



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:46 AM UTC

PDB ID : 7MNM / pdb_00007mnm
Title : Crystal structure of the N-terminal domain of NUP358/RanBP2 (residues 1-752) T585M mutant in complex with Fab fragment
Authors : Bley, C.J.; Nie, S.; Mobbs, G.W.; Petrovic, S.; Gres, A.T.; Liu, X.; Mukherjee, S.; Harvey, S.; Huber, F.M.; Lin, D.H.; Brown, B.; Tang, A.W.; Rundlet, E.J.; Correia, A.R.; Chen, S.; Regmi, S.G.; Stevens, T.A.; Jette, C.A.; Dasso, M.; Patke, A.; Palazzo, A.F.; Kossiakoff, A.A.; Hoelz, A.
Deposited on : 2021-05-01
Resolution : 4.70 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

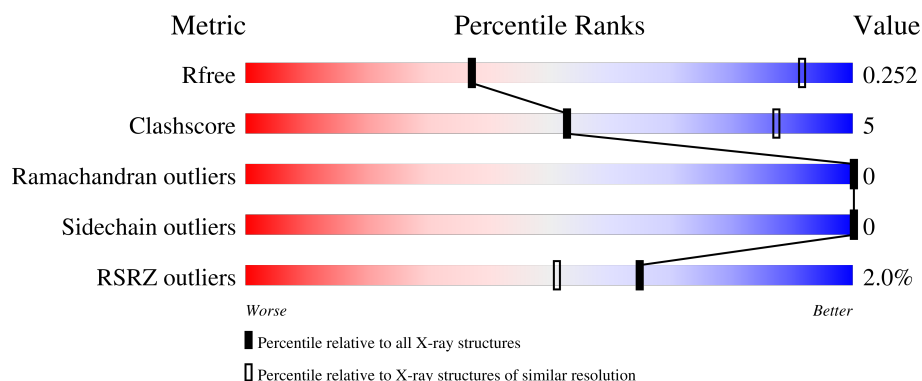
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

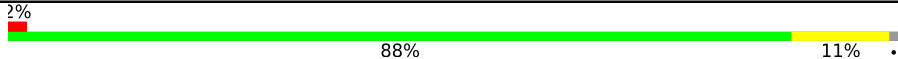
The reported resolution of this entry is 4.70 Å.

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	1020 (5.48-3.92)
Clashscore	190562	1005 (5.40-3.96)
Ramachandran outliers	187476	1095 (5.50-3.90)
Sidechain outliers	187428	1077 (5.50-3.90)
RSRZ outliers	180081	1015 (5.48-3.92)

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	753	
1	B	753	
2	H	240	
2	K	240	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	215	2% 93% 7%
3	M	215	2% 93% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34746 atoms, of which 17293 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 E3 SUMO-protein ligase RanBP2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	746	Total	C	H	N	O	S	0	0	0
			12030	3817	6023	1036	1125	29			
1	B	602	Total	C	H	N	O	S	0	0	0
			9652	3059	4832	835	902	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P49792
A	585	MET	THR	engineered mutation	UNP P49792
A	599	MET	ILE	engineered mutation	UNP P49792
B	0	SER	-	expression tag	UNP P49792
B	585	MET	THR	engineered mutation	UNP P49792
B	599	MET	ILE	engineered mutation	UNP P49792

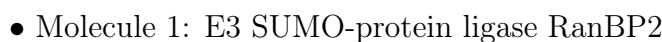
- Molecule 2 is a protein called Antibody Fab14 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	227	Total	C	H	N	O	S	0	0	0
			3329	1072	1636	282	334	5			
2	K	227	Total	C	H	N	O	S	0	0	0
			3329	1072	1636	282	334	5			

- Molecule 3 is a protein called Antibody Fab14 Light Chain.

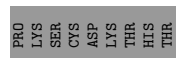
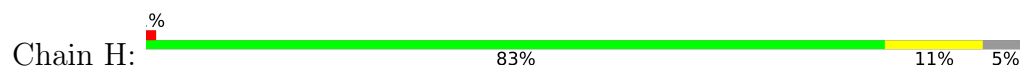
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	213	Total	C	H	N	O	S	0	0	0
			3203	1009	1583	273	333	5			
3	M	213	Total	C	H	N	O	S	0	0	0
			3203	1009	1583	273	333	5			

- Molecule 1: E3 SUMO-protein ligase RanBP2

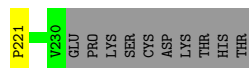
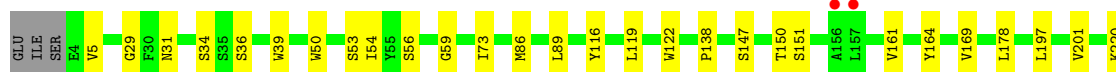
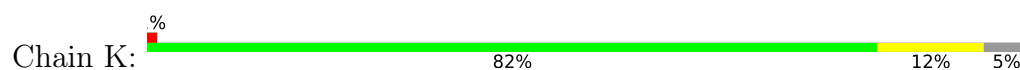




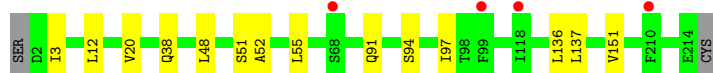
• Molecule 2: Antibody Fab14 Heavy Chain



• Molecule 2: Antibody Fab14 Heavy Chain



• Molecule 3: Antibody Fab14 Light Chain



• Molecule 3: Antibody Fab14 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	160.41 Å 160.41 Å 642.17 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 4.70 29.86 – 4.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.86-4.70) 99.3 (29.86-4.70)	Depositor EDS
R_{merge}	0.59	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.61 Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.204 , 0.254 0.205 , 0.252	Depositor DCC
R_{free} test set	1304 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	228.4	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 276.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	34746	wwPDB-VP
Average B, all atoms (Å ²)	270.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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	0.11	0/6130	0.28	0/8289
1	B	0.12	0/4917	0.32	0/6655
2	H	0.11	0/1738	0.29	0/2370
2	K	0.11	0/1738	0.29	0/2370
3	L	0.11	0/1652	0.28	0/2241
3	M	0.11	0/1652	0.28	0/2241
All	All	0.11	0/17827	0.30	0/24166

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6007	6023	6022	58	0
1	B	4820	4832	4831	67	0
2	H	1693	1636	1636	18	0
2	K	1693	1636	1636	22	0
3	L	1620	1583	1583	10	0
3	M	1620	1583	1583	8	0
All	All	17453	17293	17291	173	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 5.

All (173) 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:B:677:VAL:HG21	1:B:731:VAL:HG13	1.48	0.96
1:B:158:LEU:CD1	1:B:171:LEU:HD22	2.07	0.84
1:A:677:VAL:HG21	1:A:731:VAL:HG13	1.65	0.77
2:H:54:ILE:HD11	2:H:73:ILE:HG23	1.66	0.75
1:A:472:GLU:HG2	1:A:473:THR:HG23	1.69	0.74
2:K:54:ILE:HD11	2:K:73:ILE:HG23	1.68	0.74
1:A:385:LEU:HD23	1:A:401:LEU:HD11	1.69	0.73
1:A:371:GLU:O	1:A:375:THR:HG22	1.91	0.70
1:B:158:LEU:HD11	1:B:171:LEU:HD22	1.73	0.70
1:B:371:GLU:O	1:B:375:THR:HG22	1.93	0.69
1:A:406:ILE:HG23	1:A:409:ILE:HD11	1.75	0.67
1:A:541:ARG:NH2	2:H:56:SER:O	2.28	0.67
2:K:116:TYR:HD2	3:M:97:ILE:HD11	1.60	0.66
1:A:357:MET:HE1	1:A:514:CYS:O	1.95	0.66
1:A:482:LEU:HD13	1:A:601:ARG:HG3	1.77	0.66
1:A:158:LEU:HD23	1:A:158:LEU:O	1.99	0.63
1:A:468:THR:HG21	1:A:478:SER:HB2	1.81	0.62
2:H:39:TRP:HD1	2:H:73:ILE:HD12	1.64	0.62
1:B:157:GLU:CB	1:B:167:VAL:HG11	2.30	0.62
1:B:360:ASN:ND2	1:B:443:GLN:OE1	2.33	0.61
1:A:161:ARG:NH2	1:A:164:ASP:OD2	2.32	0.61
1:B:468:THR:HG21	1:B:478:SER:HB2	1.81	0.61
1:B:482:LEU:HD13	1:B:601:ARG:HG3	1.82	0.61
1:B:599:MET:HE1	1:B:653:THR:HG23	1.82	0.61
3:L:3:ILE:HG21	3:L:91:GLN:OE1	2.01	0.61
1:A:368:PHE:CZ	1:A:372:ILE:HD11	2.36	0.60
1:A:609:VAL:HG12	1:A:613:LEU:HG	1.84	0.59
1:A:222:GLU:OE1	1:B:388:ALA:HA	2.03	0.58
1:B:541:ARG:NH2	2:K:56:SER:O	2.37	0.58
2:K:39:TRP:HD1	2:K:73:ILE:HD12	1.70	0.57
2:H:169:VAL:CG2	2:H:197:LEU:HD21	2.33	0.57
1:B:263:ASP:OD1	1:B:264:SER:N	2.38	0.57
2:K:150:THR:HG23	2:K:151:SER:N	2.21	0.56
2:K:116:TYR:CD2	3:M:97:ILE:HD11	2.40	0.56
1:B:321:LEU:HD22	1:B:369:LEU:HD11	1.88	0.55
1:B:157:GLU:HB3	1:B:167:VAL:HG11	1.88	0.55
1:B:368:PHE:CZ	1:B:372:ILE:HD11	2.42	0.55
1:B:652:ILE:HD13	1:B:678:VAL:CG1	2.38	0.54
1:A:699:LEU:HD12	1:A:700:SER:O	2.08	0.54
2:H:153:GLY:O	2:H:205:SER:N	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:LEU:HD12	1:A:465:PRO:HD2	1.90	0.54
1:B:157:GLU:HB2	1:B:167:VAL:HG11	1.90	0.54
1:B:154:ILE:HG21	1:B:171:LEU:HB2	1.90	0.53
1:A:599:MET:HE1	1:A:653:THR:HG23	1.90	0.53
2:K:169:VAL:CG2	2:K:197:LEU:HD21	2.39	0.53
1:A:221:LEU:HD22	1:B:308:GLN:OE1	2.09	0.53
1:B:370:LYS:HA	1:B:411:VAL:HG21	1.89	0.53
2:H:5:VAL:HG22	2:H:29:GLY:HA3	1.91	0.52
1:A:439:TRP:CG	1:A:517:LEU:HD13	2.44	0.52
1:B:171:LEU:HD23	1:B:187:HIS:CD2	2.44	0.52
1:A:188:CYS:SG	1:A:207:VAL:HG22	2.50	0.52
1:A:499:LEU:HD11	1:A:523:LEU:HD22	1.92	0.51
1:A:589:LEU:HD13	1:A:594:ASP:HB3	1.92	0.51
3:M:151:VAL:O	3:M:151:VAL:HG23	2.11	0.51
2:K:147:SER:OG	2:K:150:THR:HG22	2.10	0.51
1:B:154:ILE:HG21	1:B:171:LEU:HD13	1.93	0.51
3:L:151:VAL:O	3:L:151:VAL:HG23	2.10	0.51
2:K:150:THR:HG23	2:K:151:SER:H	1.75	0.51
1:B:306:ASN:OD1	1:B:307:VAL:N	2.43	0.50
1:B:228:TRP:CZ3	1:B:272:LEU:HD22	2.46	0.50
2:H:54:ILE:HG23	2:H:59:GLY:HA2	1.93	0.50
1:B:360:ASN:OD1	1:B:513:LEU:HD11	2.11	0.50
3:M:12:LEU:HD21	3:M:20:VAL:HG13	1.94	0.50
1:A:315:LEU:HD21	1:A:385:LEU:HA	1.93	0.49
1:B:357:MET:HE1	1:B:514:CYS:O	2.13	0.49
2:H:7:LEU:HD23	2:H:27:ALA:HA	1.94	0.49
1:A:575:LEU:HB3	1:A:609:VAL:CG2	2.42	0.49
1:A:599:MET:HE2	1:A:656:ILE:HB	1.95	0.48
1:B:482:LEU:O	1:B:486:VAL:HG23	2.13	0.48
1:B:544:VAL:O	1:B:548:VAL:HG23	2.13	0.48
2:K:5:VAL:HG22	2:K:29:GLY:HA3	1.95	0.48
1:A:233:THR:HG22	1:A:278:LEU:HA	1.95	0.48
1:B:385:LEU:HD23	1:B:401:LEU:HD11	1.94	0.48
3:L:55:LEU:HD12	3:L:55:LEU:O	2.14	0.48
2:H:197:LEU:C	2:H:197:LEU:HD12	2.40	0.47
1:A:330:LYS:HB2	1:A:333:LEU:HD12	1.97	0.47
1:A:568:HIS:O	1:A:568:HIS:ND1	2.48	0.47
1:B:359:LEU:HD21	1:B:414:PRO:HG2	1.97	0.47
3:M:136:LEU:C	3:M:137:LEU:HD12	2.40	0.47
1:A:12:ILE:HG21	1:A:393:GLN:OE1	2.14	0.47
1:B:700:SER:OG	1:B:703:GLU:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASN:OD1	1:A:379:LYS:N	2.49	0.46
3:L:136:LEU:C	3:L:137:LEU:HD12	2.40	0.46
2:K:36:SER:OG	2:K:56:SER:N	2.48	0.46
1:B:244:LEU:HD11	1:B:430:HIS:NE2	2.29	0.46
1:A:699:LEU:HD12	1:A:699:LEU:C	2.41	0.46
1:B:427:ILE:HD11	1:B:456:TRP:CG	2.51	0.46
2:K:31:ASN:ND2	2:K:34:SER:OG	2.48	0.46
1:B:411:VAL:HG22	1:B:411:VAL:O	2.16	0.46
3:M:51:SER:O	3:M:52:ALA:HB3	2.16	0.46
1:A:113:ARG:N	1:B:375:THR:OG1	2.49	0.46
1:B:381:GLY:O	1:B:385:LEU:N	2.43	0.46
3:M:38:GLN:HB2	3:M:48:LEU:HD11	1.98	0.46
1:B:356:HIS:O	1:B:360:ASN:ND2	2.48	0.45
1:B:368:PHE:CE1	1:B:372:ILE:HD11	2.52	0.45
1:B:468:THR:HG22	1:B:470:ARG:H	1.81	0.45
2:K:164:TYR:CE2	2:K:169:VAL:HG13	2.51	0.45
1:A:285:MET:HE1	1:A:346:MET:HE2	1.98	0.45
1:B:609:VAL:HG12	1:B:613:LEU:HG	1.98	0.45
1:B:314:GLU:HG2	1:B:372:ILE:HD11	1.99	0.45
1:B:483:ASP:OD1	1:B:601:ARG:NH2	2.48	0.45
3:L:51:SER:O	3:L:52:ALA:HB3	2.17	0.45
1:A:541:ARG:O	1:A:541:ARG:HG2	2.16	0.45
1:B:215:LEU:HD11	1:B:235:LEU:HD22	1.98	0.45
2:H:36:SER:OG	2:H:56:SER:N	2.50	0.44
1:A:544:VAL:O	1:A:548:VAL:HG23	2.17	0.44
1:B:541:ARG:O	1:B:541:ARG:HG2	2.18	0.44
1:B:464:LEU:HD12	1:B:465:PRO:HD2	1.98	0.44
2:H:178:LEU:HD21	2:H:201:VAL:HG21	2.00	0.44
1:A:111:ASP:OD2	1:A:179:LYS:NZ	2.50	0.44
3:L:12:LEU:HD21	3:L:20:VAL:HG13	1.98	0.44
1:A:285:MET:HE1	1:A:346:MET:CE	2.47	0.44
1:A:297:LEU:HG	1:A:389:LEU:HD21	1.99	0.44
1:B:499:LEU:HD11	1:B:523:LEU:HD22	1.99	0.44
1:A:157:GLU:OE2	1:A:161:ARG:NH1	2.50	0.44
1:A:322:ILE:O	1:A:326:VAL:HG23	2.18	0.44
2:H:116:TYR:HD2	3:L:97:ILE:HD11	1.82	0.44
2:K:178:LEU:HD21	2:K:201:VAL:HG21	2.00	0.44
1:A:609:VAL:O	1:A:612:LEU:N	2.51	0.44
1:B:575:LEU:HB3	1:B:609:VAL:CG2	2.47	0.44
1:A:517:LEU:HB3	1:A:518:PRO:HD3	2.00	0.43
1:B:511:GLN:N	1:B:512:PRO:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:OD1	1:A:95:ASP:N	2.49	0.43
2:H:113:GLY:HA3	3:L:94:SER:HB2	1.99	0.43
1:B:605:TYR:O	1:B:609:VAL:HG23	2.18	0.43
2:K:178:LEU:HD21	2:K:201:VAL:HG11	2.00	0.43
2:K:197:LEU:HD12	2:K:197:LEU:C	2.44	0.43
2:K:50:TRP:NE1	2:K:53:SER:OG	2.42	0.43
1:B:365:LYS:HB2	1:B:368:PHE:HB2	2.01	0.43
1:B:214:TYR:CD2	1:B:231:THR:HG21	2.54	0.43
1:B:410:ASP:O	1:B:411:VAL:HG12	2.19	0.43
3:M:109:ARG:HG2	3:M:110:THR:N	2.34	0.43
1:A:411:VAL:O	1:A:411:VAL:HG22	2.18	0.42
3:L:38:GLN:HB2	3:L:48:LEU:HD11	2.01	0.42
1:B:457:LEU:HD13	1:B:484:LEU:HB2	2.01	0.42
1:A:158:LEU:HD23	1:A:158:LEU:C	2.44	0.42
2:H:86:MET:HB3	2:H:89:LEU:HD21	2.01	0.42
2:H:112:GLY:O	3:L:94:SER:HB2	2.20	0.42
2:K:220:LYS:N	2:K:221:PRO:CD	2.83	0.42
1:A:109:VAL:O	1:A:109:VAL:HG12	2.19	0.42
1:B:214:TYR:CE2	1:B:231:THR:HG21	2.54	0.42
1:B:478:SER:O	1:B:563:ARG:NH2	2.52	0.42
1:A:486:VAL:HG13	1:A:578:TRP:CD2	2.55	0.42
1:A:599:MET:HE2	1:A:656:ILE:CG2	2.49	0.42
1:B:171:LEU:HD11	1:B:175:TYR:CZ	2.55	0.42
2:H:157:LEU:HD13	2:H:230:VAL:HG21	2.02	0.42
2:K:119:LEU:HD12	2:K:122:TRP:CZ2	2.55	0.42
1:A:613:LEU:O	1:A:617:LYS:N	2.49	0.41
2:K:86:MET:HB3	2:K:89:LEU:HD21	2.02	0.41
2:H:101:ARG:CZ	2:H:103:PRO:HG3	2.50	0.41
1:B:214:TYR:O	1:B:220:CYS:HB2	2.21	0.41
1:A:360:ASN:ND2	1:A:443:GLN:OE1	2.53	0.41
1:B:571:GLN:NE2	1:B:633:PHE:O	2.48	0.41
1:B:213:GLU:O	1:B:217:SER:HB3	2.20	0.41
1:B:568:HIS:O	1:B:568:HIS:ND1	2.53	0.41
1:A:382:GLN:CG	1:A:406:ILE:HD12	2.50	0.41
1:A:467:GLU:OE2	1:A:471:LEU:HD13	2.21	0.41
1:B:378:ASN:OD1	1:B:379:LYS:N	2.53	0.41
1:A:410:ASP:O	1:A:411:VAL:HG12	2.21	0.41
1:A:468:THR:HG22	1:A:470:ARG:H	1.84	0.41
1:A:572:PRO:HB2	1:A:638:ILE:HD12	2.01	0.41
1:B:154:ILE:CG2	1:B:171:LEU:HB2	2.51	0.41
1:B:352:SER:HB2	1:B:423:ASP:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:54:ILE:HG23	2:K:59:GLY:HA2	2.02	0.41
2:K:138:PRO:HB2	2:K:161:VAL:HG13	2.03	0.41
1:A:222:GLU:HG3	1:A:223:SER:N	2.36	0.41
1:A:694:ILE:O	1:A:694:ILE:HG22	2.20	0.41
1:B:296:LEU:HD23	1:B:296:LEU:C	2.45	0.40
1:B:160:VAL:O	1:B:160:VAL:HG12	2.21	0.40
1:A:482:LEU:O	1:A:486:VAL:HG23	2.21	0.40
1:B:154:ILE:HD13	1:B:171:LEU:HA	2.03	0.40
1:B:579:ALA:HB1	1:B:606:TRP:NE1	2.37	0.40
2:H:220:LYS:N	2:H:221:PRO:CD	2.85	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	742/753 (98%)	731 (98%)	11 (2%)	0	100	100
1	B	598/753 (79%)	588 (98%)	10 (2%)	0	100	100
2	H	225/240 (94%)	219 (97%)	6 (3%)	0	100	100
2	K	225/240 (94%)	220 (98%)	5 (2%)	0	100	100
3	L	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
3	M	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
All	All	2212/2416 (92%)	2175 (98%)	37 (2%)	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	666/673 (99%)	666 (100%)	0	100	100
1	B	539/673 (80%)	539 (100%)	0	100	100
2	H	187/200 (94%)	187 (100%)	0	100	100
2	K	187/200 (94%)	187 (100%)	0	100	100
3	L	188/190 (99%)	188 (100%)	0	100	100
3	M	188/190 (99%)	188 (100%)	0	100	100
All	All	1955/2126 (92%)	1955 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	303	HIS
1	A	360	ASN
1	A	382	GLN
1	A	466	HIS
1	A	498	GLN
1	A	632	HIS
1	B	583	GLN
1	B	688	HIS
2	H	87	ASN
2	H	183	HIS
3	L	80	GLN
2	K	85	GLN
2	K	87	ASN
3	M	80	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	746/753 (99%)	0.29	15 (2%) 65 51	186, 263, 335, 414	0
1	B	602/753 (79%)	0.32	17 (2%) 55 44	196, 265, 361, 413	0
2	H	227/240 (94%)	0.12	3 (1%) 75 60	192, 250, 302, 357	0
2	K	227/240 (94%)	0.16	2 (0%) 81 66	215, 271, 345, 399	0
3	L	213/215 (99%)	0.14	4 (1%) 66 52	195, 262, 309, 327	0
3	M	213/215 (99%)	0.21	4 (1%) 66 52	212, 286, 338, 361	0
All	All	2228/2416 (92%)	0.25	45 (2%) 65 51	186, 264, 345, 414	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	ALA	4.0
3	M	210	PHE	4.0
1	B	385	LEU	3.9
1	B	154	ILE	3.7
1	B	312	LEU	3.6
1	B	315	LEU	3.5
3	L	118	ILE	3.3
1	A	132	TYR	3.1
1	A	167	VAL	3.1
1	A	290	TYR	2.9
1	B	389	LEU	2.8
1	B	569	GLY	2.7
1	A	134	LEU	2.6
3	M	114	PRO	2.6
1	A	577	HIS	2.5
3	L	210	PHE	2.5
1	A	318	LEU	2.5
2	K	157	LEU	2.5
1	B	314	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	193	ARG	2.4
2	H	145	PRO	2.4
3	L	68	SER	2.4
3	M	120	PRO	2.4
1	A	681	TRP	2.3
1	A	461	PHE	2.3
2	K	156	ALA	2.3
2	H	118	ALA	2.3
3	M	88	TYR	2.2
1	A	437	LEU	2.2
1	A	460	LEU	2.2
1	B	155	GLN	2.2
1	B	290	TYR	2.2
1	B	557	HIS	2.2
2	H	230	VAL	2.2
1	A	469	SER	2.2
3	L	99	PHE	2.2
1	B	318	LEU	2.2
1	B	479	ILE	2.1
1	B	172	VAL	2.1
1	B	169	ILE	2.1
1	A	353	GLN	2.1
1	A	532	TRP	2.1
1	A	135	LYS	2.1
1	B	376	PHE	2.1
1	A	289	PHE	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.