



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2022 – 06:08 PM EDT

PDB ID : 7MNL
Title : Crystal structure of the N-terminal domain of NUP358/RanBP2 (residues 1-752) 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 : 3.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

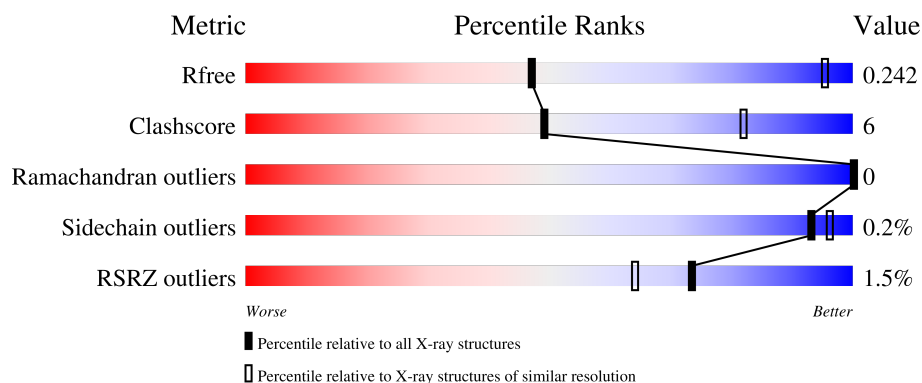
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	B	753	<div> <div>68%</div> <div>11%</div> <div>21%</div> </div>
2	H	240	<div> <div>81%</div> <div>13%</div> <div>5%</div> </div>
2	K	240	<div> <div>4%</div> <div>77%</div> <div>17%</div> <div>5%</div> </div>
3	L	215	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	215	<div><div>%</div><div><div></div></div><div>90%</div><div>8%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34556 atoms, of which 17198 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
			12026	3816	6020	1036	1126	28			
1	B	594	Total	C	H	N	O	S	0	0	0
			9481	3008	4746	819	886	22			

There are 4 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
B	0	SER	-	expression tag	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
			3328	1072	1635	282	334	5			
2	K	227	Total	C	H	N	O	S	0	0	0
			3330	1072	1637	282	334	5			

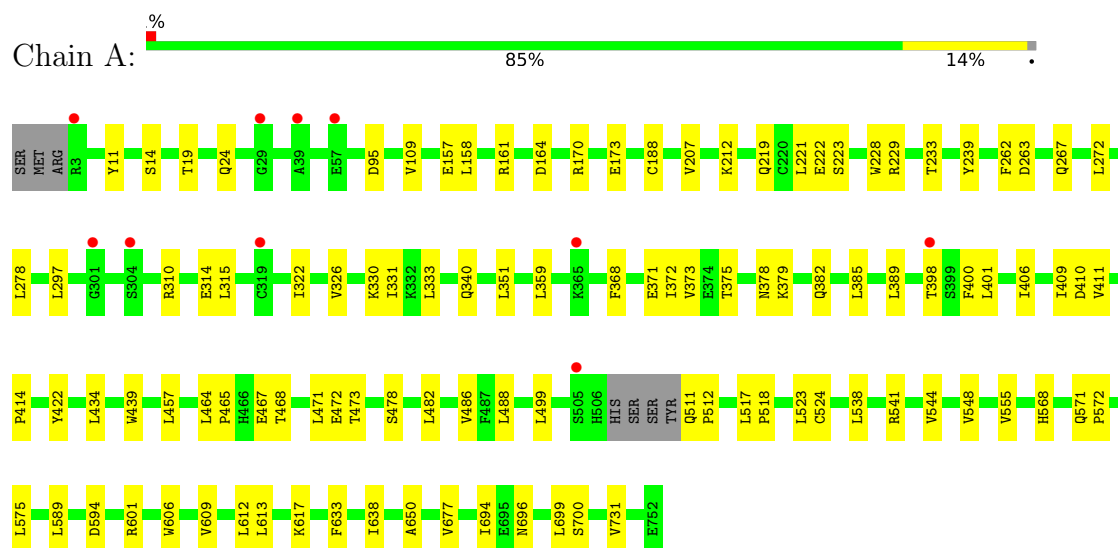
- Molecule 3 is a protein called Antibody Fab14 Light Chain.

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			

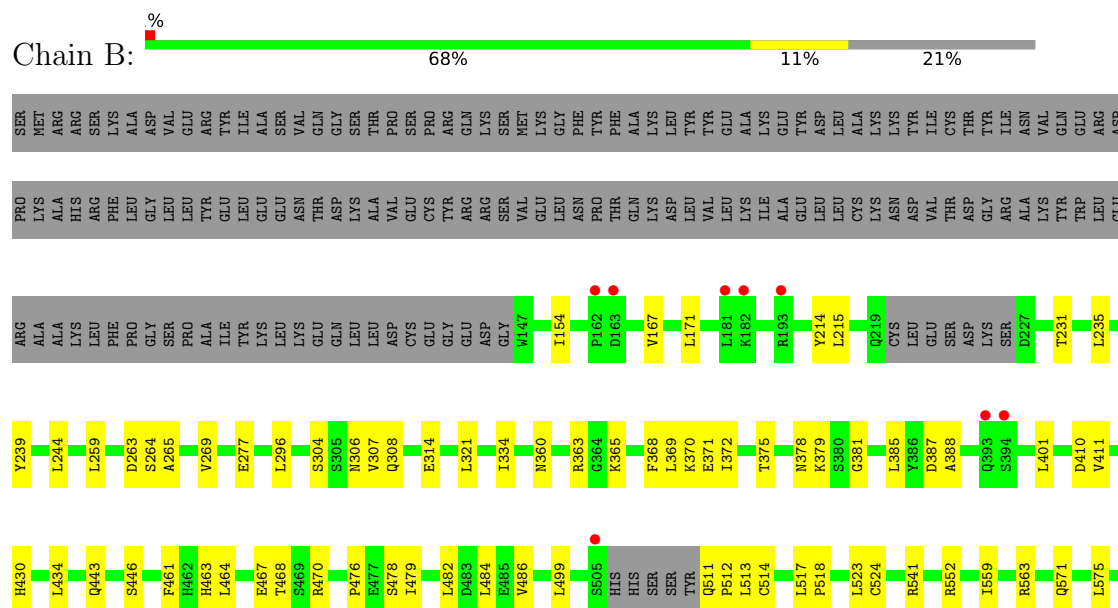
3 Residue-property plots [i](#)

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: E3 SUMO-protein ligase RanBP2

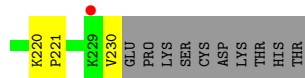
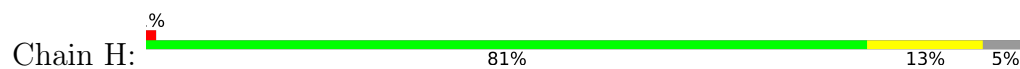


• Molecule 1: E3 SUMO-protein ligase RanBP2

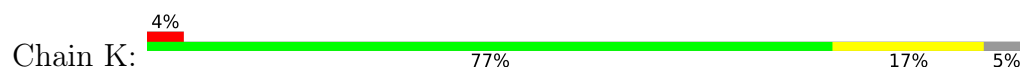




• Molecule 2: Antibody Fab14 Heavy Chain



• 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	161.42Å 161.42Å 644.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.95 19.97 – 3.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.97-3.95) 100.0 (19.97-3.95)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.94Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.192 , 0.241 0.193 , 0.242	Depositor DCC
R_{free} test set	2214 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	170.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 145.2	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	0.95	EDS
Total number of atoms	34556	wwPDB-VP
Average B, all atoms (Å ²)	224.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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	0.25	0/6129	0.39	0/8289
1	B	0.24	0/4828	0.39	0/6536
2	H	0.26	0/1738	0.46	0/2370
2	K	0.26	0/1738	0.46	0/2370
3	L	0.25	0/1652	0.45	0/2241
3	M	0.25	0/1643	0.44	0/2229
All	All	0.25	0/17728	0.42	0/24035

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	6006	6020	6020	74	0
1	B	4735	4746	4745	64	0
2	H	1693	1635	1636	22	0
2	K	1693	1637	1636	29	0
3	L	1620	1583	1583	10	0
3	M	1611	1577	1577	12	0
All	All	17358	17198	17197	202	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 (202) 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:221:LEU:HD22	1:B:308:GLN:OE1	1.72	0.90
1:B:677:VAL:HG21	1:B:731:VAL:HG13	1.57	0.86
2:K:54:ILE:HD11	2:K:73:ILE:HG23	1.57	0.85
2:H:50:TRP:HE1	2:H:53:SER:HG	1.29	0.81
1:A:677:VAL:HG21	1:A:731:VAL:HG13	1.63	0.80
2:K:50:TRP:HE1	2:K:53:SER:HG	1.31	0.78
2:H:54:ILE:HD11	2:H:73:ILE:HG23	1.69	0.75
1:A:368:PHE:CZ	1:A:372:ILE:HD11	2.24	0.73
1:A:385:LEU:HD23	1:A:401:LEU:HD11	1.71	0.72
1:B:541:ARG:NH2	2:K:56:SER:O	2.23	0.71
1:B:371:GLU:O	1:B:375:THR:HG22	1.91	0.70
1:A:472:GLU:HG2	1:A:473:THR:HG23	1.72	0.70
1:A:371:GLU:O	1:A:375:THR:HG22	1.94	0.68
1:A:499:LEU:HD11	1:A:523:LEU:HD22	1.74	0.68
1:B:468:THR:HG21	1:B:478:SER:HB2	1.75	0.68
2:H:169:VAL:CG2	2:H:197:LEU:HD21	2.24	0.68
1:A:406:ILE:HG23	1:A:409:ILE:HD11	1.75	0.67
1:A:609:VAL:HG12	1:A:613:LEU:HG	1.77	0.67
1:B:154:ILE:HG21	1:B:171:LEU:HB2	1.77	0.65
1:A:331:ILE:HG23	1:A:340:GLN:HB2	1.79	0.65
1:A:482:LEU:HD13	1:A:601:ARG:HG3	1.79	0.64
2:H:39:TRP:HD1	2:H:73:ILE:HD12	1.61	0.64
1:A:158:LEU:HD23	1:A:158:LEU:O	1.98	0.64
1:B:652:ILE:HD13	1:B:678:VAL:CG1	2.28	0.63
2:K:39:TRP:HD1	2:K:73:ILE:HD12	1.64	0.63
2:K:116:TYR:HD2	3:M:97:ILE:HD11	1.64	0.62
1:B:321:LEU:HD22	1:B:369:LEU:HD11	1.81	0.62
1:B:154:ILE:HG23	1:B:167:VAL:HG12	1.82	0.62
1:B:235:LEU:HD11	1:B:239:TYR:CE2	2.36	0.60
1:A:439:TRP:CG	1:A:517:LEU:HD13	2.38	0.59
1:B:370:LYS:HA	1:B:411:VAL:HG21	1.84	0.58
2:H:169:VAL:HG21	2:H:197:LEU:HD21	1.85	0.58
2:K:169:VAL:CG2	2:K:197:LEU:HD21	2.33	0.58
1:A:589:LEU:HD13	1:A:594:ASP:HB3	1.85	0.56
1:A:188:CYS:SG	1:A:207:VAL:HG22	2.45	0.56
2:K:150:THR:HG23	2:K:151:SER:N	2.21	0.56
1:B:482:LEU:HD13	1:B:601:ARG:HG3	1.87	0.56
1:B:482:LEU:O	1:B:486:VAL:HG23	2.05	0.56
3:L:3:ILE:HG21	3:L:91:GLN:OE1	2.06	0.56
1:A:161:ARG:NH2	1:A:164:ASP:OD2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:THR:HG23	2:H:129:THR:HA	1.88	0.55
1:A:315:LEU:HD21	1:A:385:LEU:HA	1.88	0.55
1:A:541:ARG:NH2	2:H:56:SER:O	2.39	0.55
1:B:368:PHE:CZ	1:B:372:ILE:HD11	2.41	0.55
1:A:541:ARG:O	1:A:541:ARG:HG2	2.07	0.55
2:K:169:VAL:HG21	2:K:197:LEU:HD21	1.88	0.55
1:B:263:ASP:OD1	1:B:264:SER:N	2.40	0.54
3:M:12:LEU:HD21	3:M:20:VAL:HG13	1.89	0.54
2:H:153:GLY:O	2:H:205:SER:N	2.36	0.54
1:A:699:LEU:HD12	1:A:700:SER:O	2.07	0.54
2:H:5:VAL:HG22	2:H:29:GLY:HA3	1.90	0.54
1:B:463:HIS:ND1	2:K:80:ASN:HB2	2.23	0.53
1:B:605:TYR:O	1:B:609:VAL:HG23	2.08	0.53
2:H:54:ILE:HG23	2:H:59:GLY:HA2	1.89	0.53
1:A:464:LEU:HD12	1:A:465:PRO:HD2	1.91	0.53
1:B:478:SER:O	1:B:563:ARG:NH2	2.41	0.53
1:A:699:LEU:HD12	1:A:699:LEU:C	2.30	0.53
2:H:7:LEU:HD21	2:H:30:PHE:HZ	1.74	0.52
2:K:150:THR:HG23	2:K:151:SER:H	1.73	0.52
1:A:19:THR:HB	1:A:24:GLN:HG2	1.91	0.52
1:A:222:GLU:OE1	1:B:388:ALA:HA	2.09	0.52
1:A:544:VAL:O	1:A:548:VAL:HG23	2.10	0.52
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.91	0.52
2:K:116:TYR:CD2	3:M:97:ILE:HD11	2.44	0.52
1:A:434:LEU:HD23	1:A:524:CYS:SG	2.50	0.52
2:K:119:LEU:HD12	2:K:122:TRP:CZ2	2.44	0.52
3:M:151:VAL:O	3:M:151:VAL:HG23	2.11	0.51
3:L:151:VAL:O	3:L:151:VAL:HG23	2.10	0.51
1:A:11:TYR:O	1:A:14:SER:OG	2.23	0.51
1:A:330:LYS:HB2	1:A:333:LEU:HD12	1.92	0.50
3:L:5:MET:SD	3:L:91:GLN:NE2	2.84	0.50
1:B:381:GLY:O	1:B:385:LEU:N	2.40	0.50
3:L:55:LEU:HD12	3:L:55:LEU:O	2.11	0.50
2:K:5:VAL:HG22	2:K:29:GLY:HA3	1.94	0.50
1:B:277:GLU:HG2	1:B:334:ILE:HD12	1.93	0.50
2:K:58:SER:HG	2:K:60:TYR:HE1	1.59	0.50
3:L:34:VAL:HG21	3:L:72:PHE:CZ	2.47	0.50
2:H:164:TYR:CE1	2:H:169:VAL:HG13	2.47	0.50
1:A:331:ILE:CG2	1:A:340:GLN:HB2	2.41	0.49
2:K:164:TYR:CE2	2:K:169:VAL:HG13	2.47	0.49
2:H:157:LEU:HD13	2:H:230:VAL:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:SER:CB	1:B:308:GLN:OE1	2.60	0.48
1:B:368:PHE:CE1	1:B:372:ILE:HD11	2.49	0.48
1:B:601:ARG:NH1	1:B:605:TYR:OH	2.46	0.48
1:A:613:LEU:O	1:A:617:LYS:N	2.47	0.48
2:K:147:SER:OG	2:K:150:THR:HG22	2.12	0.48
1:B:306:ASN:OD1	1:B:307:VAL:N	2.46	0.48
1:A:575:LEU:HB3	1:A:609:VAL:CG2	2.43	0.48
1:A:212:LYS:HE2	1:A:239:TYR:OH	2.14	0.48
1:A:229:ARG:CZ	1:A:278:LEU:HD23	2.44	0.47
1:A:297:LEU:HG	1:A:389:LEU:HD21	1.95	0.47
1:B:314:GLU:HG2	1:B:372:ILE:HD11	1.96	0.47
2:K:176:GLY:O	2:K:179:THR:HG23	2.14	0.47
1:A:228:TRP:HZ3	1:A:272:LEU:CD2	2.27	0.47
1:A:378:ASN:OD1	1:A:379:LYS:N	2.48	0.47
1:B:363:ARG:NH2	1:B:446:SER:OG	2.47	0.47
1:B:513:LEU:HD12	1:B:514:CYS:N	2.30	0.47
1:A:382:GLN:CG	1:A:406:ILE:HD12	2.45	0.47
1:B:360:ASN:ND2	1:B:443:GLN:OE1	2.48	0.47
1:A:382:GLN:HG2	1:A:406:ILE:HD12	1.97	0.46
1:A:439:TRP:CB	1:A:517:LEU:HD13	2.45	0.46
1:B:411:VAL:HG22	1:B:411:VAL:O	2.16	0.46
1:A:95:ASP:N	1:A:95:ASP:OD1	2.48	0.46
1:A:157:GLU:OE2	1:A:161:ARG:NH1	2.49	0.46
1:A:263:ASP:OD1	1:A:400:PHE:HB3	2.15	0.46
1:A:468:THR:HG21	1:A:478:SER:HB2	1.98	0.46
1:A:233:THR:HG22	1:A:278:LEU:HA	1.98	0.46
1:B:215:LEU:HD11	1:B:235:LEU:HD22	1.98	0.46
1:B:265:ALA:O	1:B:269:VAL:HG23	2.15	0.46
1:B:541:ARG:O	1:B:541:ARG:HG2	2.16	0.46
1:B:464:LEU:HD11	1:B:479:ILE:O	2.16	0.46
2:K:36:SER:O	2:K:101:ARG:HA	2.16	0.46
1:B:214:TYR:CD2	1:B:231:THR:HG21	2.51	0.45
1:B:541:ARG:NH2	2:K:55:TYR:O	2.50	0.45
2:H:86:MET:HB3	2:H:89:LEU:HD21	1.98	0.45
3:M:202:LEU:HD13	3:M:206:VAL:HG12	1.98	0.45
3:L:12:LEU:HD21	3:L:20:VAL:HG13	1.98	0.45
1:B:434:LEU:HD23	1:B:524:CYS:SG	2.57	0.45
1:A:170:ARG:NH2	1:A:173:GLU:OE1	2.50	0.45
1:B:369:LEU:HG	1:B:411:VAL:HG23	1.98	0.45
1:B:652:ILE:HD13	1:B:678:VAL:HG11	2.00	0.44
2:H:176:GLY:O	2:H:179:THR:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:GLN:NE2	1:B:633:PHE:O	2.44	0.44
1:B:244:LEU:HD11	1:B:430:HIS:NE2	2.32	0.44
2:K:178:LEU:HD21	2:K:201:VAL:HG11	2.00	0.44
3:M:38:GLN:HB2	3:M:48:LEU:HD11	2.00	0.44
1:B:499:LEU:HD11	1:B:523:LEU:HD22	1.99	0.44
1:B:613:LEU:O	1:B:617:LYS:N	2.49	0.44
1:A:322:ILE:O	1:A:326:VAL:HG23	2.18	0.44
1:B:365:LYS:HB2	1:B:368:PHE:HB2	2.00	0.43
1:B:575:LEU:HB3	1:B:609:VAL:CG2	2.48	0.43
2:H:197:LEU:C	2:H:197:LEU:HD12	2.38	0.43
3:L:7:GLN:NE2	3:L:103:THR:OG1	2.51	0.43
1:B:468:THR:HG22	1:B:470:ARG:H	1.83	0.43
1:A:517:LEU:HB3	1:A:518:PRO:HD3	2.00	0.43
2:K:144:ALA:HB2	2:K:230:VAL:CG1	2.48	0.43
2:K:36:SER:OG	2:K:56:SER:N	2.51	0.43
1:A:411:VAL:O	1:A:411:VAL:HG22	2.18	0.43
1:B:511:GLN:N	1:B:512:PRO:HD2	2.33	0.43
2:K:86:MET:HB3	2:K:89:LEU:HD21	2.01	0.43
1:A:606:TRP:CE3	1:A:650:ALA:HB2	2.54	0.42
1:A:222:GLU:HG3	1:A:223:SER:N	2.34	0.42
1:A:351:LEU:HD13	1:A:422:TYR:CZ	2.54	0.42
3:M:109:ARG:HG2	3:M:110:THR:N	2.34	0.42
1:A:538:LEU:HD12	1:A:555:VAL:HG21	2.00	0.42
1:B:360:ASN:OD1	1:B:513:LEU:HD11	2.20	0.42
1:B:410:ASP:O	1:B:411:VAL:HG12	2.19	0.42
2:K:7:LEU:HD21	2:K:30:PHE:CZ	2.54	0.42
1:A:315:LEU:HG	1:A:385:LEU:HD13	2.01	0.42
1:A:373:VAL:HG21	1:A:411:VAL:HB	2.01	0.42
1:A:571:GLN:NE2	1:A:633:PHE:O	2.46	0.42
1:B:385:LEU:HD23	1:B:401:LEU:HD11	2.00	0.42
1:A:229:ARG:O	1:A:233:THR:HG23	2.19	0.42
1:A:572:PRO:HB2	1:A:638:ILE:HD12	2.01	0.42
1:A:467:GLU:OE2	1:A:471:LEU:HD13	2.19	0.42
1:B:259:LEU:HD22	1:B:296:LEU:HD13	2.01	0.42
2:H:120:ASP:OD1	2:H:121:TYR:N	2.50	0.42
3:M:40:LYS:HB3	3:M:41:PRO:HD2	2.02	0.42
1:A:239:TYR:HB3	1:A:262:PHE:CD2	2.55	0.42
1:B:378:ASN:OD1	1:B:379:LYS:N	2.52	0.42
1:A:359:LEU:HD21	1:A:414:PRO:HG2	2.01	0.42
2:K:138:PRO:HB2	2:K:161:VAL:HG13	2.01	0.42
1:A:511:GLN:N	1:A:512:PRO:CD	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ILE:O	1:A:694:ILE:HG22	2.20	0.41
3:M:12:LEU:CD2	3:M:20:VAL:HG13	2.49	0.41
1:A:568:HIS:O	1:A:568:HIS:ND1	2.52	0.41
2:H:36:SER:O	2:H:101:ARG:HA	2.20	0.41
1:A:222:GLU:OE2	1:B:387:ASP:OD1	2.39	0.41
1:B:479:ILE:HD11	1:B:559:ILE:HD11	2.02	0.41
2:H:220:LYS:N	2:H:221:PRO:CD	2.83	0.41
1:A:310:ARG:O	1:A:314:GLU:HG3	2.21	0.41
2:H:119:LEU:HD12	2:H:122:TRP:CZ2	2.55	0.41
2:K:54:ILE:HG23	2:K:59:GLY:HA2	2.02	0.41
2:K:220:LYS:N	2:K:221:PRO:CD	2.84	0.41
1:A:385:LEU:CD2	1:A:401:LEU:HD11	2.47	0.41
1:A:609:VAL:O	1:A:612:LEU:N	2.54	0.41
1:B:517:LEU:HB3	1:B:518:PRO:HD3	2.03	0.41
1:B:609:VAL:HG12	1:B:613:LEU:HG	2.02	0.41
1:B:652:ILE:HD13	1:B:678:VAL:HG13	2.01	0.41
1:A:410:ASP:O	1:A:411:VAL:HG12	2.21	0.41
3:M:107:ILE:O	3:M:167:GLN:NE2	2.45	0.41
1:A:267:GLN:HG2	1:A:398:THR:O	2.21	0.41
2:H:52:ALA:HB1	2:H:73:ILE:HG21	2.03	0.41
3:L:51:SER:O	3:L:52:ALA:HB3	2.21	0.41
3:M:51:SER:O	3:M:52:ALA:HB3	2.21	0.41
3:M:116:VAL:HA	3:M:136:LEU:O	2.20	0.41
1:A:219:GLN:HA	1:A:222:GLU:OE2	2.20	0.41
1:B:479:ILE:CD1	1:B:559:ILE:HD11	2.50	0.41
2:K:153:GLY:O	2:K:205:SER:N	2.51	0.40
1:A:109:VAL:O	1:A:109:VAL:HG12	2.20	0.40
2:K:15:VAL:CG1	2:K:130:VAL:HG22	2.52	0.40
1:A:158:LEU:HD23	1:A:158:LEU:C	2.41	0.40
1:B:235:LEU:HD11	1:B:239:TYR:CZ	2.57	0.40
3:L:136:LEU:C	3:L:137:LEU:HD12	2.41	0.40
1:A:457:LEU:HD21	1:A:488:LEU:CD1	2.50	0.40
1:A:482:LEU:O	1:A:486:VAL:HG23	2.21	0.40
1:B:235:LEU:CD1	1:B:239:TYR:CE2	3.03	0.40
1:B:461:PHE:CE2	1:B:484:LEU:HD13	2.57	0.40
1:B:606:TRP:CE3	1:B:650:ALA:HB2	2.57	0.40
2:H:36:SER:OG	2:H:56:SER:N	2.55	0.40
1:B:467:GLU:OE1	1:B:601:ARG:NE	2.55	0.40
1:B:476:PRO:HG2	1:B:552:ARG:HG2	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	742/753 (98%)	733 (99%)	9 (1%)	0	100	100
1	B	588/753 (78%)	580 (99%)	8 (1%)	0	100	100
2	H	225/240 (94%)	221 (98%)	4 (2%)	0	100	100
2	K	225/240 (94%)	221 (98%)	4 (2%)	0	100	100
3	L	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
3	M	210/215 (98%)	208 (99%)	2 (1%)	0	100	100
All	All	2201/2416 (91%)	2172 (99%)	29 (1%)	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%)	665 (100%)	1 (0%)	93	96
1	B	527/673 (78%)	527 (100%)	0	100	100
2	H	187/200 (94%)	186 (100%)	1 (0%)	88	93
2	K	187/200 (94%)	186 (100%)	1 (0%)	88	93
3	L	188/190 (99%)	188 (100%)	0	100	100
3	M	187/190 (98%)	187 (100%)	0	100	100
All	All	1942/2126 (91%)	1939 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	696	ASN
2	H	101	ARG
2	K	101	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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%)	-0.27	10 (1%) 77 68	110, 194, 291, 398	0
1	B	594/753 (78%)	-0.32	8 (1%) 77 68	109, 190, 334, 432	0
2	H	227/240 (94%)	-0.26	3 (1%) 77 68	112, 180, 256, 340	0
2	K	227/240 (94%)	-0.12	9 (3%) 38 31	132, 213, 288, 357	0
3	L	213/215 (99%)	-0.22	1 (0%) 91 85	135, 199, 258, 301	0
3	M	212/215 (98%)	-0.10	3 (1%) 75 66	137, 217, 286, 299	0
All	All	2219/2416 (91%)	-0.25	34 (1%) 73 64	109, 196, 299, 432	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	158	GLY	6.7
1	B	181	LEU	5.3
2	K	159	CYS	5.0
1	B	162	PRO	4.5
3	L	89	CYS	4.3
1	A	29	GLY	4.1
1	A	57	GLU	3.3
1	B	393	GLN	3.2
1	A	304	SER	2.9
2	H	159	CYS	2.9
2	H	229	LYS	2.9
2	K	146	SER	2.8
1	B	394	SER	2.8
1	A	301	GLY	2.8
1	B	505	SER	2.7
3	M	35	ALA	2.7
2	H	38	HIS	2.7
2	K	148	LYS	2.5
1	A	39	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	38	HIS	2.4
2	K	149	SER	2.4
1	A	365	LYS	2.3
2	K	99	CYS	2.3
1	B	163	ASP	2.3
3	M	2	ASP	2.3
1	B	182	LYS	2.2
2	K	147	SER	2.2
3	M	89	CYS	2.2
1	A	3	ARG	2.2
1	B	193	ARG	2.2
1	A	505	SER	2.2
1	A	319	CYS	2.2
2	K	150	THR	2.1
1	A	398	THR	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 monosaccharides 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.