tag	UNP Q96E14

- Molecule 4 is a protein called RecQ-mediated genome instability protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	G	145	Total	C	H	N	O	S	32	0	0
			2303	726	1176	179	213	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	479	UNK	-	expression tag	UNP Q9H9A7

- Molecule 5 is a protein called RecQ-mediated genome instability protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	H	139	Total	C	H	N	O	S	16	0	0
			2103	649	1053	203	189	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	UNK	-	expression tag	UNP Q96E14
H	9	UNK	-	expression tag	UNP Q96E14
H	10	UNK	-	expression tag	UNP Q96E14
H	11	UNK	-	expression tag	UNP Q96E14
H	12	UNK	-	expression tag	UNP Q96E14
H	13	UNK	-	expression tag	UNP Q96E14

- Molecule 6 is a protein called L3 peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	C	15	Total	C	H	N	O	S	3	0	1
			253	90	124	20	18	1			
6	F	15	Total	C	H	N	O	S	3	0	1
			253	90	124	20	18	1			
6	I	15	Total	C	H	N	O	S	3	0	1
			253	90	124	20	18	1			
6	L	15	Total	C	H	N	O	S	3	0	1
			253	90	124	20	18	1			

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total	O	0	0
			39	39		

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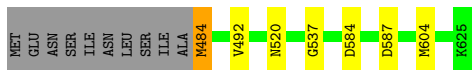
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	34	Total 34	O 34	0	0
7	D	48	Total 48	O 48	0	0
7	E	20	Total 20	O 20	0	0
7	G	34	Total 34	O 34	0	0
7	H	28	Total 28	O 28	0	0
7	J	36	Total 36	O 36	0	0
7	K	34	Total 34	O 34	0	0
7	C	2	Total 2	O 2	0	0
7	F	7	Total 7	O 7	0	0
7	I	4	Total 4	O 4	0	0
7	L	3	Total 3	O 3	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: RecQ-mediated genome instability protein 1

Chain A: 




- Molecule 1: RecQ-mediated genome instability protein 1

Chain D: 




- Molecule 1: RecQ-mediated genome instability protein 1

Chain J: 




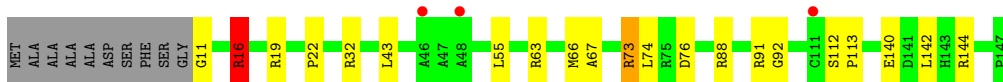
- Molecule 2: RecQ-mediated genome instability protein 2

Chain B: 

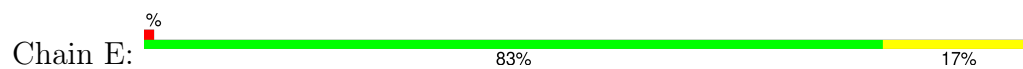


- Molecule 2: RecQ-mediated genome instability protein 2

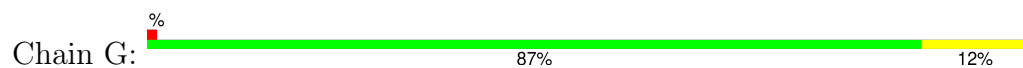
Chain K: 



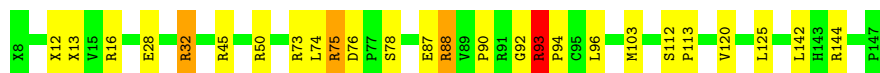
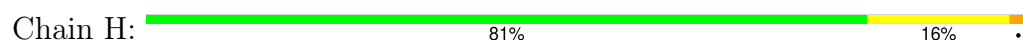
- Molecule 3: RecQ-mediated genome instability protein 2



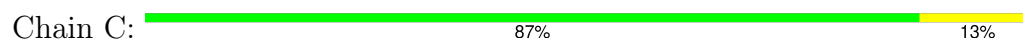
- Molecule 4: RecQ-mediated genome instability protein 1



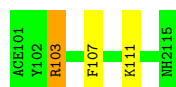
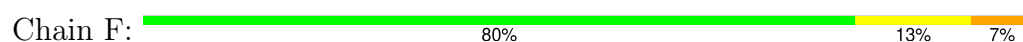
- Molecule 5: RecQ-mediated genome instability protein 2



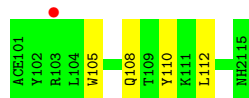
- Molecule 6: L3 peptide



- Molecule 6: L3 peptide



- Molecule 6: L3 peptide



- Molecule 6: L3 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.15Å 50.62Å 181.22Å 90.00° 118.05° 90.00°	Depositor
Resolution (Å)	48.27 – 2.35 48.27 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.27-2.35) 99.1 (48.27-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.203 , 0.247 0.204 , 0.247	Depositor DCC
R_{free} test set	3181 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18874	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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: NH2, ACE

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	0.83	0/1143	1.25	3/1542 (0.2%)
1	D	0.80	0/1163	1.20	1/1569 (0.1%)
1	J	0.82	0/1135	1.28	7/1531 (0.5%)
2	B	0.85	0/1057	1.23	5/1431 (0.3%)
2	K	0.81	0/1069	1.24	5/1448 (0.3%)
3	E	0.85	0/1052	1.27	1/1424 (0.1%)
4	G	0.84	0/1140	1.29	10/1538 (0.7%)
5	H	0.89	1/1048 (0.1%)	1.29	4/1419 (0.3%)
6	C	0.75	0/132	1.18	0/179
6	F	0.68	0/132	1.23	1/179 (0.6%)
6	I	0.65	0/132	1.59	1/179 (0.6%)
6	L	0.70	0/132	1.28	0/179
All	All	0.83	1/9335 (0.0%)	1.26	38/12618 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	4
2	K	0	5
3	E	0	8
5	H	0	7
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	76	ASP	C-O	-5.59	1.17	1.24

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	484	MET	CA-C-N	8.17	132.32	120.71
1	J	484	MET	C-N-CA	8.17	132.32	120.71
3	E	76	ASP	CA-CB-CG	7.86	120.46	112.60
1	A	484	MET	CA-C-N	7.86	131.86	120.71
1	A	484	MET	C-N-CA	7.86	131.86	120.71
1	J	485	ASP	CA-CB-CG	7.57	120.17	112.60
4	G	572	GLN	CB-CG-CD	-7.01	100.69	112.60
4	G	484	MET	CA-C-N	7.00	131.94	120.94
4	G	484	MET	C-N-CA	7.00	131.94	120.94
5	H	76	ASP	CA-CB-CG	6.93	119.53	112.60
5	H	76	ASP	O-C-N	-6.75	113.56	121.32
2	K	76	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	584	ASP	CA-CB-CG	6.52	119.12	112.60
2	K	16	ARG	NE-CZ-NH1	-6.48	115.02	121.50
4	G	485	ASP	CA-CB-CG	6.25	118.85	112.60
1	J	520	ASN	CA-CB-CG	-6.17	106.43	112.60
4	G	485	ASP	N-CA-CB	-6.12	101.35	110.17
2	B	54	ASP	CB-CA-C	5.98	119.63	109.53
2	K	11	GLY	CA-C-N	5.88	125.50	119.56
2	K	11	GLY	C-N-CA	5.88	125.50	119.56
6	I	108	GLN	CB-CA-C	-5.88	100.53	109.99
2	B	14	GLY	CA-C-N	5.83	130.45	122.34
2	B	14	GLY	C-N-CA	5.83	130.45	122.34
1	J	594	ILE	N-CA-CB	-5.75	102.01	111.44
1	J	617	GLU	CB-CG-CD	5.67	122.25	112.60
5	H	93	ARG	CB-CA-C	5.66	118.50	109.62
1	J	624	ASN	CA-CB-CG	5.52	118.12	112.60
4	G	501	LYS	CB-CA-C	5.49	115.78	111.00
2	B	87	GLU	CB-CG-CD	5.46	121.88	112.60
6	F	103	ARG	CB-CG-CD	5.40	123.71	111.30
4	G	582	GLN	CB-CG-CD	5.36	121.71	112.60
4	G	584	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	76	ASP	CA-CB-CG	5.24	117.84	112.60
4	G	582	GLN	CB-CA-C	-5.21	102.20	110.84
2	K	76	ASP	CB-CA-C	5.13	117.65	109.96
5	H	87	GLU	CB-CG-CD	5.08	121.23	112.60
1	D	507	THR	CA-CB-OG1	-5.07	101.99	109.60
4	G	558	VAL	O-C-N	-5.07	117.18	120.42

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	31	ARG	Sidechain
2	B	63	ARG	Sidechain
2	B	73	ARG	Sidechain
2	B	91	ARG	Sidechain
3	E	144	ARG	Sidechain
3	E	31	ARG	Sidechain
3	E	32	ARG	Sidechain
3	E	45	ARG	Sidechain
3	E	50	ARG	Sidechain
3	E	84	ARG	Sidechain
3	E	88	ARG	Sidechain
3	E	91	ARG	Sidechain
5	H	16	ARG	Sidechain
5	H	32	ARG	Sidechain
5	H	45	ARG	Sidechain
5	H	50	ARG	Sidechain
5	H	75	ARG	Sidechain
5	H	88	ARG	Sidechain
5	H	93	ARG	Sidechain
2	K	16	ARG	Sidechain
2	K	63	ARG	Sidechain
2	K	73	ARG	Sidechain
2	K	88	ARG	Sidechain
2	K	91	ARG	Sidechain

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	1119	1169	1169	8	0
1	D	1142	1188	1186	7	0
1	J	1117	1160	1157	8	0
2	B	1035	1049	1046	12	0
2	K	1046	1059	1056	12	0
3	E	1035	1048	1044	7	0
4	G	1127	1176	1173	7	0
5	H	1050	1053	1043	18	0
6	C	129	124	123	3	0
6	F	129	124	123	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	129	124	123	4	0
6	L	129	124	123	1	0
7	A	39	0	0	0	0
7	B	34	0	0	1	0
7	C	2	0	0	0	0
7	D	48	0	0	0	0
7	E	20	0	0	0	0
7	F	7	0	0	0	0
7	G	34	0	0	1	0
7	H	28	0	0	1	0
7	I	4	0	0	0	0
7	J	36	0	0	1	0
7	K	34	0	0	0	0
7	L	3	0	0	2	0
All	All	9476	9398	9366	73	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 (73) 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:A:484:MET:HE2	1:A:492:VAL:HG12	1.53	0.86
5:H:12:UNK:O	5:H:13:UNK:O	1.97	0.82
2:K:19:ARG:HG3	7:L:203:HOH:O	1.86	0.74
2:B:31:ARG:HD3	7:B:223:HOH:O	1.88	0.71
4:G:579:GLN:O	4:G:582:GLN:HB3	1.96	0.66
5:H:93:ARG:NH1	5:H:94:PRO:HD2	2.10	0.65
2:B:43:LEU:HB2	2:B:55:LEU:HD22	1.81	0.62
2:B:41:TRP:HB2	2:B:55:LEU:O	1.98	0.62
5:H:12:UNK:O	5:H:13:UNK:C	2.50	0.60
2:K:66:MET:HG2	2:K:67:ALA:N	2.15	0.60
5:H:88:ARG:HG2	5:H:88:ARG:HH11	1.67	0.59
5:H:28:GLU:HG2	5:H:78:SER:HB2	1.85	0.59
1:A:520:ASN:OD1	6:C:105:TRP:HH2	1.86	0.59
5:H:93:ARG:HH11	5:H:94:PRO:HD2	1.69	0.58
2:K:19:ARG:CG	7:L:203:HOH:O	2.49	0.58
1:D:582[A]:GLN:HG3	6:F:107:PHE:CD2	2.39	0.57
5:H:120:VAL:HA	6:I:112:LEU:HD13	1.88	0.56
1:D:582[B]:GLN:HG2	6:F:107:PHE:CE2	2.41	0.56
4:G:587:ASP:OD1	5:H:92:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG21	2:B:122:MET:HE2	1.89	0.55
3:E:67:ALA:HB1	3:E:96:LEU:HD22	1.88	0.55
4:G:572:GLN:O	4:G:576:GLU:HG3	2.05	0.54
2:B:112:SER:HA	2:B:113:PRO:C	2.33	0.54
1:A:484:MET:HE1	1:A:492:VAL:HA	1.90	0.53
1:A:484:MET:CE	1:A:492:VAL:HG12	2.34	0.53
5:H:12:UNK:CA	6:I:105:TRP:CD1	2.91	0.53
4:G:562:LYS:NZ	7:G:702:HOH:O	2.41	0.53
1:J:594:ILE:HG23	1:J:603:ALA:HB1	1.90	0.52
1:D:564:SER:HA	1:D:570:GLN:HE21	1.75	0.50
1:J:494:LEU:O	1:J:498:MET:HG2	2.11	0.50
4:G:600:LEU:HD23	4:G:602:LYS:HE2	1.94	0.49
1:A:537:GLY:HA2	2:B:22:PRO:O	2.13	0.48
5:H:112:SER:HA	5:H:113:PRO:C	2.40	0.47
1:D:582[B]:GLN:HG2	6:F:107:PHE:CZ	2.49	0.47
2:B:16:ARG:HD3	6:C:101:ACE:O	2.13	0.47
2:K:112:SER:HA	2:K:113:PRO:C	2.40	0.47
2:B:28:GLU:HG3	2:B:29:GLN:N	2.29	0.47
1:A:520:ASN:OD1	6:C:105:TRP:CH2	2.68	0.47
1:D:527:ILE:HB	1:D:547:ASP:HB2	1.97	0.46
1:J:484:MET:HE3	1:J:492:VAL:HG12	1.98	0.46
1:J:509:LYS:HE3	7:J:705:HOH:O	2.15	0.46
4:G:527:ILE:HB	4:G:547:ASP:HB2	1.98	0.46
5:H:73:ARG:C	5:H:74:LEU:HD12	2.41	0.46
1:J:537:GLY:HA2	2:K:22:PRO:O	2.17	0.44
3:E:95:CYS:HB3	3:E:124:ASP:HB2	1.99	0.44
5:H:120:VAL:HG13	6:I:112:LEU:CD1	2.48	0.44
2:B:34:ALA:O	1:D:569:LEU:HD21	2.18	0.44
3:E:146:ILE:HA	3:E:147:PRO:HD3	1.86	0.43
1:A:587:ASP:OD1	2:B:92:GLY:HA3	2.18	0.43
3:E:112:SER:HA	3:E:113:PRO:C	2.44	0.43
5:H:90:PRO:HG3	6:I:110:TYR:CD2	2.54	0.43
1:J:594:ILE:HG23	1:J:603:ALA:CB	2.49	0.43
1:J:604:MET:HE2	1:J:604:MET:HB2	1.93	0.43
6:F:103:ARG:HD2	6:F:111:LYS:HG2	2.00	0.42
5:H:73:ARG:HH21	5:H:73:ARG:HD3	1.67	0.42
2:K:16:ARG:HD3	6:L:101:ACE:O	2.19	0.42
1:J:587:ASP:OD1	2:K:92:GLY:HA3	2.20	0.42
2:K:140:GLU:O	2:K:144:ARG:HG3	2.20	0.42
2:B:73:ARG:C	2:B:74:LEU:HD12	2.45	0.42
5:H:75:ARG:HD3	7:H:222:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:103:MET:HE3	5:H:103:MET:HB2	1.99	0.41
2:K:43:LEU:HB2	2:K:55:LEU:HD22	2.03	0.41
3:E:42:ARG:HA	3:E:53:LEU:O	2.21	0.41
5:H:125:LEU:HD23	5:H:125:LEU:HA	1.91	0.41
3:E:56:ALA:O	3:E:107:VAL:HG13	2.19	0.41
1:A:484:MET:HE2	1:A:492:VAL:CG1	2.39	0.41
2:K:32:ARG:O	2:K:32:ARG:HG2	2.21	0.41
2:K:142:LEU:C	2:K:142:LEU:HD23	2.46	0.41
3:E:142:LEU:HD23	3:E:142:LEU:C	2.46	0.40
5:H:142:LEU:HD23	5:H:142:LEU:C	2.46	0.40
2:B:35:GLU:OE2	1:D:572:GLN:HG2	2.21	0.40
2:K:73:ARG:C	2:K:74:LEU:HD12	2.46	0.40
4:G:557:SER:HB2	4:G:559:PRO:HD2	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	142/152 (93%)	139 (98%)	3 (2%)	0	100	100
1	D	145/152 (95%)	142 (98%)	3 (2%)	0	100	100
1	J	141/152 (93%)	137 (97%)	4 (3%)	0	100	100
2	B	133/147 (90%)	125 (94%)	8 (6%)	0	100	100
2	K	135/147 (92%)	127 (94%)	8 (6%)	0	100	100
3	E	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
4	G	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
5	H	131/139 (94%)	124 (95%)	7 (5%)	0	100	100
6	C	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
6	F	13/15 (87%)	11 (85%)	2 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	I	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
6	L	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	1153/1229 (94%)	1101 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	132/139 (95%)	131 (99%)	1 (1%)	79	88
1	D	134/139 (96%)	133 (99%)	1 (1%)	81	89
1	J	131/139 (94%)	130 (99%)	1 (1%)	79	88
2	B	109/115 (95%)	108 (99%)	1 (1%)	75	85
2	K	110/115 (96%)	110 (100%)	0	100	100
3	E	109/109 (100%)	108 (99%)	1 (1%)	75	85
4	G	131/131 (100%)	129 (98%)	2 (2%)	60	73
5	H	109/109 (100%)	106 (97%)	3 (3%)	38	49
6	C	13/13 (100%)	13 (100%)	0	100	100
6	F	13/13 (100%)	13 (100%)	0	100	100
6	I	13/13 (100%)	13 (100%)	0	100	100
6	L	13/13 (100%)	13 (100%)	0	100	100
All	All	1017/1048 (97%)	1007 (99%)	10 (1%)	73	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	604	MET
2	B	144	ARG
1	D	501	LYS
3	E	28	GLU

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Mol	Chain	Res	Type
4	G	503	LYS
4	G	544	ASP
5	H	32	ARG
5	H	96	LEU
5	H	144	ARG
1	J	614	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	563	GLN
1	A	579	GLN
1	D	570	GLN
1	D	618	ASN
4	G	582	GLN
1	J	570	GLN
1	J	579	GLN
1	J	582	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1
5	H	1
4	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	12:UNK	C	14:GLY	N	4.18
1	H	13:UNK	C	15:VAL	N	4.18
1	G	479:UNK	C	482:ILE	N	3.44

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	142/152 (93%)	-0.48	0 100 100	21, 34, 61, 81	2 (1%)
1	D	145/152 (95%)	-0.53	2 (1%) 73 77	15, 31, 63, 85	2 (1%)
1	J	142/152 (93%)	-0.55	0 100 100	15, 32, 59, 75	1 (0%)
2	B	135/147 (91%)	-0.10	5 (3%) 45 52	22, 38, 83, 97	0
2	K	137/147 (93%)	-0.10	3 (2%) 62 67	22, 39, 87, 105	0
3	E	134/135 (99%)	-0.22	1 (0%) 84 86	24, 38, 74, 90	0
4	G	144/145 (99%)	-0.48	1 (0%) 84 86	23, 35, 59, 75	0
5	H	133/139 (95%)	-0.29	0 100 100	23, 39, 66, 97	0
6	C	13/15 (86%)	-0.33	0 100 100	23, 35, 60, 67	0
6	F	13/15 (86%)	-0.29	0 100 100	27, 35, 54, 69	0
6	I	13/15 (86%)	0.85	1 (7%) 21 24	37, 53, 70, 83	0
6	L	13/15 (86%)	-0.58	0 100 100	25, 34, 53, 63	0
All	All	1164/1229 (94%)	-0.34	13 (1%) 77 82	15, 36, 74, 105	5 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	481	SER	4.6
2	B	13	ALA	4.4
4	G	482	ILE	3.5
1	D	482	ILE	3.4
3	E	47	ALA	3.0
2	B	14	GLY	2.6
6	I	103	ARG	2.3
2	K	46	ALA	2.2
2	K	111	CYS	2.2
2	K	48	ALA	2.1
2	B	52	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	53	LEU	2.1
2	B	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.