



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:57 am GMT

PDB ID : 3HHW
Title : Complex of a vesicular stomatitis virus empty capsid with the nucleocapsid-binding domain of the phosphoprotein
Authors : Green, T.J.; Luo, M.
Deposited on : 2009-05-18
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

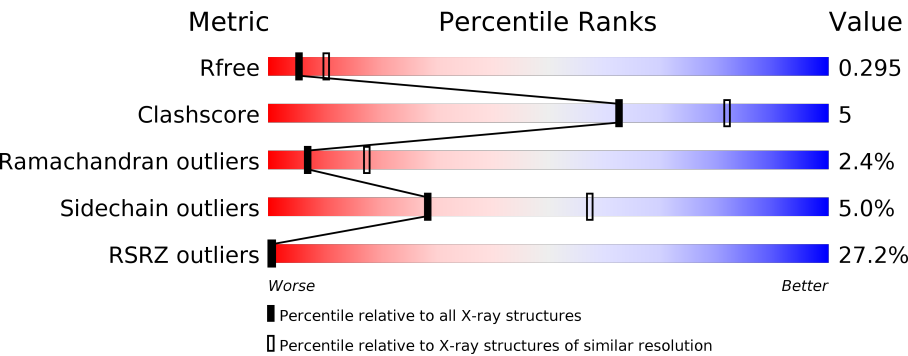
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	87	<div><div>22%</div><div><div>74%</div><div>9%</div><div>•</div><div>16%</div></div></div>
1	B	87	<div><div>74%</div><div><div>74%</div><div>10%</div><div>•</div><div>16%</div></div></div>
1	C	87	<div><div>25%</div><div><div>69%</div><div>13%</div><div>•</div><div>16%</div></div></div>
1	D	87	<div><div>63%</div><div><div>72%</div><div>9%</div><div>•</div><div>16%</div></div></div>
1	E	87	<div><div>67%</div><div><div>75%</div><div>9%</div><div>•</div><div>16%</div></div></div>
2	K	421	<div><div>17%</div><div><div>80%</div><div>18%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
2	L	421	
2	M	421	
2	N	421	
2	O	421	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TAR	K	423	X	-	-	X
3	TAR	K	424	X	-	-	-
3	TAR	K	425	X	-	-	-
3	TAR	K	426	X	-	-	X
3	TAR	M	1	X	-	-	-
3	TAR	O	423	X	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19615 atoms, of which 0 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	B	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	C	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	D	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	E	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	GLY	-	EXPRESSION TAG	UNP P04880
A	180	SER	-	EXPRESSION TAG	UNP P04880
A	181	HIS	-	EXPRESSION TAG	UNP P04880
A	182	MET	-	EXPRESSION TAG	UNP P04880
B	179	GLY	-	EXPRESSION TAG	UNP P04880
B	180	SER	-	EXPRESSION TAG	UNP P04880
B	181	HIS	-	EXPRESSION TAG	UNP P04880
B	182	MET	-	EXPRESSION TAG	UNP P04880
C	179	GLY	-	EXPRESSION TAG	UNP P04880
C	180	SER	-	EXPRESSION TAG	UNP P04880
C	181	HIS	-	EXPRESSION TAG	UNP P04880
C	182	MET	-	EXPRESSION TAG	UNP P04880
D	179	GLY	-	EXPRESSION TAG	UNP P04880
D	180	SER	-	EXPRESSION TAG	UNP P04880
D	181	HIS	-	EXPRESSION TAG	UNP P04880
D	182	MET	-	EXPRESSION TAG	UNP P04880
E	179	GLY	-	EXPRESSION TAG	UNP P04880
E	180	SER	-	EXPRESSION TAG	UNP P04880
E	181	HIS	-	EXPRESSION TAG	UNP P04880

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Chain	Residue	Modelled	Actual	Comment	Reference
E	182	MET	-	EXPRESSION TAG	UNP P04880

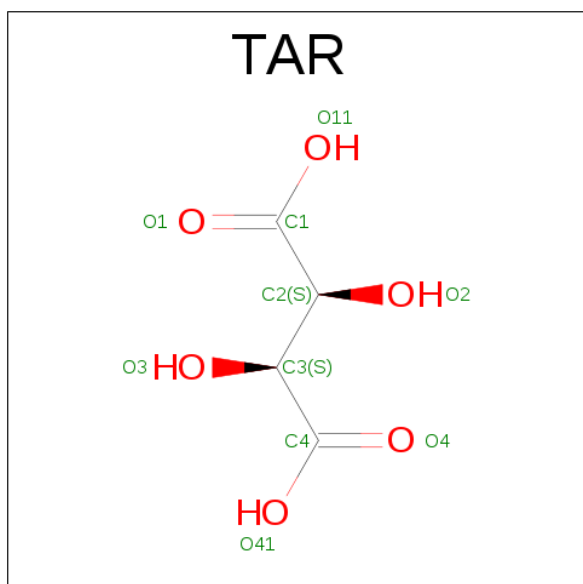
- Molecule 2 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	L	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	M	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	N	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	O	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	290	TRP	SER	ENGINEERED	UNP Q77E03
L	290	TRP	SER	ENGINEERED	UNP Q77E03
M	290	TRP	SER	ENGINEERED	UNP Q77E03
N	290	TRP	SER	ENGINEERED	UNP Q77E03
O	290	TRP	SER	ENGINEERED	UNP Q77E03

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).

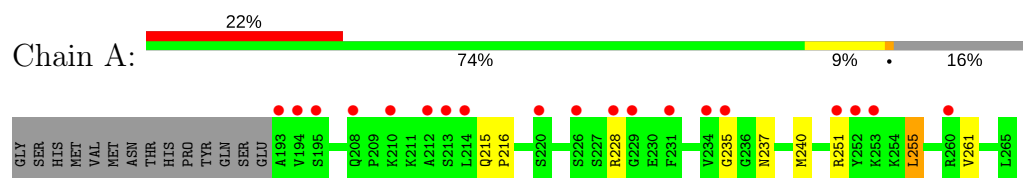


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	O	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		

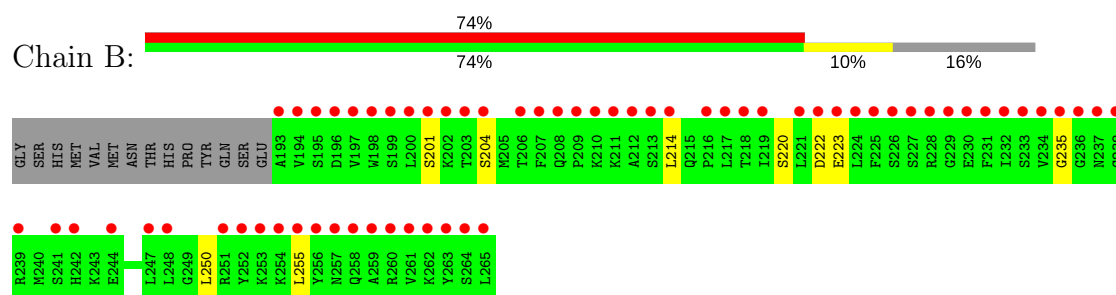
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

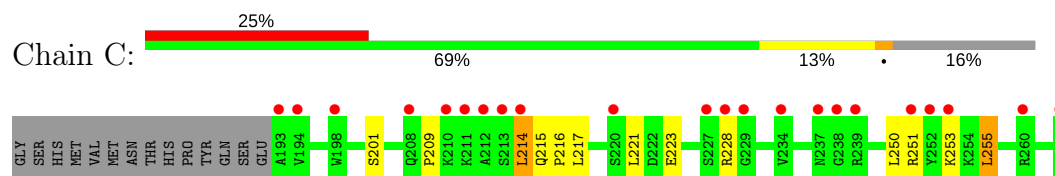
• Molecule 1: Phosphoprotein



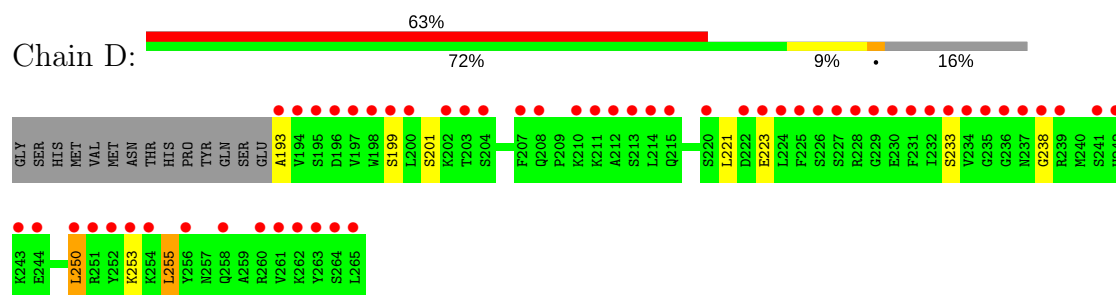
• Molecule 1: Phosphoprotein



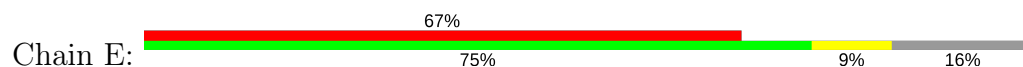
• Molecule 1: Phosphoprotein

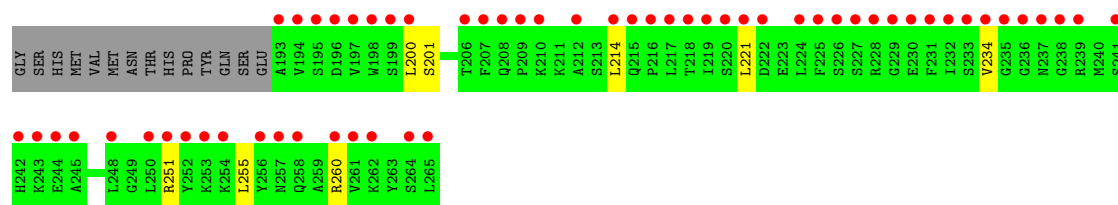


• Molecule 1: Phosphoprotein

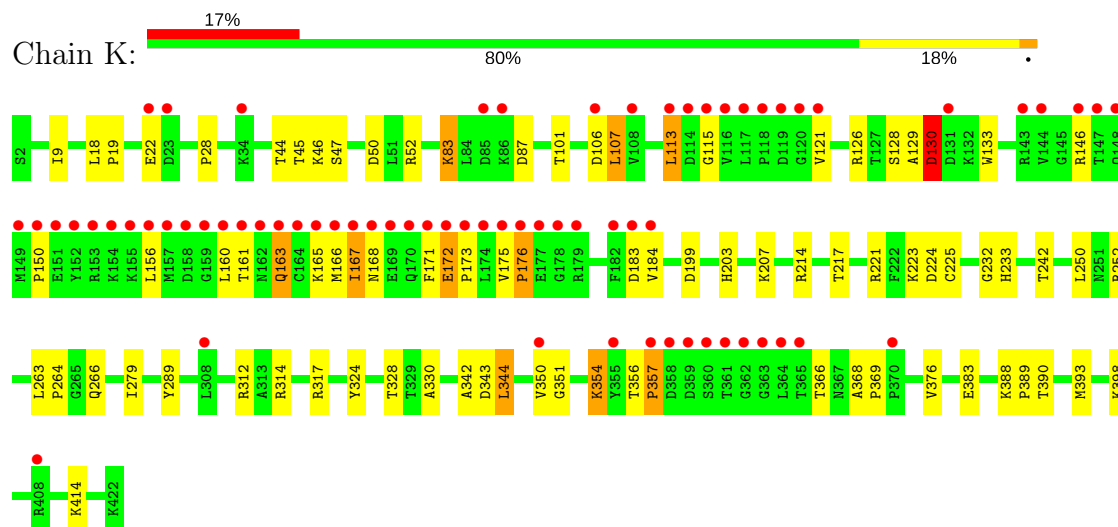


• Molecule 1: Phosphoprotein

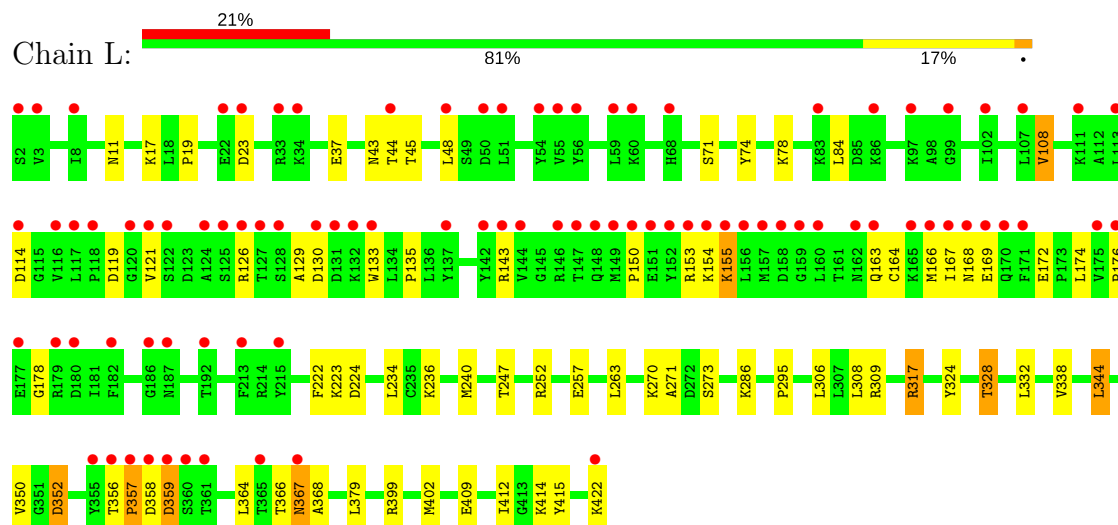




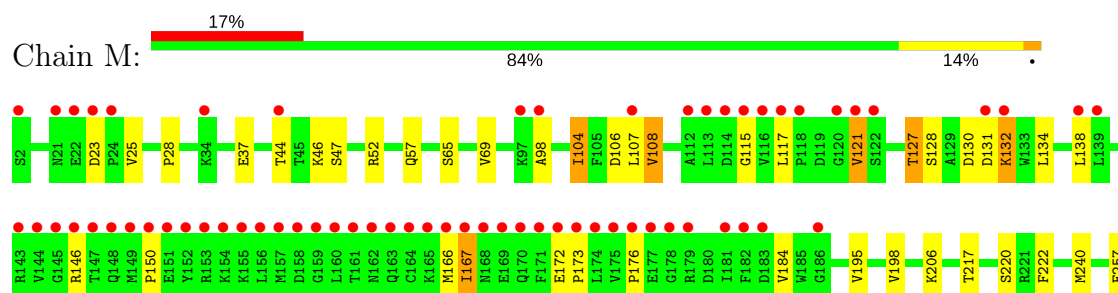
• Molecule 2: Nucleoprotein

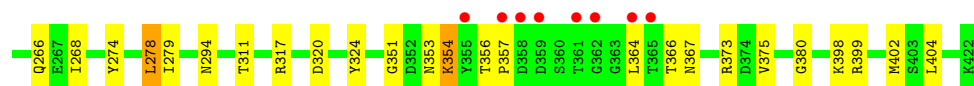


• Molecule 2: Nucleoprotein

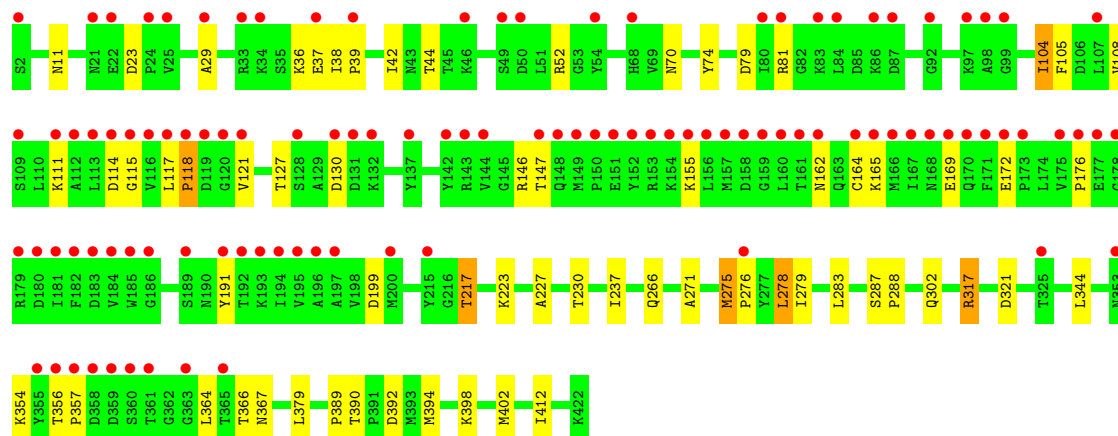
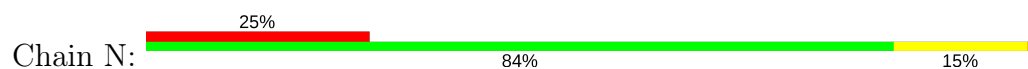


• Molecule 2: Nucleoprotein

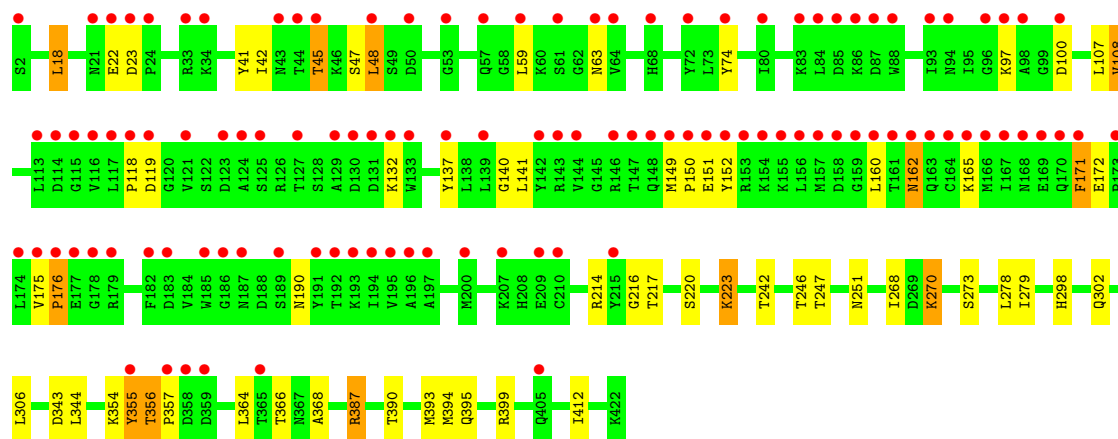
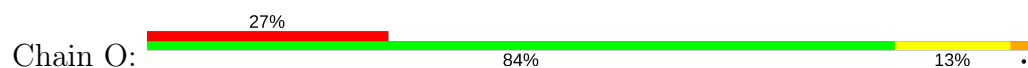




• Molecule 2: Nucleoprotein



• Molecule 2: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.60Å 234.52Å 95.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	73.7 (30.00-2.70) 73.7 (29.95-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.263 , 0.296 0.262 , 0.295	Depositor DCC
R_{free} test set	3839 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19615	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAR

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	0.34	0/584	0.49	0/778
1	B	0.34	0/584	0.49	0/778
1	C	0.34	0/584	0.54	0/778
1	D	0.33	0/584	0.50	0/778
1	E	0.33	0/584	0.47	0/778
2	K	0.36	0/3413	0.50	0/4622
2	L	0.35	0/3413	0.49	0/4622
2	M	0.35	0/3413	0.50	0/4622
2	N	0.34	0/3413	0.47	0/4622
2	O	0.35	0/3413	0.50	0/4622
All	All	0.35	0/19985	0.49	0/27000

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	576	0	597	12	0
1	B	576	0	597	3	0
1	C	576	0	597	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	576	0	597	4	0
1	E	576	0	597	3	0
2	K	3335	0	3292	52	0
2	L	3335	0	3292	37	0
2	M	3335	0	3292	43	0
2	N	3335	0	3292	31	0
2	O	3335	0	3292	32	0
3	K	40	0	16	0	0
3	M	10	0	4	0	0
3	O	10	0	4	0	0
All	All	19615	0	19469	197	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 (197) 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:255:LEU:CD2	2:K:366:THR:HG23	2.00	0.90
2:M:356:THR:H	2:M:357:PRO:HD2	1.41	0.83
2:M:356:THR:N	2:M:357:PRO:HD2	1.95	0.82
2:K:214:ARG:HA	2:K:217:THR:HG22	1.63	0.79
2:O:220:SER:O	2:O:223:LYS:HG3	1.82	0.77
2:K:389:PRO:HA	2:K:393:MET:HE3	1.66	0.76
2:N:302:GLN:HB2	2:N:412:ILE:HD13	1.68	0.74
2:K:324:TYR:O	2:K:328:THR:HG23	1.87	0.74
2:L:324:TYR:O	2:L:328:THR:HG23	1.89	0.71
2:O:302:GLN:HB3	2:O:412:ILE:HD13	1.70	0.71
1:A:255:LEU:HD22	2:K:366:THR:CG2	2.22	0.70
1:A:261:VAL:HG21	2:K:376:VAL:HG12	1.72	0.70
2:L:317:ARG:NE	2:L:317:ARG:H	1.89	0.70
1:A:255:LEU:HD22	2:K:366:THR:HG23	1.75	0.69
2:O:356:THR:N	2:O:357:PRO:HD3	2.09	0.67
2:M:366:THR:HG23	2:M:367:ASN:H	1.61	0.66
2:M:356:THR:H	2:M:357:PRO:CD	2.09	0.65
2:M:320:ASP:HA	2:M:324:TYR:OH	1.96	0.65
1:A:251:ARG:HH21	1:A:251:ARG:HG2	1.61	0.64
2:M:356:THR:N	2:M:357:PRO:CD	2.61	0.63
1:A:255:LEU:CD2	2:K:366:THR:CG2	2.74	0.62
2:K:160:LEU:HD13	2:K:171:PHE:HD2	1.65	0.62
2:N:29:ALA:H	2:N:266:GLN:HE22	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:172:GLU:H	2:K:173:PRO:HD3	1.65	0.62
2:M:130:ASP:C	2:M:132:LYS:H	2.04	0.61
2:L:17:LYS:HB2	2:M:268:ILE:HD11	1.81	0.61
2:K:172:GLU:N	2:K:173:PRO:CD	2.63	0.61
2:K:9:ILE:HD13	2:L:252:ARG:HH22	1.64	0.61
2:N:146:ARG:HE	2:N:223:LYS:HE2	1.65	0.61
2:L:422:LYS:HE2	2:M:399:ARG:HB3	1.82	0.61
2:K:172:GLU:H	2:K:173:PRO:CD	2.13	0.60
2:K:47:SER:HB2	2:K:50:ASP:HB2	1.85	0.59
2:N:390:THR:HG22	2:N:392:ASP:H	1.68	0.59
1:D:250:LEU:HD12	1:D:255:LEU:HD13	1.85	0.58
2:K:342:ALA:HB1	2:K:344:LEU:HD23	1.84	0.58
2:L:317:ARG:HE	2:L:317:ARG:H	1.50	0.58
2:L:366:THR:C	2:L:368:ALA:H	2.07	0.58
2:O:387:ARG:HH11	2:O:387:ARG:CG	2.17	0.57
2:N:70:ASN:HD21	2:N:191:TYR:HB2	1.68	0.57
2:M:37:GLU:HB2	2:M:108:VAL:HG21	1.87	0.57
2:M:240:MET:HE2	2:M:373:ARG:HD3	1.87	0.57
2:M:28:PRO:HG3	2:M:278:LEU:HD23	1.86	0.56
2:O:395:GLN:O	2:O:399:ARG:HG2	2.06	0.56
2:N:278:LEU:HA	2:N:283:LEU:HD12	1.88	0.56
2:O:107:LEU:O	2:O:108:VAL:HB	2.06	0.56
2:K:160:LEU:HD23	2:K:163:GLN:HE21	1.71	0.55
2:K:354:LYS:HE3	2:K:356:THR:HA	1.88	0.55
2:M:65:SER:HB2	2:M:117:LEU:HD22	1.87	0.55
1:A:251:ARG:NH2	1:A:251:ARG:HG2	2.22	0.55
2:K:106:ASP:OD1	2:K:107:LEU:N	2.39	0.55
2:K:366:THR:O	2:K:366:THR:HG23	2.07	0.55
1:A:255:LEU:HD23	2:K:366:THR:HG23	1.87	0.55
2:L:379:LEU:HB3	2:M:354:LYS:HD2	1.89	0.54
2:O:270:LYS:HD2	2:O:273:SER:HB2	1.89	0.54
2:L:240:MET:CE	2:L:338:VAL:HG22	2.37	0.54
2:K:224:ASP:OD1	2:K:279:ILE:HG21	2.08	0.54
2:K:184:VAL:HG11	2:L:164:CYS:HB2	1.89	0.54
2:K:350:VAL:HG23	2:O:247:THR:HG21	1.90	0.54
2:N:398:LYS:O	2:N:402:MET:HB2	2.07	0.54
2:O:364:LEU:C	2:O:366:THR:H	2.12	0.53
2:K:52:ARG:HD3	2:K:130:ASP:HB3	1.88	0.53
2:N:44:THR:H	2:N:111:LYS:HE3	1.74	0.52
2:K:390:THR:H	2:K:393:MET:CE	2.23	0.52
2:K:113:LEU:HD13	2:K:113:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:SER:HB2	1:B:222:ASP:HB2	1.91	0.51
2:M:240:MET:CE	2:M:373:ARG:HD3	2.40	0.51
2:M:106:ASP:C	2:M:107:LEU:HD12	2.31	0.51
2:M:57:GLN:HB3	2:M:121:VAL:HB	1.93	0.51
2:O:45:THR:HG21	2:O:48:LEU:HD12	1.90	0.51
2:O:140:GLY:HA2	2:O:216:GLY:HA3	1.92	0.51
2:L:223:LYS:O	2:L:224:ASP:HB2	2.10	0.51
2:O:387:ARG:HG2	2:O:387:ARG:HH11	1.76	0.51
2:N:389:PRO:HB2	2:N:394:MET:HE1	1.93	0.51
1:E:234:VAL:HG12	1:E:251:ARG:HH21	1.75	0.51
1:A:255:LEU:HD22	2:K:366:THR:HG21	1.93	0.51
2:M:130:ASP:O	2:M:132:LYS:N	2.44	0.51
2:K:223:LYS:O	2:K:224:ASP:HB2	2.11	0.50
2:M:172:GLU:HB2	2:M:173:PRO:HD3	1.91	0.50
2:O:242:THR:O	2:O:246:THR:HG23	2.11	0.50
1:C:201:SER:HA	1:C:221:LEU:HB2	1.93	0.50
1:D:253:LYS:HD2	2:N:367:ASN:HB2	1.94	0.50
2:M:184:VAL:HG13	2:N:165:LYS:HG2	1.94	0.50
2:N:389:PRO:HB2	2:N:394:MET:CE	2.41	0.49
2:K:167:ILE:HG12	2:K:168:ASN:H	1.77	0.49
2:O:41:TYR:HB2	2:O:190:ASN:HD21	1.75	0.49
2:M:132:LYS:HG3	2:M:166:MET:HB2	1.94	0.49
2:L:174:LEU:HB2	2:L:178:GLY:HA3	1.94	0.48
2:L:133:TRP:HE3	2:L:163:GLN:HE22	1.61	0.48
2:O:390:THR:H	2:O:393:MET:HE3	1.78	0.48
2:K:83:LYS:HB2	2:K:101:THR:HG22	1.95	0.48
2:L:257:GLU:OE2	2:L:295:PRO:HD2	2.14	0.48
2:M:130:ASP:C	2:M:132:LYS:N	2.67	0.48
2:L:399:ARG:HA	2:L:402:MET:HE2	1.94	0.48
2:M:132:LYS:HG2	2:M:167:ILE:HG12	1.96	0.48
1:E:260:ARG:HG2	2:K:357:PRO:HB3	1.95	0.48
2:K:376:VAL:HG21	2:L:352:ASP:HB3	1.95	0.48
2:O:387:ARG:NH1	2:O:387:ARG:HG2	2.29	0.47
2:L:328:THR:HG21	2:L:415:TYR:OH	2.15	0.47
2:K:203:HIS:HD2	2:K:214:ARG:HH22	1.62	0.47
2:M:44:THR:HG23	2:M:46:LYS:HE2	1.97	0.47
2:N:147:THR:HG21	2:N:155:LYS:HG3	1.97	0.47
2:K:232:GLY:HA2	2:O:18:LEU:HD21	1.97	0.47
2:O:42:ILE:HD13	2:O:74:TYR:HB2	1.96	0.47
1:D:201:SER:HA	1:D:221:LEU:HB2	1.97	0.47
2:N:164:CYS:HB3	2:N:169:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:162:ASN:HA	2:O:165:LYS:HE3	1.96	0.47
2:K:203:HIS:CG	2:K:221:ARG:HH21	2.33	0.46
2:K:225:CYS:HA	2:K:289:TYR:HB2	1.96	0.46
2:O:214:ARG:HA	2:O:217:THR:OG1	2.15	0.46
1:C:223:GLU:HB3	2:M:364:LEU:HD21	1.97	0.46
2:M:278:LEU:HD13	2:M:279:ILE:HG12	1.96	0.46
2:K:242:THR:HG22	2:O:18:LEU:HD22	1.97	0.46
2:K:45:THR:HG22	2:K:46:LYS:H	1.81	0.45
2:M:132:LYS:HG3	2:M:166:MET:CB	2.46	0.45
2:M:217:THR:O	2:M:220:SER:HB3	2.16	0.45
2:N:275:MET:HG3	2:N:276:PRO:HD3	1.98	0.45
1:C:209:PRO:HB3	1:C:214:LEU:HB3	1.98	0.45
2:K:368:ALA:HB1	2:K:369:PRO:HD2	1.98	0.45
2:L:270:LYS:HD3	2:L:273:SER:HB2	1.99	0.45
2:M:380:GLY:HA2	2:N:354:LYS:HE2	1.99	0.45
1:C:253:LYS:HB2	1:C:255:LEU:HG	1.99	0.44
2:O:366:THR:C	2:O:368:ALA:H	2.21	0.44
2:K:133:TRP:HB2	2:K:163:GLN:HG3	2.00	0.44
2:L:37:GLU:HB2	2:L:108:VAL:HG21	1.99	0.44
2:L:306:LEU:HD22	2:L:412:ILE:HD12	2.00	0.44
2:N:364:LEU:C	2:N:366:THR:H	2.20	0.44
2:K:161:THR:HG22	2:K:165:LYS:HE3	1.99	0.44
2:L:350:VAL:HG12	2:L:350:VAL:O	2.18	0.44
2:M:69:VAL:HG13	2:M:138:LEU:HD13	2.00	0.44
2:L:143:ARG:HH21	2:L:155:LYS:HE2	1.82	0.44
2:M:320:ASP:HA	2:M:324:TYR:HH	1.82	0.44
2:M:364:LEU:O	2:M:366:THR:HG22	2.18	0.44
2:N:104:ILE:HG22	2:N:105:PHE:H	1.83	0.44
2:N:162:ASN:HA	2:N:165:LYS:HE3	2.00	0.44
2:L:357:PRO:C	2:L:359:ASP:H	2.21	0.44
2:L:422:LYS:HB3	2:M:402:MET:SD	2.58	0.44
2:N:37:GLU:HB2	2:N:108:VAL:HG21	2.00	0.44
2:L:167:ILE:HG22	2:L:168:ASN:N	2.32	0.43
2:O:160:LEU:HD22	2:O:171:PHE:HD2	1.83	0.43
2:K:28:PRO:HD2	2:K:266:GLN:OE1	2.19	0.43
2:L:130:ASP:O	2:L:135:PRO:HD3	2.17	0.43
2:O:298:HIS:O	2:O:302:GLN:HB2	2.19	0.43
2:O:387:ARG:NH1	2:O:387:ARG:CG	2.81	0.43
1:A:235:GLY:HA3	2:L:364:LEU:HD13	2.00	0.43
2:K:175:VAL:HB	2:K:176:PRO:HD3	2.01	0.43
2:L:126:ARG:HH21	2:L:129:ALA:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ALA:N	1:D:199:SER:HG	2.17	0.43
2:N:79:ASP:HB2	2:N:81:ARG:HG3	2.00	0.43
1:A:215:GLN:HA	1:A:216:PRO:HD3	1.95	0.43
2:L:409:GLU:HA	2:L:414:LYS:HD2	2.01	0.43
1:A:237:ASN:HB2	1:A:240:MSE:HG3	2.01	0.42
2:K:126:ARG:NH2	2:K:129:ALA:HB3	2.34	0.42
2:O:278:LEU:HG	2:O:279:ILE:HD12	2.00	0.42
2:M:195:VAL:HG13	2:M:217:THR:HG22	2.00	0.42
2:M:366:THR:HG23	2:M:367:ASN:N	2.31	0.42
2:O:137:TYR:O	2:O:141:LEU:HG	2.19	0.42
2:L:366:THR:C	2:L:368:ALA:N	2.73	0.42
2:L:74:TYR:O	2:L:78:LYS:HB2	2.19	0.42
2:M:52:ARG:HD3	2:M:130:ASP:OD2	2.20	0.42
2:N:317:ARG:HG2	2:N:317:ARG:H	1.56	0.42
2:L:164:CYS:SG	2:L:169:GLU:HG2	2.60	0.42
2:M:104:ILE:HD13	2:M:198:VAL:HG22	2.02	0.42
2:N:117:LEU:N	2:N:118:PRO:CD	2.83	0.42
1:B:220:SER:HB3	1:B:223:GLU:HG2	2.01	0.42
2:K:390:THR:H	2:K:393:MET:HE2	1.85	0.42
2:L:23:ASP:HB3	2:L:286:LYS:HE3	2.02	0.42
2:K:19:PRO:HB3	2:L:222:PHE:CZ	2.55	0.42
2:M:257:GLU:HB3	2:M:294:ASN:HD22	1.85	0.42
2:O:387:ARG:CB	2:O:387:ARG:HH11	2.32	0.42
1:C:215:GLN:HA	1:C:216:PRO:HD3	1.95	0.41
2:K:314:ARG:HG2	2:K:314:ARG:H	1.60	0.41
2:N:278:LEU:HD13	2:N:279:ILE:HG12	2.02	0.41
2:O:387:ARG:HH11	2:O:387:ARG:HB3	1.86	0.41
1:C:253:LYS:HD2	2:M:367:ASN:HB2	2.02	0.41
2:O:149:MET:C	2:O:151:GLU:H	2.23	0.41
1:E:201:SER:HA	1:E:221:LEU:HB2	2.02	0.41
2:N:38:ILE:HA	2:N:39:PRO:HD3	1.86	0.41
2:N:287:SER:HA	2:N:288:PRO:HD3	1.86	0.41
2:L:19:PRO:HB3	2:M:222:PHE:CZ	2.56	0.41
2:K:330:ALA:HB2	2:L:344:LEU:HD21	2.03	0.41
2:M:127:THR:OG1	2:M:128:SER:N	2.52	0.41
2:K:199:ASP:OD1	2:K:217:THR:HG23	2.21	0.41
2:M:107:LEU:HD23	2:M:274:TYR:HE2	1.86	0.41
2:N:199:ASP:HB2	2:N:217:THR:HG22	2.01	0.41
2:M:28:PRO:HD2	2:M:266:GLN:OE1	2.21	0.41
2:K:224:ASP:CG	2:K:279:ILE:HG21	2.41	0.41
2:N:227:ALA:HA	2:N:230:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:175:VAL:HB	2:O:176:PRO:HD3	2.03	0.41
2:N:52:ARG:NH2	2:N:127:THR:HA	2.36	0.40
2:K:263:LEU:HA	2:K:264:PRO:HD3	1.93	0.40
2:N:356:THR:N	2:N:357:PRO:HD3	2.36	0.40
2:N:42:ILE:HD13	2:N:74:TYR:HB2	2.04	0.40
2:K:233:HIS:CE1	2:K:312:ARG:HD2	2.57	0.40
2:L:43:ASN:HA	2:L:44:THR:HA	1.74	0.40
1:B:204:SER:HB3	1:B:220:SER:HB2	2.03	0.40
1:C:214:LEU:HD23	1:C:215:GLN:H	1.86	0.40
2:O:355:TYR:HB2	2:O:357:PRO:HD3	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	71/87 (82%)	62 (87%)	8 (11%)	1 (1%)	13	33
1	B	71/87 (82%)	59 (83%)	11 (16%)	1 (1%)	13	33
1	C	71/87 (82%)	60 (84%)	10 (14%)	1 (1%)	13	33
1	D	71/87 (82%)	58 (82%)	11 (16%)	2 (3%)	6	14
1	E	71/87 (82%)	64 (90%)	7 (10%)	0	100	100
2	K	419/421 (100%)	377 (90%)	29 (7%)	13 (3%)	5	11
2	L	419/421 (100%)	373 (89%)	35 (8%)	11 (3%)	6	15
2	M	419/421 (100%)	372 (89%)	37 (9%)	10 (2%)	7	17
2	N	419/421 (100%)	376 (90%)	36 (9%)	7 (2%)	11	27
2	O	419/421 (100%)	369 (88%)	37 (9%)	13 (3%)	5	11
All	All	2450/2540 (96%)	2170 (89%)	221 (9%)	59 (2%)	7	17

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	44	THR
2	K	357	PRO
2	L	357	PRO
2	M	176	PRO
2	K	115	GLY
2	K	176	PRO
2	M	98	ALA
2	M	131	ASP
2	N	118	PRO
2	N	130	ASP
2	N	176	PRO
2	O	22	GLU
2	O	108	VAL
1	D	238	GLY
2	K	146	ARG
2	K	351	GLY
2	L	150	PRO
2	L	176	PRO
2	L	271	ALA
2	M	115	GLY
2	M	127	THR
2	N	271	ALA
2	O	47	SER
2	O	119	ASP
2	O	343	ASP
1	A	228	ARG
1	C	251	ARG
2	L	45	THR
2	L	121	VAL
2	L	358	ASP
2	L	359	ASP
2	O	63	ASN
2	O	344	LEU
1	D	233	SER
2	K	130	ASP
2	K	150	PRO
2	K	172	GLU
2	K	343	ASP
2	K	344	LEU
2	L	172	GLU
2	L	367	ASN
2	M	47	SER

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Mol	Chain	Res	Type
2	M	108	VAL
2	O	45	THR
2	O	118	PRO
2	K	121	VAL
2	K	167	ILE
2	L	108	VAL
2	M	351	GLY
1	B	235	GLY
2	N	115	GLY
2	O	356	THR
2	M	150	PRO
2	M	167	ILE
2	N	121	VAL
2	O	172	GLU
2	N	172	GLU
2	O	150	PRO
2	O	176	PRO

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	64/75 (85%)	63 (98%)	1 (2%)	68	89
1	B	64/75 (85%)	61 (95%)	3 (5%)	30	60
1	C	64/75 (85%)	59 (92%)	5 (8%)	15	33
1	D	64/75 (85%)	61 (95%)	3 (5%)	30	60
1	E	64/75 (85%)	61 (95%)	3 (5%)	30	60
2	K	362/362 (100%)	341 (94%)	21 (6%)	23	50
2	L	362/362 (100%)	339 (94%)	23 (6%)	20	45
2	M	362/362 (100%)	346 (96%)	16 (4%)	33	63
2	N	362/362 (100%)	349 (96%)	13 (4%)	40	70
2	O	362/362 (100%)	343 (95%)	19 (5%)	27	55
All	All	2130/2185 (98%)	2023 (95%)	107 (5%)	28	57

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	LEU
1	B	214	LEU
1	B	250	LEU
1	B	255	LEU
1	C	214	LEU
1	C	217	LEU
1	C	228	ARG
1	C	250	LEU
1	C	255	LEU
1	D	223	GLU
1	D	250	LEU
1	D	255	LEU
1	E	200	LEU
1	E	214	LEU
1	E	255	LEU
2	K	18	LEU
2	K	22	GLU
2	K	83	LYS
2	K	87	ASP
2	K	107	LEU
2	K	113	LEU
2	K	128	SER
2	K	130	ASP
2	K	156	LEU
2	K	163	GLN
2	K	166	MET
2	K	183	ASP
2	K	207	LYS
2	K	250	LEU
2	K	252	ARG
2	K	317	ARG
2	K	354	LYS
2	K	383	GLU
2	K	388	LYS
2	K	398	LYS
2	K	414	LYS
2	L	11	ASN
2	L	48	LEU
2	L	71	SER
2	L	84	LEU
2	L	114	ASP
2	L	119	ASP

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Mol	Chain	Res	Type
2	L	153	ARG
2	L	154	LYS
2	L	155	LYS
2	L	166	MET
2	L	234	LEU
2	L	236	LYS
2	L	247	THR
2	L	263	LEU
2	L	308	LEU
2	L	309	ARG
2	L	317	ARG
2	L	328	THR
2	L	332	LEU
2	L	344	LEU
2	L	352	ASP
2	L	356	THR
2	L	367	ASN
2	M	23	ASP
2	M	25	VAL
2	M	104	ILE
2	M	121	VAL
2	M	132	LYS
2	M	134	LEU
2	M	146	ARG
2	M	206	LYS
2	M	278	LEU
2	M	311	THR
2	M	317	ARG
2	M	353	ASN
2	M	354	LYS
2	M	375	VAL
2	M	398	LYS
2	M	404	LEU
2	N	11	ASN
2	N	23	ASP
2	N	36	LYS
2	N	104	ILE
2	N	114	ASP
2	N	217	THR
2	N	237	ILE
2	N	275	MET
2	N	278	LEU

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Mol	Chain	Res	Type
2	N	317	ARG
2	N	321	ASP
2	N	344	LEU
2	N	379	LEU
2	O	18	LEU
2	O	23	ASP
2	O	48	LEU
2	O	59	LEU
2	O	97	LYS
2	O	100	ASP
2	O	132	LYS
2	O	152	TYR
2	O	162	ASN
2	O	171	PHE
2	O	223	LYS
2	O	251	ASN
2	O	268	ILE
2	O	270	LYS
2	O	306	LEU
2	O	354	LYS
2	O	355	TYR
2	O	387	ARG
2	O	394	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	B	237	ASN
1	B	258	GLN
2	K	163	GLN
2	K	203	HIS
2	K	294	ASN
2	K	395	GLN
2	L	163	GLN
2	L	187	ASN
2	L	251	ASN
2	L	386	ASN
2	L	395	GLN
2	M	57	GLN
2	M	203	HIS
2	M	251	ASN

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Mol	Chain	Res	Type
2	M	294	ASN
2	M	347	GLN
2	M	371	GLN
2	N	11	ASN
2	N	57	GLN
2	N	70	ASN
2	N	251	ASN
2	N	266	GLN
2	N	294	ASN
2	N	302	GLN
2	N	385	GLN
2	O	70	ASN
2	O	203	HIS
2	O	251	ASN
2	O	347	GLN
2	O	395	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAR	K	423	-	3,9,9	0.54	0	6,12,12	0.49	0
3	TAR	K	424	-	3,9,9	0.57	0	6,12,12	0.78	0
3	TAR	K	425	-	3,9,9	0.58	0	6,12,12	0.74	0
3	TAR	K	426	-	3,9,9	0.47	0	6,12,12	0.73	0
3	TAR	M	1	-	3,9,9	0.47	0	6,12,12	0.91	0
3	TAR	O	423	-	3,9,9	0.50	0	6,12,12	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAR	K	423	-	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	K	424	-	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	K	425	-	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	K	426	-	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	M	1	-	1/1/4/4	0/4/12/12	0/0/0/0
3	TAR	O	423	-	1/1/4/4	0/4/12/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	K	424	TAR	C2
3	K	423	TAR	C2
3	M	1	TAR	C2
3	K	426	TAR	C2
3	O	423	TAR	C2
3	K	425	TAR	C2

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	71/87 (81%)	1.60	19 (26%) 1 0	59, 84, 88, 89	0
1	B	71/87 (81%)	5.58	64 (90%) 0 0	137, 145, 147, 147	0
1	C	71/87 (81%)	1.82	22 (30%) 0 0	71, 87, 92, 92	0
1	D	71/87 (81%)	4.27	55 (77%) 0 0	107, 126, 127, 127	0
1	E	71/87 (81%)	4.39	58 (81%) 0 0	119, 133, 135, 135	0
2	K	421/421 (100%)	1.07	70 (16%) 2 1	31, 49, 111, 120	0
2	L	421/421 (100%)	1.30	90 (21%) 1 1	33, 62, 132, 139	0
2	M	421/421 (100%)	1.21	73 (17%) 2 1	31, 53, 116, 126	0
2	N	421/421 (100%)	1.52	106 (25%) 1 0	36, 66, 139, 145	0
2	O	421/421 (100%)	1.49	113 (26%) 1 0	34, 62, 135, 139	0
All	All	2460/2540 (96%)	1.64	670 (27%) 1 0	31, 64, 137, 147	0

All (670) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	ASN	18.7
1	D	252	TYR	17.5
2	O	148	GLN	17.3
1	B	252	TYR	16.9
2	O	157	MET	15.1
2	O	162	ASN	15.1
1	B	228	ARG	15.0
1	D	253	LYS	14.8
1	D	194	VAL	14.8
2	N	150	PRO	14.5
2	M	162	ASN	13.2
2	M	167	ILE	13.0
1	E	198	TRP	13.0

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Mol	Chain	Res	Type	RSRZ
2	M	178	GLY	12.6
2	L	149	MET	12.4
1	C	194	VAL	12.2
1	E	193	ALA	12.0
1	B	229	GLY	12.0
2	O	149	MET	12.0
1	B	201	SER	12.0
1	E	253	LYS	11.8
2	M	149	MET	11.5
1	B	198	TRP	11.5
2	N	154	LYS	11.3
2	N	153	ARG	11.1
2	L	131	ASP	11.0
1	B	193	ALA	10.9
1	B	223	GLU	10.8
2	N	152	TYR	10.7
1	E	239	ARG	10.6
2	N	180	ASP	10.2
1	B	253	LYS	10.2
2	L	150	PRO	10.1
2	M	163	GLN	10.0
1	B	194	VAL	9.9
2	K	117	LEU	9.9
2	N	169	GLU	9.9
2	O	147	THR	9.8
1	E	227	SER	9.7
2	K	166	MET	9.7
1	B	195	SER	9.6
1	E	196	ASP	9.6
2	K	177	GLU	9.6
1	B	200	LEU	9.6
1	B	261	VAL	9.6
2	N	151	GLU	9.5
2	N	2	SER	9.5
1	B	222	ASP	9.4
2	O	176	PRO	9.4
1	B	237	ASN	9.3
2	K	167	ILE	9.3
1	D	234	VAL	9.2
2	L	144	VAL	9.2
1	E	234	VAL	9.1
1	E	195	SER	9.1

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Mol	Chain	Res	Type	RSRZ
2	L	147	THR	9.1
2	K	168	ASN	9.0
2	M	151	GLU	9.0
2	K	149	MET	9.0
2	O	151	GLU	8.9
2	N	149	MET	8.9
2	L	160	LEU	8.9
1	E	214	LEU	8.8
2	M	152	TYR	8.8
2	K	176	PRO	8.8
2	N	160	LEU	8.8
2	M	150	PRO	8.7
2	N	117	LEU	8.7
2	N	155	LYS	8.7
2	M	357	PRO	8.7
2	O	150	PRO	8.6
2	O	357	PRO	8.6
2	K	178	GLY	8.6
2	O	168	ASN	8.6
2	L	171	PHE	8.5
2	O	358	ASP	8.5
2	N	186	GLY	8.5
2	K	154	LYS	8.5
2	K	165	LYS	8.3
2	L	170	GLN	8.3
1	E	194	VAL	8.3
2	M	131	ASP	8.2
2	M	2	SER	8.2
2	M	176	PRO	8.1
2	M	159	GLY	8.1
2	N	168	ASN	8.1
2	O	365	THR	8.1
2	N	148	GLN	8.1
1	D	226	SER	8.0
1	E	235	GLY	8.0
1	B	227	SER	7.9
2	O	152	TYR	7.9
2	L	166	MET	7.9
1	E	197	VAL	7.8
2	L	152	TYR	7.8
2	L	151	GLU	7.8
1	E	252	TYR	7.8

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Mol	Chain	Res	Type	RSRZ
2	L	153	ARG	7.8
1	A	252	TYR	7.8
2	K	364	LEU	7.7
1	B	212	ALA	7.7
1	B	238	GLY	7.7
2	N	159	GLY	7.7
1	E	215	GLN	7.7
2	M	164	CYS	7.6
2	O	131	ASP	7.6
1	D	213	SER	7.6
2	K	175	VAL	7.5
1	B	230	GLU	7.5
2	L	132	LYS	7.5
2	L	177	GLU	7.4
2	M	154	LYS	7.4
2	L	182	PHE	7.3
1	E	233	SER	7.3
2	M	153	ARG	7.3
2	N	176	PRO	7.2
1	D	211	LYS	7.2
2	L	358	ASP	7.2
2	N	165	LYS	7.2
2	N	182	PHE	7.2
2	K	150	PRO	7.1
1	B	199	SER	7.1
2	N	177	GLU	7.1
2	K	171	PHE	7.1
2	N	158	ASP	7.0
2	O	144	VAL	7.0
2	N	161	THR	6.9
2	N	147	THR	6.9
1	B	221	LEU	6.9
1	A	194	VAL	6.9
2	M	148	GLN	6.8
2	K	147	THR	6.8
1	A	212	ALA	6.8
1	E	222	ASP	6.8
2	N	357	PRO	6.7
2	M	118	PRO	6.7
1	B	231	PHE	6.7
1	C	253	LYS	6.7
1	B	233	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	193	ALA	6.7
2	L	154	LYS	6.7
2	M	157	MET	6.7
1	E	229	GLY	6.6
1	D	195	SER	6.6
1	D	210	LYS	6.6
2	M	145	GLY	6.6
2	K	148	GLN	6.6
1	B	214	LEU	6.5
2	M	170	GLN	6.5
2	N	178	GLY	6.5
1	A	226	SER	6.5
1	B	213	SER	6.5
2	N	81	ARG	6.4
1	E	208	GLN	6.4
1	D	212	ALA	6.4
2	M	161	THR	6.4
1	D	220	SER	6.4
2	K	179	ARG	6.4
2	O	118	PRO	6.3
2	O	175	VAL	6.3
2	O	173	PRO	6.3
1	B	217	LEU	6.2
2	L	159	GLY	6.2
1	D	230	GLU	6.2
2	N	167	ILE	6.2
2	K	361	THR	6.1
2	M	168	ASN	6.1
2	M	175	VAL	6.1
2	O	160	LEU	6.1
2	L	157	MET	6.1
2	K	151	GLU	6.1
2	M	364	LEU	6.1
2	O	167	ILE	6.1
2	O	156	LEU	6.0
2	O	130	ASP	6.0
2	K	120	GLY	6.0
1	D	258	GLN	6.0
2	O	45	THR	6.0
1	D	229	GLY	6.0
2	K	144	VAL	5.9
2	K	119	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	258	GLN	5.9
2	N	175	VAL	5.8
2	L	2	SER	5.8
2	M	166	MET	5.8
2	L	148	GLN	5.8
2	N	68	HIS	5.8
2	M	358	ASP	5.8
2	K	114	ASP	5.8
1	C	252	TYR	5.8
1	B	218	THR	5.7
2	O	171	PHE	5.7
2	M	120	GLY	5.7
2	K	170	GLN	5.7
2	M	165	LYS	5.6
1	D	236	GLY	5.6
2	K	363	GLY	5.6
2	L	56	TYR	5.6
2	N	114	ASP	5.6
1	B	197	VAL	5.6
2	M	144	VAL	5.6
1	E	261	VAL	5.5
2	O	163	GLN	5.5
2	K	159	GLY	5.5
2	K	116	VAL	5.5
2	O	153	ARG	5.5
1	E	216	PRO	5.4
2	K	365	THR	5.4
2	N	120	GLY	5.4
1	E	199	SER	5.4
2	N	181	ILE	5.4
2	N	118	PRO	5.4
2	L	168	ASN	5.4
1	A	193	ALA	5.3
2	N	131	ASP	5.3
1	B	254	LYS	5.3
2	K	355	TYR	5.2
1	E	220	SER	5.2
1	B	241	SER	5.2
2	N	164	CYS	5.2
2	O	68	HIS	5.2
1	D	260	ARG	5.2
2	K	143	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	222	ASP	5.2
1	E	232	ILE	5.2
2	K	153	ARG	5.1
2	M	22	GLU	5.1
2	L	113	LEU	5.1
2	M	114	ASP	5.1
2	M	365	THR	5.1
1	B	251	ARG	5.0
2	M	147	THR	5.0
1	B	239	ARG	5.0
2	O	177	GLU	5.0
1	C	208	GLN	5.0
1	B	263	TYR	5.0
1	D	196	ASP	5.0
2	L	127	THR	5.0
2	N	137	TYR	5.0
2	L	117	LEU	5.0
2	L	155	LYS	5.0
2	N	83	LYS	5.0
1	B	234	VAL	5.0
2	O	125	SER	4.9
2	N	361	THR	4.9
2	O	169	GLU	4.9
2	M	169	GLU	4.9
2	M	160	LEU	4.9
2	N	98	ALA	4.9
2	O	161	THR	4.8
2	M	171	PHE	4.8
1	C	213	SER	4.8
1	E	212	ALA	4.8
2	N	50	ASP	4.8
1	D	250	LEU	4.8
2	N	113	LEU	4.8
2	L	121	VAL	4.8
2	L	107	LEU	4.8
2	O	174	LEU	4.8
1	B	211	LYS	4.7
2	O	215	TYR	4.7
2	L	365	THR	4.7
1	D	264	SER	4.7
2	K	113	LEU	4.7
1	A	213	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	O	143	ARG	4.7
2	L	124	ALA	4.7
1	D	251	ARG	4.7
1	C	212	ALA	4.7
2	M	177	GLU	4.7
2	L	162	ASN	4.7
2	K	360	SER	4.7
1	E	230	GLU	4.6
2	M	174	LEU	4.6
1	D	202	LYS	4.6
2	K	161	THR	4.5
2	L	34	LYS	4.5
2	O	97	LYS	4.5
2	M	155	LYS	4.5
2	O	183	ASP	4.5
2	L	125	SER	4.5
1	B	260	ARG	4.5
2	K	164	CYS	4.4
2	N	183	ASP	4.4
2	K	169	GLU	4.4
1	B	242	HIS	4.4
2	O	83	LYS	4.4
1	B	264	SER	4.4
2	L	175	VAL	4.4
2	N	171	PHE	4.4
2	O	146	ARG	4.3
2	M	182	PHE	4.3
1	D	238	GLY	4.3
2	M	143	ARG	4.3
1	D	228	ARG	4.3
1	B	208	GLN	4.3
2	O	115	GLY	4.2
1	B	206	THR	4.2
2	K	155	LYS	4.2
1	E	209	PRO	4.2
2	N	34	LYS	4.2
2	L	357	PRO	4.2
2	L	130	ASP	4.2
2	K	162	ASN	4.2
1	D	208	GLN	4.2
2	K	146	ARG	4.2
1	D	214	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	L	176	PRO	4.1
2	O	154	LYS	4.1
1	D	198	TRP	4.1
2	O	57	GLN	4.1
1	B	257	ASN	4.1
2	O	159	GLY	4.1
2	L	114	ASP	4.1
2	O	2	SER	4.1
1	E	217	LEU	4.1
1	D	261	VAL	4.0
1	C	234	VAL	4.0
2	O	93	ILE	4.0
2	O	96	GLY	4.0
1	E	226	SER	4.0
1	B	247	LEU	4.0
1	C	220	SER	4.0
1	B	265	LEU	4.0
1	E	219	ILE	4.0
1	E	225	PHE	4.0
1	E	231	PHE	3.9
2	M	158	ASP	3.9
1	B	226	SER	3.9
2	N	144	VAL	3.9
1	C	251	ARG	3.9
1	B	232	ILE	3.9
2	N	87	ASP	3.9
1	E	251	ARG	3.9
2	O	179	ARG	3.9
2	M	113	LEU	3.9
1	D	227	SER	3.8
1	B	256	TYR	3.8
2	M	23	ASP	3.8
1	C	214	LEU	3.8
1	E	228	ARG	3.8
1	B	224	LEU	3.8
2	L	143	ARG	3.8
2	O	127	THR	3.8
2	K	183	ASP	3.8
2	M	21	ASN	3.8
1	B	236	GLY	3.8
1	E	262	LYS	3.8
2	O	63	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	N	162	ASN	3.7
1	C	211	LYS	3.7
1	D	241	SER	3.7
2	M	361	THR	3.7
2	N	143	ARG	3.7
2	N	179	ARG	3.7
2	L	120	GLY	3.7
2	L	359	ASP	3.7
2	N	107	LEU	3.7
2	O	53	GLY	3.7
1	B	255	LEU	3.7
1	D	193	ALA	3.7
1	E	245	ALA	3.7
2	L	116	VAL	3.7
2	K	115	GLY	3.7
2	L	169	GLU	3.7
2	M	98	ALA	3.7
2	K	157	MET	3.7
2	N	109	SER	3.6
1	B	216	PRO	3.6
1	E	210	LYS	3.6
2	N	86	LYS	3.6
2	K	359	ASP	3.6
2	N	358	ASP	3.6
2	N	360	SER	3.6
2	N	37	GLU	3.6
2	N	359	ASP	3.6
1	E	258	GLN	3.6
2	M	117	LEU	3.6
1	A	253	LYS	3.5
2	K	131	ASP	3.5
1	C	229	GLY	3.5
2	O	117	LEU	3.5
2	O	197	ALA	3.5
1	D	233	SER	3.5
2	M	116	VAL	3.5
2	N	356	THR	3.5
2	O	182	PHE	3.5
1	D	243	LYS	3.4
2	O	22	GLU	3.4
2	L	118	PRO	3.4
2	O	207	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	M	156	LEU	3.4
2	N	156	LEU	3.4
2	K	118	PRO	3.4
1	C	227	SER	3.4
1	E	221	LEU	3.4
2	L	111	LYS	3.4
2	N	195	VAL	3.4
2	O	48	LEU	3.4
2	L	167	ILE	3.4
2	L	186	GLY	3.4
2	L	126	ARG	3.4
1	B	196	ASP	3.4
2	L	355	TYR	3.4
1	A	228	ARG	3.4
2	O	114	ASP	3.4
1	D	263	TYR	3.4
2	K	152	TYR	3.4
1	D	224	LEU	3.4
2	M	146	ARG	3.3
2	M	121	VAL	3.3
2	L	367	ASN	3.3
2	L	133	TRP	3.3
1	B	225	PHE	3.3
1	B	259	ALA	3.3
2	K	160	LEU	3.3
2	N	365	THR	3.3
2	L	33	ARG	3.3
2	L	146	ARG	3.3
2	O	170	GLN	3.3
2	O	34	LYS	3.3
2	L	361	THR	3.2
2	L	97	LYS	3.2
1	C	228	ARG	3.2
1	D	239	ARG	3.2
2	K	358	ASP	3.2
1	D	232	ILE	3.2
2	O	164	CYS	3.2
1	B	202	LYS	3.2
2	O	132	LYS	3.2
2	N	173	PRO	3.2
2	N	166	MET	3.2
2	N	33	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	360	SER	3.2
2	O	133	TRP	3.2
1	B	209	PRO	3.2
1	D	262	LYS	3.2
2	O	119	ASP	3.1
2	N	39	PRO	3.1
2	K	121	VAL	3.1
1	D	254	LYS	3.1
2	N	157	MET	3.1
2	N	80	ILE	3.1
2	K	362	GLY	3.1
1	E	254	LYS	3.1
1	D	265	LEU	3.1
2	O	113	LEU	3.1
2	L	68	HIS	3.1
1	A	229	GLY	3.1
1	B	207	PHE	3.1
2	M	107	LEU	3.1
2	O	74	TYR	3.1
2	M	34	LYS	3.1
2	N	115	GLY	3.1
2	N	21	ASN	3.1
1	E	264	SER	3.1
2	N	363	GLY	3.0
2	K	23	ASP	3.0
2	M	179	ARG	3.0
2	N	121	VAL	3.0
2	O	196	ALA	3.0
1	E	243	LYS	3.0
2	N	193	LYS	3.0
2	M	172	GLU	3.0
2	N	325	THR	3.0
1	A	220	SER	3.0
2	K	34	LYS	3.0
2	O	121	VAL	3.0
2	L	60	LYS	3.0
2	N	132	LYS	3.0
2	N	196	ALA	3.0
1	D	215	GLN	3.0
2	N	49	SER	3.0
2	O	44	THR	3.0
1	B	248	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	235	GLY	3.0
2	N	112	ALA	3.0
2	K	86	LYS	3.0
2	N	128	SER	3.0
1	A	231	PHE	2.9
2	M	362	GLY	2.9
2	O	186	GLY	2.9
2	N	197	ALA	2.9
2	L	158	ASP	2.9
1	C	260	ARG	2.9
2	O	192	THR	2.9
2	O	355	TYR	2.9
2	M	186	GLY	2.9
2	O	137	TYR	2.9
1	E	237	ASN	2.9
2	K	357	PRO	2.9
2	N	353	ASN	2.9
2	O	21	ASN	2.9
2	N	22	GLU	2.9
1	D	256	TYR	2.9
2	L	99	GLY	2.8
2	O	178	GLY	2.8
1	E	236	GLY	2.8
2	L	3	VAL	2.8
1	D	207	PHE	2.8
1	E	207	PHE	2.8
2	O	33	ARG	2.8
1	B	262	LYS	2.8
1	D	235	GLY	2.8
2	O	124	ALA	2.8
2	O	193	LYS	2.8
2	L	55	VAL	2.8
1	C	265	LEU	2.8
2	O	129	ALA	2.8
1	B	244	GLU	2.8
2	O	209	GLU	2.8
2	L	50	ASP	2.7
2	L	180	ASP	2.7
2	O	50	ASP	2.7
2	O	158	ASP	2.7
1	C	198	TRP	2.7
2	M	97	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	244	GLU	2.7
2	K	22	GLU	2.7
2	O	80	ILE	2.7
1	A	234	VAL	2.7
2	N	184	VAL	2.7
2	L	165	LYS	2.7
1	D	199	SER	2.7
2	M	24	PRO	2.7
2	N	130	ASP	2.7
1	A	260	ARG	2.7
2	M	132	LYS	2.7
1	B	204	SER	2.7
2	K	156	LEU	2.7
2	L	156	LEU	2.7
2	N	185	TRP	2.7
2	N	172	GLU	2.7
2	O	86	LYS	2.7
2	N	200	MET	2.7
2	M	181	ILE	2.7
2	N	29	ALA	2.6
2	O	195	VAL	2.6
2	N	111	LYS	2.6
2	L	142	TYR	2.6
1	D	223	GLU	2.6
2	O	23	ASP	2.6
2	L	128	SER	2.6
1	A	214	LEU	2.6
2	L	48	LEU	2.6
1	D	225	PHE	2.6
2	O	123	ASP	2.6
1	E	218	THR	2.6
2	N	54	TYR	2.6
1	D	204	SER	2.6
2	K	172	GLU	2.6
1	D	203	THR	2.6
2	L	102	ILE	2.6
2	O	43	ASN	2.6
2	N	99	GLY	2.6
2	K	173	PRO	2.5
2	N	142	TYR	2.5
2	M	359	ASP	2.5
2	O	194	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	256	TYR	2.5
1	E	206	THR	2.5
2	K	158	ASP	2.5
1	E	257	ASN	2.5
1	E	242	HIS	2.5
1	A	251	ARG	2.5
2	L	54	TYR	2.5
1	D	244	GLU	2.5
2	K	85	ASP	2.5
2	L	83	LYS	2.5
2	O	59	LEU	2.5
1	E	260	ARG	2.5
2	O	87	ASP	2.5
1	B	203	THR	2.5
2	K	350	VAL	2.5
2	O	359	ASP	2.5
1	A	195	SER	2.5
1	D	197	VAL	2.5
2	K	106	ASP	2.5
2	L	215	TYR	2.4
2	M	355	TYR	2.4
2	N	191	TYR	2.4
2	O	116	VAL	2.4
1	D	231	PHE	2.4
2	O	142	TYR	2.4
2	O	200	MET	2.4
2	L	22	GLU	2.4
1	D	200	LEU	2.4
2	M	112	ALA	2.4
2	M	139	LEU	2.4
2	L	213	PHE	2.4
2	N	276	PRO	2.4
2	N	92	GLY	2.4
1	D	242	HIS	2.3
1	B	210	LYS	2.3
2	O	84	LEU	2.3
2	N	194	ILE	2.3
2	O	185	TRP	2.3
2	O	405	GLN	2.3
2	L	187	ASN	2.3
2	K	108	VAL	2.3
2	O	165	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	N	192	THR	2.3
1	C	239	ARG	2.3
2	K	174	LEU	2.3
2	N	84	LEU	2.3
2	N	215	TYR	2.3
2	O	191	TYR	2.3
2	N	119	ASP	2.3
2	M	44	THR	2.3
2	K	184	VAL	2.3
2	O	64	VAL	2.3
2	M	115	GLY	2.2
2	O	24	PRO	2.2
2	O	61	SER	2.2
2	O	98	ALA	2.2
1	E	238	GLY	2.2
2	N	189	SER	2.2
2	O	100	ASP	2.2
1	C	210	LYS	2.2
2	N	24	PRO	2.2
1	A	235	GLY	2.2
2	L	163	GLN	2.2
2	O	166	MET	2.2
2	L	356	THR	2.2
2	K	182	PHE	2.2
2	M	122	SER	2.2
2	O	94	ASN	2.2
1	E	200	LEU	2.2
1	E	224	LEU	2.2
1	E	248	LEU	2.2
2	O	139	LEU	2.2
2	K	370	PRO	2.1
2	L	179	ARG	2.1
2	L	422	LYS	2.1
2	L	192	THR	2.1
1	C	237	ASN	2.1
2	O	210	CYS	2.1
2	L	122	SER	2.1
2	N	170	GLN	2.1
2	N	355	TYR	2.1
2	L	86	LYS	2.1
2	K	408	ARG	2.1
2	O	88	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	97	LYS	2.1
2	L	51	LEU	2.1
2	L	59	LEU	2.1
1	B	219	ILE	2.1
2	L	8	ILE	2.1
2	L	137	TYR	2.1
1	E	241	SER	2.1
2	N	116	VAL	2.1
1	E	265	LEU	2.0
2	K	163	GLN	2.0
2	O	72	TYR	2.0
1	A	210	LYS	2.0
2	N	46	LYS	2.0
2	M	138	LEU	2.0
2	O	187	ASN	2.0
1	C	238	GLY	2.0
2	L	23	ASP	2.0
2	L	44	THR	2.0
2	O	189	SER	2.0
1	A	208	GLN	2.0
1	E	250	LEU	2.0
2	K	308	LEU	2.0
2	O	155	LYS	2.0
2	M	183	ASP	2.0
2	O	85	ASP	2.0
2	M	173	PRO	2.0
2	N	25	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	TAR	K	423	10/10	0.56	0.51	5.74	120,120,120,120	0
3	TAR	O	423	10/10	0.73	0.41	4.60	108,108,108,108	0
3	TAR	K	426	10/10	0.75	0.32	2.96	87,88,88,88	0
3	TAR	K	425	10/10	0.65	0.38	1.30	67,69,70,71	0
3	TAR	M	1	10/10	0.80	0.31	0.04	117,118,118,118	0
3	TAR	K	424	10/10	0.71	0.31	-	92,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.