



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:55 AM UTC

PDB ID : 7MNN / pdb_00007mnn
Title : Crystal structure of the N-terminal domain of NUP358/RanBP2 (residues 1-752) T653I 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 : 6.70 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

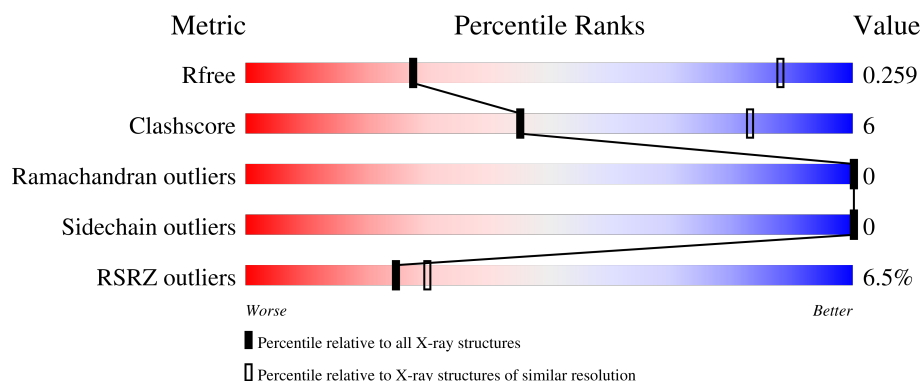
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.70 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	1162 (9.00-4.00)
Clashscore	190562	1001 (9.32-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	7% 86% 14%
1	B	753	6% 68% 12% 20%
2	H	240	6% 81% 14% 5%
2	K	240	4% 78% 17% 5%

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Mol	Chain	Length	Quality of chain
3	L	215	3% 88% 11%
3	M	215	9% 90% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34833 atoms, of which 17334 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	750	Total	C	H	N	O	S	0	0	0
			12093	3839	6052	1042	1132	28			
1	B	604	Total	C	H	N	O	S	0	0	0
			9691	3074	4850	838	906	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	653	ILE	THR	engineered mutation	UNP P49792
B	0	SER	-	expression tag	UNP P49792
B	599	MET	ILE	engineered mutation	UNP P49792
B	653	ILE	THR	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			

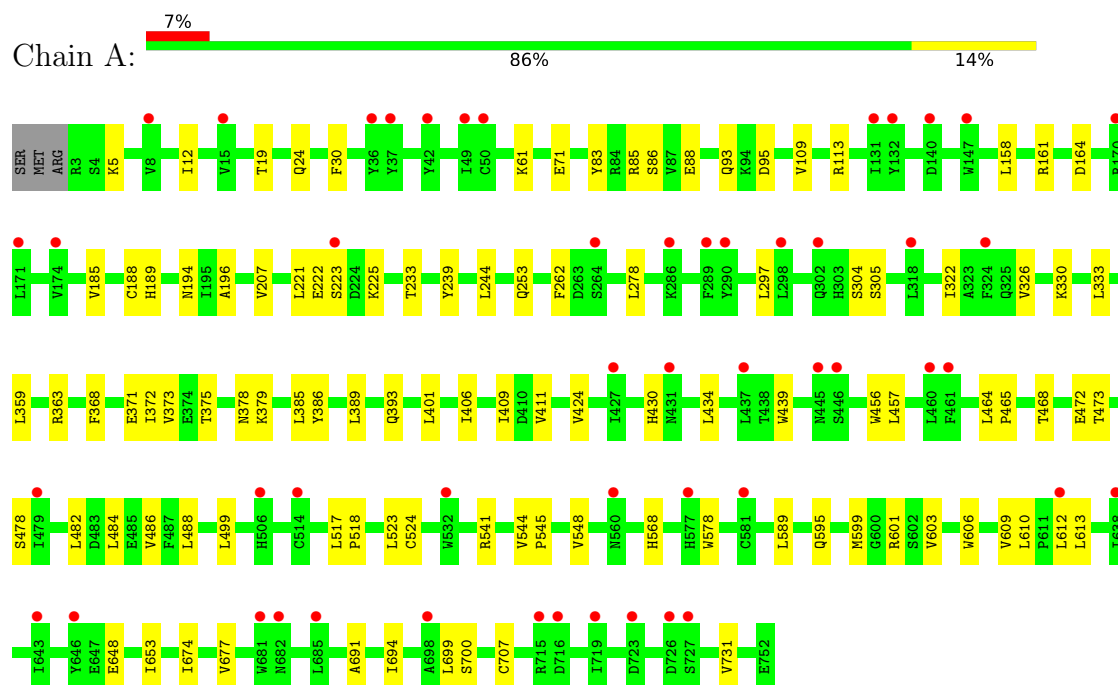
- Molecule 3 is a protein called Antibody Fab14 Light Chain.

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	212	Total	C	H	N	O	S	0	0	0
			3188	1004	1577	272	330	5			

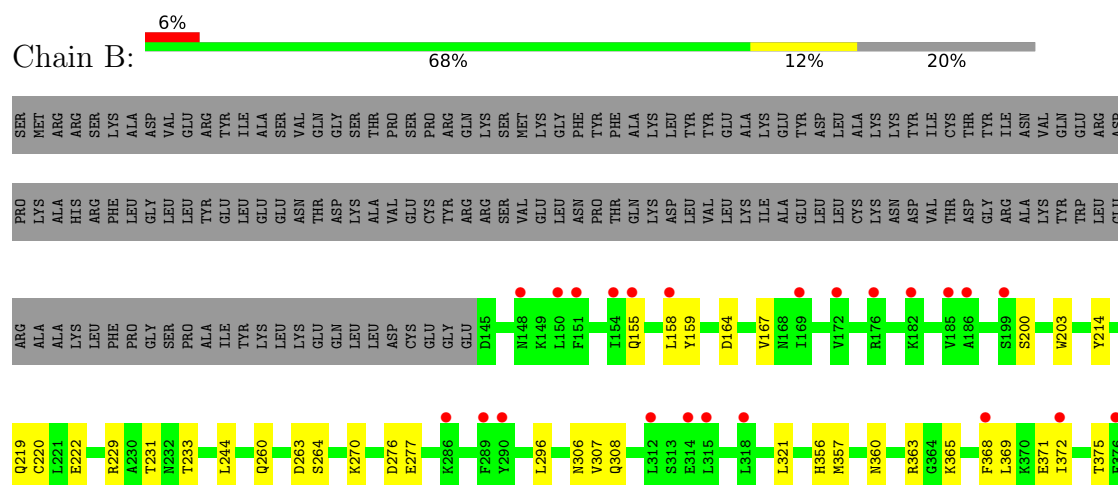
3 Residue-property plots

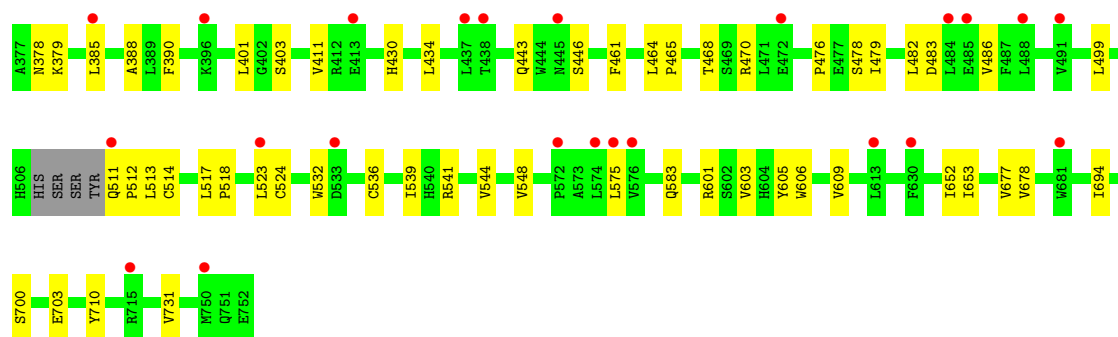
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: E3 SUMO-protein ligase RanBP2

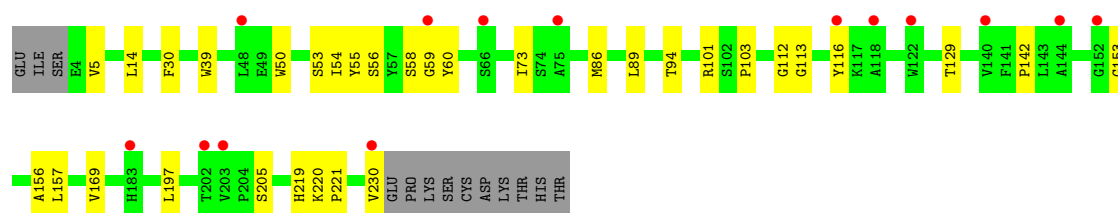
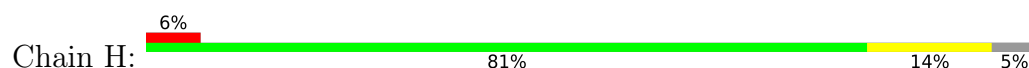


• Molecule 1: E3 SUMO-protein ligase RanBP2

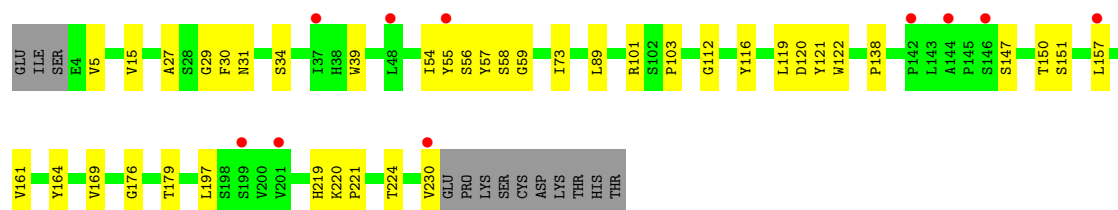
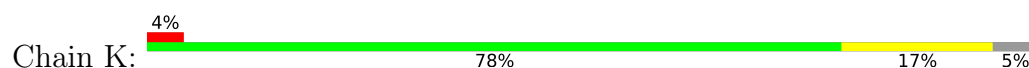




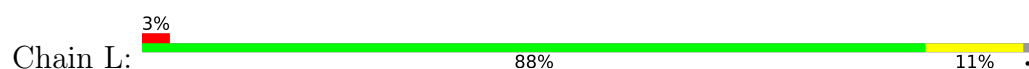
• Molecule 2: Antibody Fab14 Heavy Chain



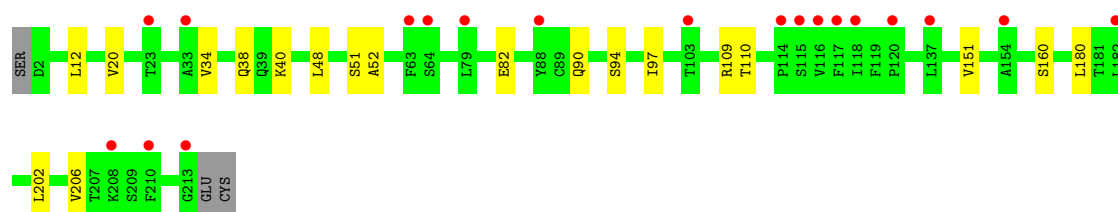
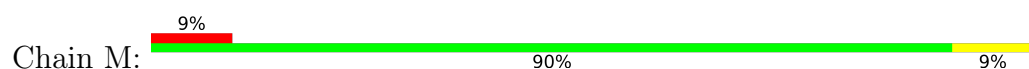
• Molecule 2: Antibody Fab14 Heavy Chain



• 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	161.54Å 161.54Å 647.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 6.70 30.00 – 6.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-6.70) 98.4 (30.00-6.70)	Depositor EDS
R_{merge}	0.78	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 6.58Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.217 , 0.263 0.220 , 0.259	Depositor DCC
R_{free} test set	457 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	384.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 340.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	34833	wwPDB-VP
Average B, all atoms (Å ²)	363.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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	0.17	0/6167	0.38	0/8342
1	B	0.18	0/4940	0.39	0/6688
2	H	0.16	0/1738	0.35	0/2370
2	K	0.17	0/1738	0.37	0/2370
3	L	0.15	0/1652	0.35	0/2241
3	M	0.18	0/1643	0.38	0/2229
All	All	0.17	0/17878	0.38	0/24240

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	6041	6052	6051	74	0
1	B	4841	4850	4848	66	0
2	H	1693	1636	1636	26	0
2	K	1693	1636	1636	31	0
3	L	1620	1583	1583	17	0
3	M	1611	1577	1577	14	0
All	All	17499	17334	17331	207	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 6.

All (207) 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	1.47	0.97
2:H:54:ILE:HD11	2:H:73:ILE:HG23	1.66	0.76
2:K:116:TYR:HD2	3:M:97:ILE:HD11	1.48	0.76
1:A:677:VAL:HG21	1:A:731:VAL:HG13	1.68	0.75
1:A:385:LEU:HD23	1:A:401:LEU:HD11	1.71	0.72
1:A:406:ILE:HG23	1:A:409:ILE:HD11	1.72	0.71
1:B:360:ASN:ND2	1:B:443:GLN:OE1	2.24	0.71
1:B:468:THR:HG21	1:B:478:SER:HB2	1.71	0.70
1:B:158:LEU:HD23	1:B:158:LEU:O	1.96	0.66
2:K:54:ILE:HD11	2:K:73:ILE:HG23	1.78	0.66
2:H:116:TYR:HD2	3:L:97:ILE:HD11	1.59	0.65
1:A:472:GLU:HG2	1:A:473:THR:HG23	1.77	0.64
1:A:158:LEU:HD23	1:A:158:LEU:O	1.98	0.64
2:H:169:VAL:CG2	2:H:197:LEU:HD21	2.28	0.63
1:A:371:GLU:O	1:A:375:THR:HG22	1.99	0.63
1:B:603:VAL:HG22	1:B:653:ILE:HG22	1.80	0.63
3:M:38:GLN:HB2	3:M:48:LEU:HD11	1.80	0.63
2:K:15:VAL:HG11	2:K:89:LEU:HD13	1.82	0.62
1:A:541:ARG:NH2	2:H:56:SER:O	2.33	0.61
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.82	0.61
2:H:116:TYR:CD2	3:L:97:ILE:HD11	2.36	0.60
1:A:499:LEU:HD11	1:A:523:LEU:HD22	1.83	0.60
1:A:609:VAL:HG12	1:A:613:LEU:HG	1.83	0.60
1:B:544:VAL:O	1:B:548:VAL:HG23	2.02	0.60
1:B:371:GLU:O	1:B:375:THR:HG22	2.01	0.59
1:B:499:LEU:HD11	1:B:523:LEU:HD22	1.83	0.59
1:A:5:LYS:NZ	1:A:253:GLN:OE1	2.20	0.59
3:M:202:LEU:HD13	3:M:206:VAL:HG12	1.85	0.59
1:B:369:LEU:HG	1:B:411:VAL:HG23	1.86	0.58
1:B:652:ILE:HD13	1:B:678:VAL:HG13	1.86	0.57
1:A:434:LEU:HD23	1:A:524:CYS:SG	2.44	0.57
1:B:385:LEU:HD23	1:B:401:LEU:HD11	1.86	0.57
1:A:222:GLU:OE1	1:B:388:ALA:HA	2.04	0.57
1:A:373:VAL:HG21	1:A:411:VAL:HB	1.87	0.57
1:B:360:ASN:OD1	1:B:513:LEU:HD11	2.05	0.56
1:A:88:GLU:OE1	1:B:365:LYS:HG2	2.06	0.56
1:B:260:GLN:HA	1:B:390:PHE:HE2	1.71	0.56
2:K:150:THR:HG23	2:K:151:SER:N	2.21	0.55
1:B:483:ASP:OD1	1:B:601:ARG:NH2	2.36	0.55
1:A:12:ILE:HG21	1:A:393:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:116:TYR:CD2	3:M:97:ILE:HD11	2.37	0.55
1:A:541:ARG:NH2	2:H:55:TYR:O	2.40	0.55
2:K:5:VAL:HG22	2:K:29:GLY:HA3	1.89	0.54
1:B:263:ASP:OD1	1:B:264:SER:N	2.40	0.54
1:A:439:TRP:CG	1:A:517:LEU:HD13	2.42	0.54
2:K:147:SER:OG	2:K:150:THR:HG22	2.07	0.54
1:A:648:GLU:HG2	1:A:674:ILE:HD13	1.89	0.54
1:A:88:GLU:OE1	1:B:365:LYS:CG	2.56	0.53
1:B:368:PHE:CE1	1:B:372:ILE:HD11	2.43	0.53
1:B:321:LEU:HD22	1:B:369:LEU:HD11	1.91	0.53
3:M:12:LEU:HD21	3:M:20:VAL:HG13	1.91	0.53
1:A:330:LYS:HB2	1:A:333:LEU:HD12	1.92	0.52
1:A:699:LEU:HD12	1:A:700:SER:O	2.10	0.52
1:B:605:TYR:O	1:B:609:VAL:HG23	2.10	0.52
1:B:155:GLN:HG2	1:B:159:TYR:CZ	2.44	0.52
3:M:151:VAL:HG23	3:M:151:VAL:O	2.10	0.52
1:A:221:LEU:HD12	1:A:225:LYS:HD3	1.92	0.52
1:A:482:LEU:HD13	1:A:601:ARG:HG3	1.92	0.52
3:M:109:ARG:HG2	3:M:110:THR:N	2.25	0.52
2:K:138:PRO:HD2	2:K:224:THR:HG21	1.92	0.51
1:A:188:CYS:SG	1:A:207:VAL:HG22	2.50	0.51
1:B:482:LEU:O	1:B:486:VAL:HG23	2.09	0.51
2:K:39:TRP:HD1	2:K:73:ILE:HD12	1.75	0.51
3:L:151:VAL:HG23	3:L:151:VAL:O	2.10	0.50
1:B:532:TRP:CD1	1:B:536:CYS:HG	2.30	0.50
1:B:583:GLN:OE1	1:B:653:ILE:HD11	2.11	0.49
1:B:214:TYR:CD2	1:B:231:THR:HG21	2.47	0.49
2:K:150:THR:HG23	2:K:151:SER:H	1.77	0.49
1:A:464:LEU:HD12	1:A:465:PRO:HD2	1.94	0.49
1:A:221:LEU:HD22	1:B:308:GLN:OE1	2.13	0.49
1:B:652:ILE:HD13	1:B:678:VAL:CG1	2.43	0.49
2:K:15:VAL:HG11	2:K:89:LEU:CD1	2.41	0.49
1:B:368:PHE:CZ	1:B:372:ILE:HD11	2.48	0.49
3:L:136:LEU:C	3:L:137:LEU:HD12	2.38	0.48
1:A:161:ARG:NH2	1:A:164:ASP:OD2	2.46	0.48
1:B:541:ARG:NH2	2:K:55:TYR:O	2.47	0.48
2:H:169:VAL:HG12	2:H:219:HIS:HD2	1.77	0.48
1:B:363:ARG:NH2	1:B:446:SER:OG	2.47	0.48
1:B:583:GLN:CD	1:B:653:ILE:HD11	2.38	0.48
2:H:54:ILE:HG23	2:H:59:GLY:HA2	1.95	0.48
1:B:464:LEU:HD12	1:B:465:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:3:ILE:HG21	3:L:91:GLN:OE1	2.14	0.48
1:A:603:VAL:HG22	1:A:653:ILE:HG22	1.96	0.48
3:L:30:VAL:HG21	3:L:91:GLN:CD	2.39	0.47
3:M:51:SER:O	3:M:52:ALA:HB3	2.15	0.47
1:A:517:LEU:HB3	1:A:518:PRO:HD3	1.96	0.47
1:B:229:ARG:O	1:B:233:THR:HG23	2.14	0.47
1:A:85:ARG:HA	1:A:88:GLU:OE2	2.15	0.47
2:H:39:TRP:HD1	2:H:73:ILE:HD12	1.79	0.47
2:H:197:LEU:HD12	2:H:197:LEU:C	2.40	0.47
1:A:541:ARG:O	1:A:541:ARG:HG2	2.12	0.47
3:L:55:LEU:HD12	3:L:55:LEU:O	2.14	0.47
2:K:34:SER:HA	2:K:57:TYR:CE2	2.49	0.47
2:K:197:LEU:C	2:K:197:LEU:HD12	2.40	0.47
1:B:541:ARG:O	1:B:541:ARG:HG2	2.15	0.47
2:K:31:ASN:ND2	2:K:34:SER:OG	2.48	0.47
1:B:365:LYS:HB2	1:B:368:PHE:HB2	1.97	0.46
2:H:157:LEU:HD13	2:H:230:VAL:HG21	1.96	0.46
1:A:486:VAL:HG13	1:A:578:TRP:CD2	2.50	0.46
2:K:54:ILE:HG23	2:K:59:GLY:HA2	1.97	0.46
1:B:306:ASN:OD1	1:B:307:VAL:N	2.48	0.46
1:B:270:LYS:NZ	1:B:403:SER:OG	2.49	0.46
2:K:169:VAL:CG2	2:K:197:LEU:HD21	2.46	0.46
1:A:297:LEU:HG	1:A:389:LEU:HD21	1.97	0.46
1:A:541:ARG:HG2	2:H:58:SER:O	2.16	0.46
1:A:589:LEU:O	1:A:595:GLN:NE2	2.44	0.46
1:B:164:ASP:OD2	1:B:167:VAL:HG23	2.16	0.46
1:B:378:ASN:OD1	1:B:379:LYS:N	2.49	0.46
1:A:239:TYR:HB3	1:A:262:PHE:CD2	2.51	0.46
1:A:482:LEU:O	1:A:486:VAL:HG23	2.15	0.46
2:K:169:VAL:HG12	2:K:219:HIS:HD2	1.81	0.46
2:H:50:TRP:NE1	2:H:53:SER:OG	2.38	0.46
2:K:119:LEU:HD12	2:K:122:TRP:CZ2	2.51	0.45
1:A:411:VAL:HG22	1:A:411:VAL:O	2.15	0.45
2:K:112:GLY:O	3:M:94:SER:HB2	2.16	0.45
2:K:157:LEU:HB2	2:K:230:VAL:HG11	1.96	0.45
1:B:356:HIS:O	1:B:360:ASN:ND2	2.49	0.45
1:A:424:VAL:HG22	1:A:456:TRP:CD1	2.52	0.45
1:A:568:HIS:ND1	1:A:568:HIS:O	2.50	0.45
1:B:511:GLN:N	1:B:512:PRO:HD2	2.32	0.45
2:K:176:GLY:O	2:K:179:THR:HG23	2.17	0.45
1:A:457:LEU:HD13	1:A:484:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:GLY:O	2:H:205:SER:N	2.45	0.45
2:H:169:VAL:HG12	2:H:219:HIS:CD2	2.52	0.45
3:M:109:ARG:HG2	3:M:110:THR:H	1.82	0.45
1:B:214:TYR:O	1:B:220:CYS:HB2	2.17	0.45
1:A:12:ILE:CG2	1:A:393:GLN:OE1	2.65	0.45
1:A:439:TRP:CB	1:A:517:LEU:HD13	2.46	0.45
1:A:194:ASN:OD1	1:A:196:ALA:N	2.50	0.44
1:B:700:SER:OG	1:B:703:GLU:HB3	2.17	0.44
1:A:222:GLU:HG3	1:A:223:SER:N	2.32	0.44
3:L:25:ARG:NH1	3:L:71:ASP:OD2	2.51	0.44
1:A:378:ASN:OD1	1:A:379:LYS:N	2.51	0.44
1:B:229:ARG:NH1	1:B:276:ASP:OD2	2.50	0.44
1:B:476:PRO:O	1:B:479:ILE:HG12	2.17	0.44
1:B:575:LEU:HB3	1:B:609:VAL:CG2	2.47	0.44
2:H:112:GLY:O	3:L:94:SER:HB2	2.18	0.44
2:K:169:VAL:HG12	2:K:219:HIS:CD2	2.52	0.44
1:A:694:ILE:HG22	1:A:694:ILE:O	2.18	0.44
3:M:12:LEU:CD2	3:M:20:VAL:HG13	2.48	0.44
3:L:12:LEU:HD21	3:L:20:VAL:HG13	2.00	0.44
1:A:368:PHE:CZ	1:A:372:ILE:HD11	2.53	0.43
1:B:260:GLN:CA	1:B:390:PHE:HE2	2.31	0.43
2:H:220:LYS:N	2:H:221:PRO:CD	2.81	0.43
3:L:51:SER:O	3:L:52:ALA:HB3	2.18	0.43
3:M:34:VAL:HA	3:M:90:GLN:O	2.18	0.43
2:K:220:LYS:N	2:K:221:PRO:CD	2.81	0.43
1:A:233:THR:HG22	1:A:278:LEU:HA	2.01	0.43
1:A:322:ILE:O	1:A:326:VAL:HG23	2.19	0.43
1:B:411:VAL:O	1:B:411:VAL:HG22	2.19	0.43
2:K:120:ASP:OD1	2:K:121:TYR:N	2.48	0.43
3:M:160:SER:HB3	3:M:180:LEU:HD13	2.00	0.43
1:B:694:ILE:HD12	1:B:710:TYR:CE2	2.53	0.43
2:K:101:ARG:CZ	2:K:103:PRO:HG3	2.49	0.43
1:A:603:VAL:CG2	1:A:653:ILE:HG22	2.48	0.43
1:B:468:THR:HG22	1:B:470:ARG:H	1.84	0.43
2:H:14:LEU:C	2:H:14:LEU:HD12	2.44	0.43
2:K:27:ALA:HB1	2:K:30:PHE:CZ	2.53	0.43
2:K:164:TYR:CE2	2:K:169:VAL:HG13	2.52	0.43
1:A:95:ASP:OD1	1:A:95:ASP:N	2.50	0.43
1:B:517:LEU:HB3	1:B:518:PRO:HD3	2.01	0.42
1:B:541:ARG:HG2	2:K:58:SER:O	2.19	0.42
3:M:40:LYS:NZ	3:M:82:GLU:O	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PHE:CZ	1:A:61:LYS:HG3	2.54	0.42
1:B:464:LEU:HD11	1:B:479:ILE:O	2.18	0.42
2:H:94:THR:HG23	2:H:129:THR:HA	2.02	0.42
2:H:113:GLY:HA3	3:L:94:SER:HB2	2.02	0.42
1:A:599:MET:CE	1:A:653:ILE:HG23	2.49	0.42
2:H:86:MET:HB3	2:H:89:LEU:HD21	2.01	0.42
1:A:71:GLU:OE1	1:A:83:TYR:OH	2.36	0.42
1:A:544:VAL:O	1:A:548:VAL:HG23	2.20	0.42
1:A:158:LEU:HD23	1:A:158:LEU:C	2.44	0.42
1:A:545:PRO:HD3	2:H:60:TYR:CE1	2.54	0.42
1:B:434:LEU:HD23	1:B:524:CYS:SG	2.60	0.42
1:B:296:LEU:C	1:B:296:LEU:HD23	2.45	0.42
1:A:185:VAL:O	1:A:189:HIS:N	2.47	0.41
1:B:357:MET:HE1	1:B:514:CYS:O	2.19	0.41
1:B:606:TRP:NE1	1:B:653:ILE:HG13	2.34	0.41
1:B:219:GLN:HA	1:B:222:GLU:HG2	2.02	0.41
2:H:142:PRO:O	3:L:122:SER:HB3	2.20	0.41
1:A:468:THR:HG21	1:A:478:SER:HB2	2.02	0.41
1:A:609:VAL:O	1:A:612:LEU:N	2.53	0.41
3:L:13:SER:HG	3:L:141:TYR:HH	1.67	0.41
1:A:606:TRP:O	1:A:610:LEU:HG	2.21	0.41
1:A:699:LEU:HD12	1:A:699:LEU:C	2.46	0.41
1:B:214:TYR:CE2	1:B:231:THR:HG21	2.55	0.41
1:B:244:LEU:HD11	1:B:430:HIS:NE2	2.36	0.41
2:H:101:ARG:CZ	2:H:103:PRO:HG3	2.50	0.41
1:A:304:SER:OG	1:A:305:SER:N	2.53	0.41
1:A:457:LEU:HD21	1:A:488:LEU:CD1	2.50	0.41
1:A:691:ALA:HA	1:A:707:CYS:SG	2.61	0.41
1:B:200:SER:HB3	1:B:203:TRP:HB3	2.03	0.41
1:B:541:ARG:NH2	2:K:56:SER:O	2.54	0.41
2:H:5:VAL:HG13	2:H:30:PHE:HD2	1.85	0.41
3:L:107:ILE:O	3:L:167:GLN:NE2	2.45	0.41
1:A:244:LEU:HD21	1:A:430:HIS:NE2	2.35	0.41
1:A:359:LEU:O	1:A:363:ARG:HG3	2.20	0.41
2:H:156:ALA:HB3	3:L:119:PHE:HZ	1.86	0.41
2:K:138:PRO:HB2	2:K:161:VAL:HG13	2.03	0.41
1:A:86:SER:O	1:A:93:GLN:NE2	2.55	0.40
1:A:113:ARG:N	1:B:375:THR:OG1	2.54	0.40
1:A:386:TYR:CD1	1:A:401:LEU:HD23	2.56	0.40
1:B:233:THR:HG21	1:B:277:GLU:OE2	2.20	0.40
1:B:461:PHE:HD1	1:B:539:ILE:HG21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HB	1:A:24:GLN:HG2	2.03	0.40
1:A:109:VAL:O	1:A:109:VAL:HG12	2.20	0.40
1:A:677:VAL:HG21	1:A:731:VAL:CG1	2.43	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	748/753 (99%)	736 (98%)	12 (2%)	0	100	100
1	B	600/753 (80%)	592 (99%)	8 (1%)	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	210/215 (98%)	208 (99%)	2 (1%)	0	100	100
All	All	2219/2416 (92%)	2183 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	670/673 (100%)	670 (100%)	0	100	100
1	B	541/673 (80%)	541 (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	187/190 (98%)	187 (100%)	0	100	100
All	All	1960/2126 (92%)	1960 (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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	155	GLN
1	A	288	HIS
1	A	303	HIS
1	A	463	HIS
1	A	496	HIS
1	A	498	GLN
1	A	540	HIS
1	A	632	HIS
1	A	651	HIS
1	B	241	ASN
1	B	253	GLN
1	B	556	GLN
1	B	688	HIS
2	H	85	GLN
2	H	183	HIS
3	L	39	GLN
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	750/753 (99%)	0.53	51 (6%)	23	28	322, 360, 402, 442	0
1	B	604/753 (80%)	0.57	46 (7%)	20	26	325, 357, 413, 436	0
2	H	227/240 (94%)	0.37	14 (6%)	26	31	329, 355, 399, 408	0
2	K	227/240 (94%)	0.36	10 (4%)	39	39	319, 368, 412, 459	0
3	L	213/215 (99%)	0.36	6 (2%)	55	48	329, 357, 387, 402	0
3	M	212/215 (98%)	0.50	19 (8%)	15	22	335, 365, 395, 412	0
All	All	2233/2416 (92%)	0.49	146 (6%)	25	30	319, 360, 404, 459	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	572	PRO	6.5
1	A	681	TRP	5.9
1	A	514	CYS	5.6
1	B	314	GLU	4.6
1	A	290	TYR	4.5
1	A	174	VAL	4.4
1	B	154	ILE	4.3
1	B	155	GLN	4.2
3	M	114	PRO	4.0
1	B	151	PHE	4.0
1	B	491	VAL	3.9
1	B	575	LEU	3.9
1	B	715	ARG	3.6
1	A	719	ILE	3.6
1	B	576	VAL	3.6
1	B	523	LEU	3.6
2	K	142	PRO	3.6
1	B	290	TYR	3.5
1	B	289	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
3	M	115	SER	3.4
1	B	372	ILE	3.3
1	A	318	LEU	3.3
1	B	199	SER	3.3
2	H	116	TYR	3.2
1	A	532	TRP	3.2
1	A	698	ALA	3.2
1	A	286	LYS	3.1
1	B	630	PHE	3.1
1	A	682	ASN	3.1
2	K	146	SER	3.1
2	H	118	ALA	3.1
1	A	171	LEU	3.1
1	B	385	LEU	3.0
1	A	577	HIS	3.0
1	A	289	PHE	3.0
1	B	438	THR	3.0
1	A	560	ASN	3.0
2	K	48	LEU	3.0
2	K	37	ILE	2.9
2	H	75	ALA	2.9
1	B	182	LYS	2.9
2	H	183	HIS	2.9
1	B	613	LEU	2.9
1	B	158	LEU	2.9
1	A	302	GLN	2.9
1	A	726	ASP	2.9
2	K	55	TYR	2.9
1	B	681	TRP	2.8
3	M	118	ILE	2.8
3	M	88	TYR	2.8
1	A	223	SER	2.8
3	M	120	PRO	2.8
2	K	201	VAL	2.8
1	A	445	ASN	2.7
3	M	64	SER	2.7
1	B	437	LEU	2.7
1	A	132	TYR	2.7
2	K	157	LEU	2.7
1	B	169	ILE	2.7
1	B	368	PHE	2.7
3	L	64	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	210	PHE	2.6
1	A	461	PHE	2.6
2	H	59	GLY	2.6
1	A	427	ILE	2.6
1	B	286	LYS	2.6
1	B	312	LEU	2.6
1	A	147	TRP	2.6
1	A	170	ARG	2.6
1	B	472	GLU	2.5
1	B	485	GLU	2.5
1	B	533	ASP	2.5
1	A	42	TYR	2.5
1	A	643	ILE	2.5
1	A	8	VAL	2.5
1	B	172	VAL	2.5
1	A	324	PHE	2.4
1	A	612	LEU	2.4
3	L	57	SER	2.4
2	H	203	VAL	2.4
2	H	202	THR	2.4
2	H	144	ALA	2.4
1	A	479	ILE	2.4
1	A	715	ARG	2.4
1	B	315	LEU	2.4
3	M	137	LEU	2.4
1	A	646	TYR	2.4
1	A	685	LEU	2.4
1	B	574	LEU	2.4
1	B	176	ARG	2.3
1	B	318	LEU	2.3
1	A	131	ILE	2.3
1	A	638	ILE	2.3
3	L	53	SER	2.3
1	A	723	ASP	2.3
3	M	208	LYS	2.3
1	B	511	GLN	2.3
1	A	140	ASP	2.3
1	B	484	LEU	2.3
2	K	199	SER	2.3
1	A	15	VAL	2.3
2	K	144	ALA	2.2
1	A	36	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	376	PHE	2.2
2	K	230	VAL	2.2
1	B	445	ASN	2.2
1	A	727	SER	2.2
3	L	37	TYR	2.2
1	B	148	ASN	2.2
1	B	750	MET	2.2
2	H	152	GLY	2.2
1	A	264	SER	2.2
1	B	488	LEU	2.2
1	A	506	HIS	2.2
1	A	50	CYS	2.2
1	A	581	CYS	2.2
1	A	37	TYR	2.2
1	B	185	VAL	2.2
3	M	116	VAL	2.2
1	B	186	ALA	2.1
1	A	460	LEU	2.1
2	H	66	SER	2.1
2	H	122	TRP	2.1
1	A	49	ILE	2.1
1	A	298	LEU	2.1
2	H	140	VAL	2.1
1	A	716	ASP	2.1
3	M	23	THR	2.1
3	M	103	THR	2.1
3	L	120	PRO	2.1
1	A	437	LEU	2.1
3	M	117	PHE	2.1
2	H	230	VAL	2.1
1	B	150	LEU	2.1
2	H	48	LEU	2.1
3	L	118	ILE	2.1
3	M	33	ALA	2.1
3	M	182	LEU	2.1
1	B	413	GLU	2.1
1	B	396	LYS	2.0
3	M	63	PHE	2.0
3	M	154	ALA	2.0
3	M	213	GLY	2.0
3	M	79	LEU	2.0
1	A	431	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	446	SER	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.