



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:36 AM UTC

PDB ID : 7MNO / pdb_00007mno
Title : Crystal structure of the N-terminal domain of NUP358/RanBP2 (residues 1-752) I656V mutant in complex with Fab fragment
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Deposited on : 2021-05-01
Resolution : 6.73 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

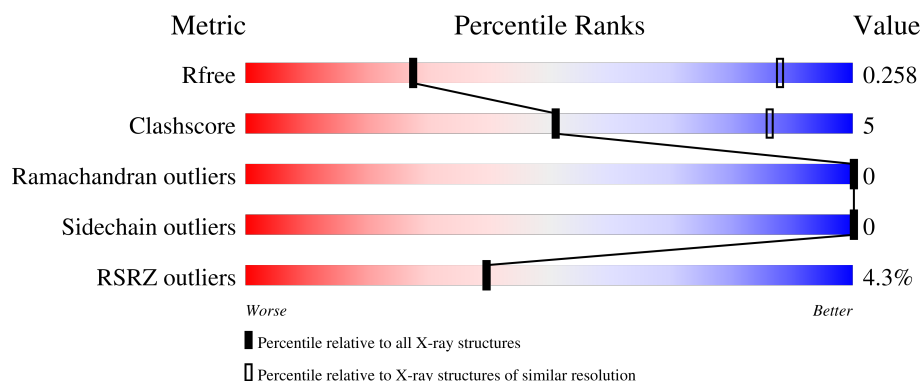
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.73 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	1163 (9.44-4.00)
Clashscore	190562	1003 (9.44-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1156 (9.44-4.00)

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	5% 88% 11% .
1	B	753	5% 68% 12% 20%
2	H	240	% 81% 14% 5%
2	K	240	3% 79% 16% 5%

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Mol	Chain	Length	Quality of chain
3	L	215	3% 90% 9%
3	M	215	3% 92% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34781 atoms, of which 17307 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
			12024	3815	6019	1036	1126	28			
1	B	604	Total	C	H	N	O	S	0	0	0
			9693	3073	4850	839	908	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P49792
A	599	MET	ILE	engineered mutation	UNP P49792
A	656	VAL	ILE	engineered mutation	UNP P49792
B	0	SER	-	expression tag	UNP P49792
B	599	MET	ILE	engineered mutation	UNP P49792
B	656	VAL	ILE	engineered mutation	UNP P49792

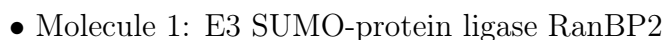
- Molecule 2 is a protein called Antibody Fab14 Heavy Chain.

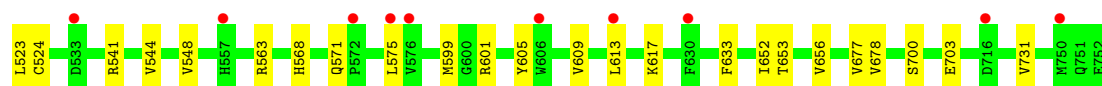
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	227	Total	C	H	N	O	S	0	0	0
			3329	1072	1636	282	334	5			
2	K	227	Total	C	H	N	O	S	0	0	0
			3329	1072	1636	282	334	5			

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

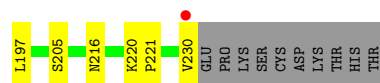
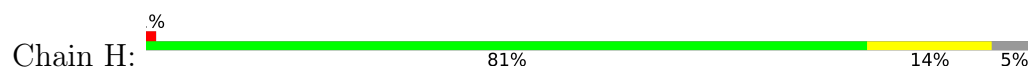
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	213	Total	C	H	N	O	S	0	0	0
			3203	1009	1583	273	333	5			
3	M	213	Total	C	H	N	O	S	0	0	0
			3203	1009	1583	273	333	5			

- Molecule 1: E3 SUMO-protein ligase RanBP2

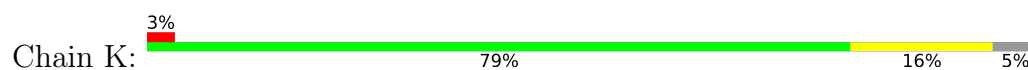




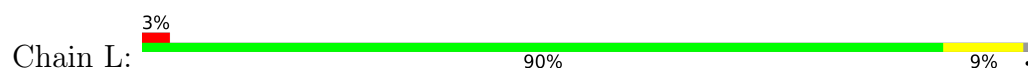
• Molecule 2: Antibody Fab14 Heavy Chain



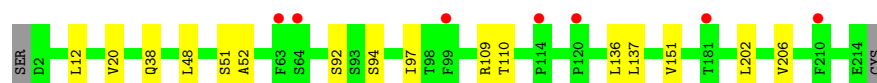
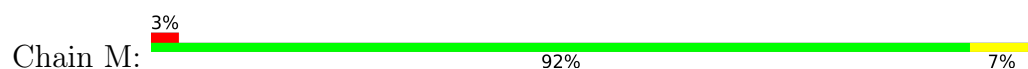
• Molecule 2: Antibody Fab14 Heavy Chain



• 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	161.56Å 161.56Å 645.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.05 – 6.73 30.05 – 6.73	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.05-6.73) 98.2 (30.05-6.73)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 6.58Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.205 , 0.254 0.206 , 0.258	Depositor DCC
R_{free} test set	445 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	370.1	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 386.5	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	0.83	EDS
Total number of atoms	34781	wwPDB-VP
Average B, all atoms (Å ²)	348.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.11	0/6128	0.31	0/8288
1	B	0.11	0/4942	0.33	0/6691
2	H	0.11	0/1738	0.31	0/2370
2	K	0.12	0/1738	0.33	0/2370
3	L	0.12	0/1652	0.31	0/2241
3	M	0.11	0/1652	0.32	0/2241
All	All	0.12	0/17850	0.32	0/24201

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	6005	6019	6018	54	0
1	B	4843	4850	4848	64	0
2	H	1693	1636	1636	23	0
2	K	1693	1636	1636	28	0
3	L	1620	1583	1583	14	0
3	M	1620	1583	1583	12	0
All	All	17474	17307	17304	182	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 (182) 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	1.55	0.86
1:A:677:VAL:HG21	1:A:731:VAL:HG13	1.61	0.80
2:K:116:TYR:HD2	3:M:97:ILE:HD11	1.45	0.78
1:A:472:GLU:HG2	1:A:473:THR:HG23	1.69	0.74
1:A:385:LEU:HD23	1:A:401:LEU:HD11	1.71	0.73
1:B:154:ILE:HG21	1:B:171:LEU:HB2	1.69	0.72
2:K:54:ILE:HD11	2:K:73:ILE:HG23	1.72	0.71
1:A:499:LEU:HD11	1:A:523:LEU:HD22	1.74	0.70
2:H:54:ILE:HD11	2:H:73:ILE:HG23	1.73	0.69
1:A:406:ILE:HG23	1:A:409:ILE:HD11	1.76	0.68
1:A:541:ARG:NH2	2:H:56:SER:O	2.26	0.67
1:A:222:GLU:OE1	1:B:388:ALA:HA	1.96	0.65
1:B:468:THR:HG21	1:B:478:SER:HB2	1.77	0.65
1:B:158:LEU:HD23	1:B:158:LEU:O	1.97	0.65
1:B:652:ILE:HD13	1:B:678:VAL:CG1	2.28	0.64
1:A:357:MET:HE1	1:A:514:CYS:O	1.97	0.64
1:A:371:GLU:O	1:A:375:THR:HG22	1.99	0.62
1:B:599:MET:HE1	1:B:653:THR:HG23	1.80	0.62
1:A:158:LEU:HD23	1:A:158:LEU:O	1.99	0.62
2:H:169:VAL:CG2	2:H:197:LEU:HD21	2.28	0.62
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.82	0.61
2:H:39:TRP:HD1	2:H:73:ILE:HD12	1.66	0.61
1:A:609:VAL:HG12	1:A:613:LEU:HG	1.83	0.60
1:A:368:PHE:CZ	1:A:372:ILE:HD11	2.37	0.60
1:A:482:LEU:HD13	1:A:601:ARG:HG3	1.82	0.60
2:K:116:TYR:CD2	3:M:97:ILE:HD11	2.33	0.59
1:B:385:LEU:HD23	1:B:401:LEU:HD11	1.85	0.59
1:B:360:ASN:ND2	1:B:443:GLN:OE1	2.35	0.59
2:H:116:TYR:HD2	3:L:97:ILE:HD11	1.67	0.58
1:B:371:GLU:O	1:B:375:THR:HG22	2.04	0.58
1:B:263:ASP:OD1	1:B:264:SER:N	2.38	0.57
1:B:321:LEU:HD22	1:B:369:LEU:HD11	1.87	0.56
1:B:360:ASN:OD1	1:B:513:LEU:HD11	2.06	0.56
1:B:363:ARG:NH2	1:B:446:SER:OG	2.38	0.56
2:K:150:THR:HG23	2:K:151:SER:N	2.22	0.55
2:K:31:ASN:ND2	2:K:34:SER:OG	2.39	0.55
3:M:12:LEU:HD21	3:M:20:VAL:HG13	1.89	0.55
2:K:119:LEU:HD12	2:K:122:TRP:CZ2	2.43	0.54
1:A:188:CYS:SG	1:A:207:VAL:HG22	2.48	0.54
1:B:482:LEU:O	1:B:486:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:169:VAL:CG2	2:K:197:LEU:HD21	2.38	0.53
1:B:541:ARG:NH2	2:K:56:SER:O	2.42	0.53
1:A:699:LEU:HD12	1:A:700:SER:O	2.09	0.53
1:B:541:ARG:NH2	2:K:55:TYR:O	2.42	0.52
3:M:38:GLN:HB2	3:M:48:LEU:HD11	1.91	0.52
1:B:306:ASN:OD1	1:B:307:VAL:N	2.43	0.52
1:A:581:CYS:O	1:A:585:THR:OG1	2.21	0.51
1:A:330:LYS:HB2	1:A:333:LEU:HD12	1.92	0.51
2:K:147:SER:OG	2:K:150:THR:HG22	2.09	0.51
1:A:589:LEU:HD13	1:A:594:ASP:HB3	1.91	0.51
2:K:39:TRP:HD1	2:K:73:ILE:HD12	1.76	0.51
1:B:605:TYR:O	1:B:609:VAL:HG23	2.11	0.51
1:A:434:LEU:HD23	1:A:524:CYS:SG	2.51	0.51
1:A:599:MET:HE1	1:A:653:THR:HG23	1.92	0.50
3:L:136:LEU:C	3:L:137:LEU:HD12	2.36	0.50
1:A:464:LEU:HD12	1:A:465:PRO:HD2	1.93	0.50
2:K:150:THR:HG23	2:K:151:SER:H	1.75	0.50
1:B:499:LEU:HD11	1:B:523:LEU:HD22	1.93	0.50
3:L:151:VAL:O	3:L:151:VAL:HG23	2.11	0.50
3:M:151:VAL:O	3:M:151:VAL:HG23	2.12	0.50
3:L:107:ILE:H	3:L:167:GLN:HE22	1.60	0.49
1:B:652:ILE:HD13	1:B:678:VAL:HG13	1.92	0.49
2:K:153:GLY:O	2:K:205:SER:N	2.43	0.49
2:H:112:GLY:O	3:L:94:SER:HB2	2.12	0.49
3:L:30:VAL:HG21	3:L:91:GLN:CD	2.38	0.49
1:A:19:THR:HB	1:A:24:GLN:HG2	1.94	0.49
3:L:3:ILE:HG21	3:L:91:GLN:OE1	2.13	0.49
1:A:315:LEU:HD21	1:A:385:LEU:HA	1.95	0.48
1:B:381:GLY:O	1:B:385:LEU:N	2.38	0.48
1:A:568:HIS:O	1:A:568:HIS:ND1	2.46	0.48
2:H:94:THR:HG23	2:H:129:THR:HA	1.95	0.48
1:B:544:VAL:O	1:B:548:VAL:HG23	2.14	0.48
1:B:228:TRP:CZ3	1:B:272:LEU:HD22	2.49	0.48
1:B:378:ASN:OD1	1:B:379:LYS:N	2.47	0.48
1:A:575:LEU:HB3	1:A:609:VAL:CG2	2.44	0.47
1:A:233:THR:HG22	1:A:278:LEU:HA	1.96	0.47
1:A:439:TRP:CG	1:A:517:LEU:HD13	2.49	0.47
1:A:482:LEU:O	1:A:486:VAL:HG23	2.15	0.47
3:L:12:LEU:HD21	3:L:20:VAL:HG13	1.97	0.47
2:H:7:LEU:HD23	2:H:27:ALA:HA	1.97	0.47
2:K:50:TRP:NE1	2:K:53:SER:OG	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:144:ALA:HB2	2:K:230:VAL:CG1	2.45	0.47
1:A:541:ARG:O	1:A:541:ARG:HG2	2.14	0.46
2:H:153:GLY:O	2:H:205:SER:N	2.42	0.46
3:L:55:LEU:HD12	3:L:55:LEU:O	2.15	0.46
2:H:157:LEU:HD13	2:H:230:VAL:HG21	1.97	0.46
2:H:197:LEU:C	2:H:197:LEU:HD12	2.41	0.46
1:B:368:PHE:CZ	1:B:372:ILE:HD11	2.51	0.46
1:B:473:THR:O	1:B:563:ARG:NH1	2.49	0.46
2:K:160:LEU:HD12	2:K:197:LEU:O	2.16	0.46
2:K:197:LEU:HD12	2:K:197:LEU:C	2.41	0.46
1:A:517:LEU:HB3	1:A:518:PRO:HD3	1.98	0.45
1:B:357:MET:HE1	1:B:514:CYS:O	2.15	0.45
2:H:116:TYR:CD2	3:L:97:ILE:HD11	2.50	0.45
1:B:161:ARG:NH2	1:B:164:ASP:OD2	2.49	0.45
1:B:541:ARG:HG2	2:K:58:SER:O	2.17	0.45
3:M:12:LEU:CD2	3:M:20:VAL:HG13	2.46	0.45
2:H:27:ALA:HB1	2:H:30:PHE:CZ	2.52	0.45
1:A:699:LEU:HD12	1:A:699:LEU:C	2.42	0.45
2:H:54:ILE:HG23	2:H:59:GLY:HA2	1.98	0.45
3:M:109:ARG:HG2	3:M:110:THR:N	2.32	0.45
3:M:136:LEU:C	3:M:137:LEU:HD12	2.42	0.45
1:A:373:VAL:HG21	1:A:411:VAL:HB	1.99	0.44
1:B:259:LEU:HD22	1:B:296:LEU:HD13	1.99	0.44
1:B:165:VAL:HG12	1:B:169:ILE:CD1	2.47	0.44
1:B:541:ARG:HG2	1:B:541:ARG:O	2.18	0.44
2:H:119:LEU:HD12	2:H:122:TRP:CZ2	2.52	0.44
1:A:222:GLU:HG3	1:A:223:SER:N	2.32	0.44
1:A:613:LEU:O	1:A:617:LYS:N	2.51	0.44
2:H:86:MET:HB3	2:H:89:LEU:HD21	1.99	0.44
1:A:609:VAL:O	1:A:612:LEU:N	2.51	0.44
1:A:411:VAL:O	1:A:411:VAL:HG22	2.16	0.44
1:B:379:LYS:HE3	1:B:382:GLN:OE1	2.18	0.44
1:A:297:LEU:HG	1:A:389:LEU:HD21	2.00	0.44
1:A:378:ASN:OD1	1:A:379:LYS:N	2.51	0.44
1:A:544:VAL:O	1:A:548:VAL:HG23	2.18	0.44
1:B:214:TYR:CE2	1:B:231:THR:HG21	2.53	0.44
2:K:164:TYR:CE2	2:K:169:VAL:HG13	2.52	0.44
1:A:694:ILE:O	1:A:694:ILE:HG22	2.18	0.43
1:B:365:LYS:HB2	1:B:368:PHE:HB2	2.00	0.43
1:B:652:ILE:O	1:B:656:VAL:HG23	2.18	0.43
1:A:95:ASP:N	1:A:95:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:ILE:HD13	1:B:678:VAL:HG11	1.97	0.43
1:B:575:LEU:HB3	1:B:609:VAL:CG2	2.48	0.43
2:H:50:TRP:NE1	2:H:53:SER:OG	2.39	0.43
1:B:296:LEU:HD23	1:B:296:LEU:C	2.43	0.43
1:B:483:ASP:OD1	1:B:601:ARG:NH2	2.44	0.43
2:H:138:PRO:HB2	2:H:161:VAL:HG13	2.00	0.43
2:K:15:VAL:HG11	2:K:89:LEU:HD13	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
1:B:434:LEU:HD23	1:B:524:CYS:SG	2.59	0.43
1:B:368:PHE:CE1	1:B:372:ILE:HD11	2.54	0.43
2:H:220:LYS:N	2:H:221:PRO:CD	2.82	0.43
3:L:51:SER:O	3:L:52:ALA:HB3	2.19	0.43
2:K:112:GLY:O	3:M:94:SER:HB2	2.18	0.43
1:B:482:LEU:HD13	1:B:601:ARG:HG3	2.00	0.43
2:K:220:LYS:N	2:K:221:PRO:CD	2.82	0.43
1:B:464:LEU:HD12	1:B:465:PRO:HD2	2.00	0.42
2:K:176:GLY:O	2:K:179:THR:HG23	2.19	0.42
3:M:51:SER:O	3:M:52:ALA:HB3	2.19	0.42
1:A:158:LEU:HD23	1:A:158:LEU:C	2.44	0.42
1:B:609:VAL:HG12	1:B:613:LEU:HG	2.00	0.42
3:L:7:GLN:NE2	3:L:103:THR:OG1	2.52	0.42
1:A:410:ASP:O	1:A:411:VAL:HG12	2.20	0.42
1:A:468:THR:HG21	1:A:478:SER:HB2	2.01	0.42
2:H:175:SER:N	2:H:216:ASN:OD1	2.45	0.42
1:A:239:TYR:HB3	1:A:262:PHE:CD2	2.55	0.42
2:K:14:LEU:HD12	2:K:14:LEU:C	2.45	0.42
2:K:115:TYR:HB2	3:M:92:SER:OG	2.19	0.42
1:B:568:HIS:O	1:B:568:HIS:ND1	2.52	0.42
1:A:221:LEU:HD22	1:B:308:GLN:OE1	2.19	0.42
1:B:613:LEU:O	1:B:617:LYS:N	2.52	0.42
1:A:285:MET:HE1	1:A:346:MET:CE	2.50	0.42
1:B:215:LEU:HD11	1:B:235:LEU:HD22	2.02	0.42
1:B:511:GLN:N	1:B:512:PRO:HD2	2.35	0.42
1:A:185:VAL:O	1:A:189:HIS:N	2.48	0.41
1:B:700:SER:OG	1:B:703:GLU:HB3	2.19	0.41
1:A:71:GLU:OE1	1:A:83:TYR:OH	2.38	0.41
1:B:427:ILE:HD11	1:B:456:TRP:CG	2.55	0.41
1:B:468:THR:HG22	1:B:470:ARG:H	1.85	0.41
1:A:109:VAL:O	1:A:109:VAL:HG12	2.19	0.41
1:B:321:LEU:O	1:B:325:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ILE:O	1:A:326:VAL:HG23	2.21	0.41
1:B:158:LEU:HD11	1:B:187:HIS:CE1	2.55	0.41
1:B:411:VAL:HG22	1:B:411:VAL:O	2.21	0.41
1:A:439:TRP:CB	1:A:517:LEU:HD13	2.50	0.41
1:B:229:ARG:HG2	1:B:278:LEU:HD22	2.02	0.41
1:B:571:GLN:NE2	1:B:633:PHE:O	2.41	0.41
2:H:7:LEU:HD21	2:H:30:PHE:HZ	1.85	0.41
2:K:5:VAL:HG22	2:K:29:GLY:HA3	2.02	0.41
2:K:18:GLY:N	2:K:89:LEU:O	2.40	0.41
1:B:200:SER:HB3	1:B:203:TRP:HB3	2.03	0.41
1:B:386:TYR:HE1	1:B:399:SER:HB2	1.86	0.41
1:A:511:GLN:N	1:A:512:PRO:CD	2.84	0.41
2:H:39:TRP:O	2:H:51:VAL:HG22	2.21	0.41
1:B:214:TYR:O	1:B:220:CYS:HB2	2.22	0.40
2:H:36:SER:O	2:H:101:ARG:HA	2.21	0.40
1:A:331:ILE:HG23	1:A:340:GLN:HB2	2.03	0.40
3:L:5:MET:SD	3:L:91:GLN:NE2	2.94	0.40
2:K:138:PRO:HD2	2:K:224:THR:HG21	2.02	0.40
3:M:202:LEU:HD13	3:M:206:VAL:HG12	2.04	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	742/753 (98%)	730 (98%)	12 (2%)	0	100	100
1	B	600/753 (80%)	591 (98%)	9 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
All	All	2214/2416 (92%)	2177 (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	542/673 (80%)	542 (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	1958/2126 (92%)	1958 (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	498	GLN
1	A	583	GLN
1	B	189	HIS
1	B	583	GLN
1	B	688	HIS
2	H	87	ASN
3	L	39	GLN
3	L	80	GLN

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Mol	Chain	Res	Type
2	K	85	GLN
2	K	87	ASN
2	K	211	GLN
3	M	80	GLN

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 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%)	0.45	39 (5%) 33 35	301, 345, 391, 464	0
1	B	604/753 (80%)	0.38	34 (5%) 30 33	303, 345, 393, 426	0
2	H	227/240 (94%)	0.29	3 (1%) 75 64	298, 336, 385, 404	0
2	K	227/240 (94%)	0.26	7 (3%) 51 46	303, 351, 407, 450	0
3	L	213/215 (99%)	0.23	6 (2%) 55 48	302, 338, 368, 379	0
3	M	213/215 (99%)	0.27	7 (3%) 49 45	320, 346, 380, 394	0
All	All	2230/2416 (92%)	0.36	96 (4%) 40 40	298, 344, 389, 464	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	681	TRP	4.6
1	B	155	GLN	4.5
1	A	132	TYR	4.2
2	K	157	LEU	4.0
3	M	210	PHE	3.9
1	B	315	LEU	3.9
1	B	314	GLU	3.8
1	A	290	TYR	3.7
1	B	154	ILE	3.6
3	L	118	ILE	3.4
3	L	210	PHE	3.3
1	A	646	TYR	3.2
1	B	572	PRO	3.2
1	B	312	LEU	3.2
1	B	318	LEU	3.2
1	B	576	VAL	3.1
1	A	65	PHE	3.1
1	A	532	TRP	3.0
1	A	479	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	577	HIS	3.0
3	M	120	PRO	3.0
1	B	151	PHE	2.9
1	A	289	PHE	2.9
1	A	721	ILE	2.8
1	B	172	VAL	2.8
1	A	147	TRP	2.8
1	B	385	LEU	2.8
1	B	290	TYR	2.7
1	A	167	VAL	2.7
1	B	613	LEU	2.7
1	A	613	LEU	2.7
3	L	64	SER	2.7
1	B	575	LEU	2.6
2	H	118	ALA	2.6
1	A	318	LEU	2.6
1	B	372	ILE	2.6
1	A	153	LEU	2.6
1	A	36	TYR	2.6
1	B	289	PHE	2.5
1	B	533	ASP	2.5
1	A	174	VAL	2.5
1	B	376	PHE	2.5
2	K	48	LEU	2.5
3	M	63	PHE	2.5
1	B	716	ASP	2.5
3	M	114	PRO	2.5
1	A	286	LYS	2.5
3	M	64	SER	2.4
1	A	727	SER	2.4
1	A	557	HIS	2.4
1	A	324	PHE	2.4
1	A	638	ILE	2.4
2	K	201	VAL	2.4
1	B	750	MET	2.4
1	A	35	LEU	2.3
3	L	79	LEU	2.3
1	A	469	SER	2.3
1	A	349	ASP	2.3
1	A	461	PHE	2.3
1	B	557	HIS	2.3
1	A	719	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	192	GLU	2.3
3	L	120	PRO	2.3
1	A	539	ILE	2.3
1	B	286	LYS	2.3
1	B	353	GLN	2.3
1	B	472	GLU	2.2
2	K	55	TYR	2.2
1	B	485	GLU	2.2
2	K	156	ALA	2.2
1	A	141	CYS	2.2
3	L	37	TYR	2.2
1	A	392	SER	2.2
1	A	685	LEU	2.2
1	B	158	LEU	2.2
1	A	391	SER	2.2
1	A	437	LEU	2.1
1	A	750	MET	2.1
1	B	186	ALA	2.1
2	H	183	HIS	2.1
1	A	48	TYR	2.1
3	M	181	THR	2.1
1	B	606	TRP	2.1
2	H	230	VAL	2.1
1	A	600	GLY	2.1
1	B	630	PHE	2.1
1	A	151	PHE	2.1
1	A	385	LEU	2.1
1	B	445	ASN	2.1
1	B	391	SER	2.1
2	K	31	ASN	2.0
1	A	218	LEU	2.0
3	M	99	PHE	2.0
1	B	310	ARG	2.0
1	B	438	THR	2.0
2	K	77	THR	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 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.