Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:12 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 ①) were used in the production of this report:

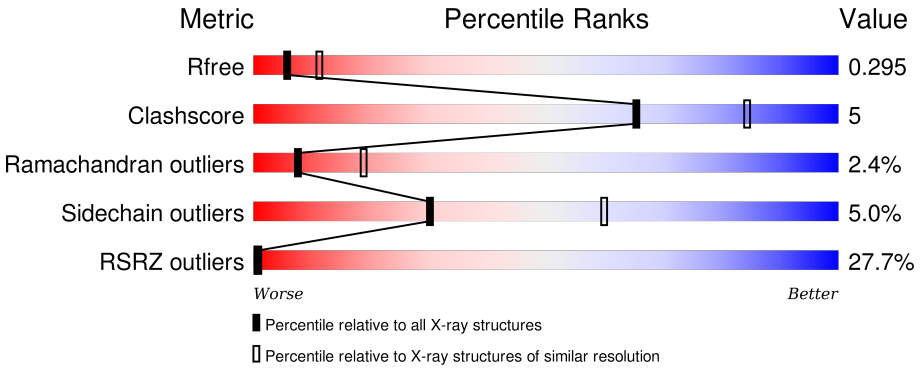
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 <=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	22%, 74%, 9%, 16%
1	B	87	74%, 74%, 10%, 16%
1	C	87	26%, 69%, 13%, 16%
1	D	87	63%, 72%, 9%, 16%
1	E	87	67%, 75%, 9%, 16%

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Mol	Chain	Length	Quality of chain
2	K	421	17% 80% 18%
2	L	421	22% 81% 17%
2	M	421	18% 84% 14%
2	N	421	26% 84% 15%
2	O	421	28% 84% 13%

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

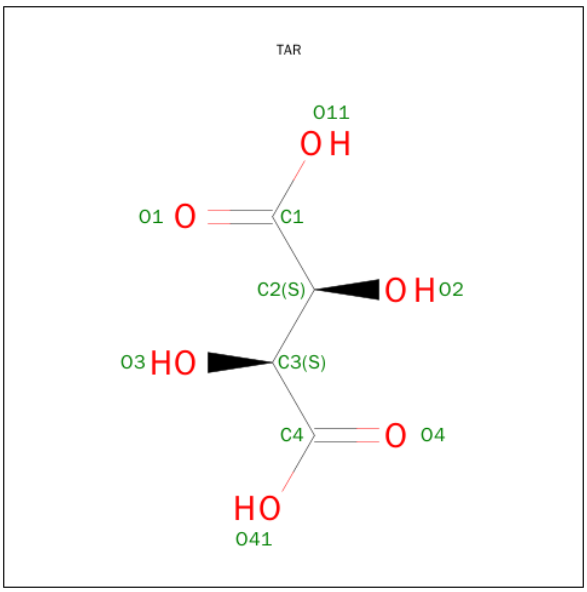
- Molecule 2 is a protein called Nucleoprotein.

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: $C_4H_6O_6$).



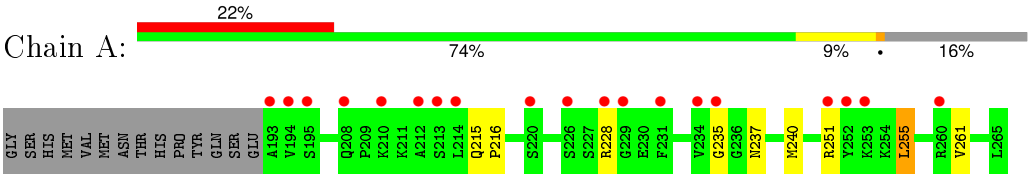
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	O	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		

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 errors 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.

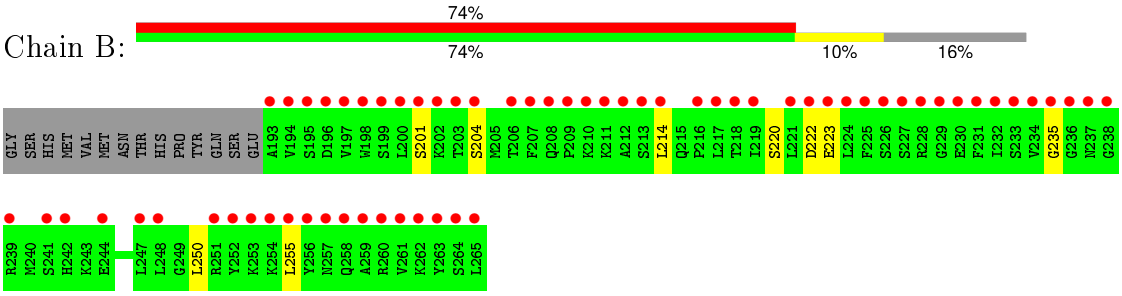
- Molecule 1: Phosphoprotein

Chain A:



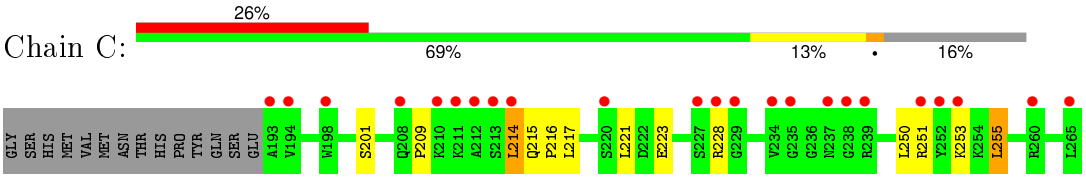
- Molecule 1: Phosphoprotein

Chain B:



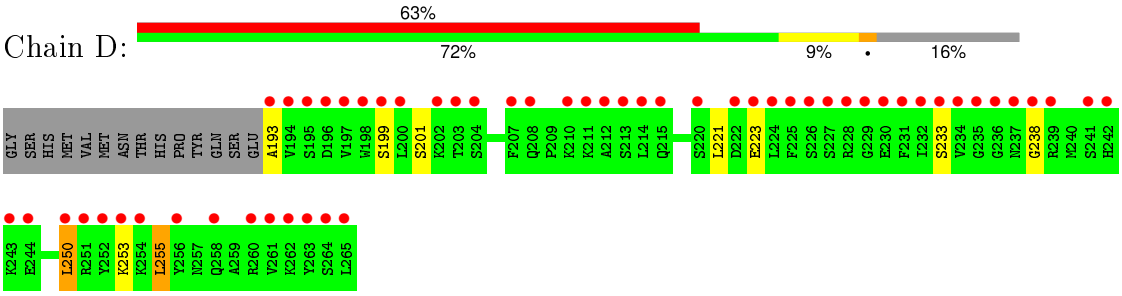
- Molecule 1: Phosphoprotein

Chain C:



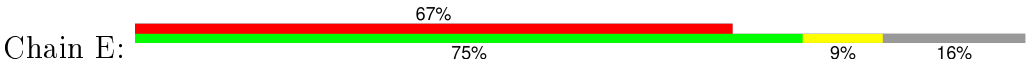
- Molecule 1: Phosphoprotein

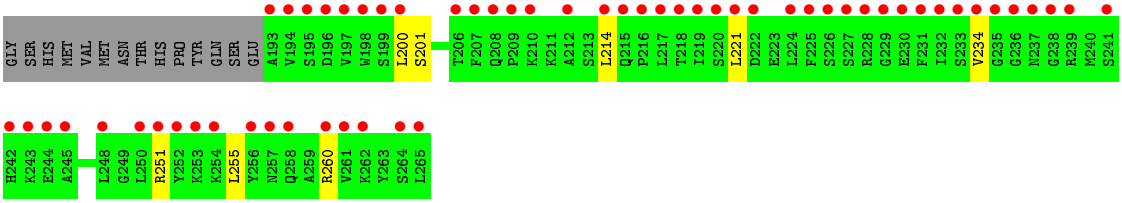
Chain D:



- Molecule 1: Phosphoprotein

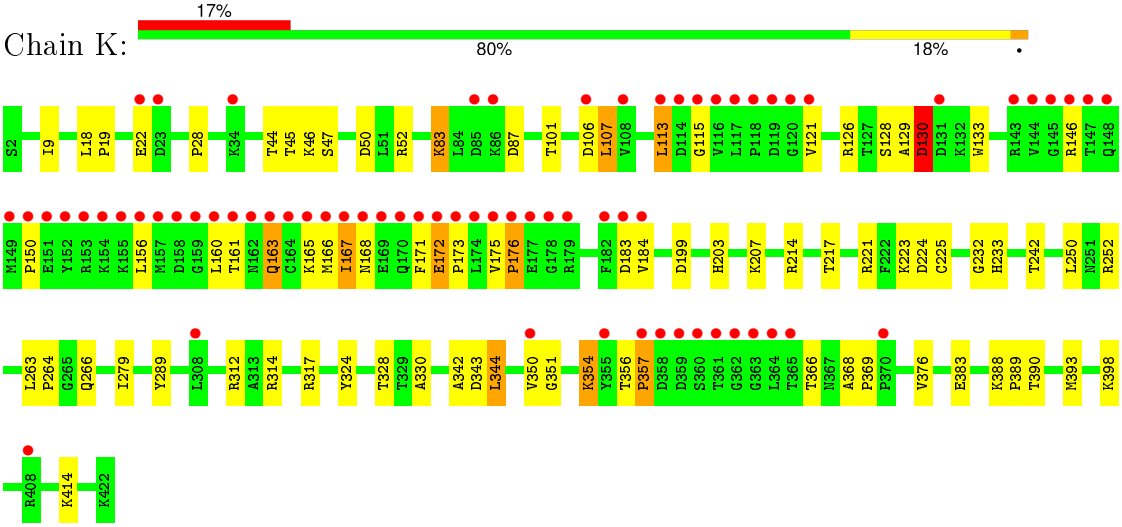
Chain E:





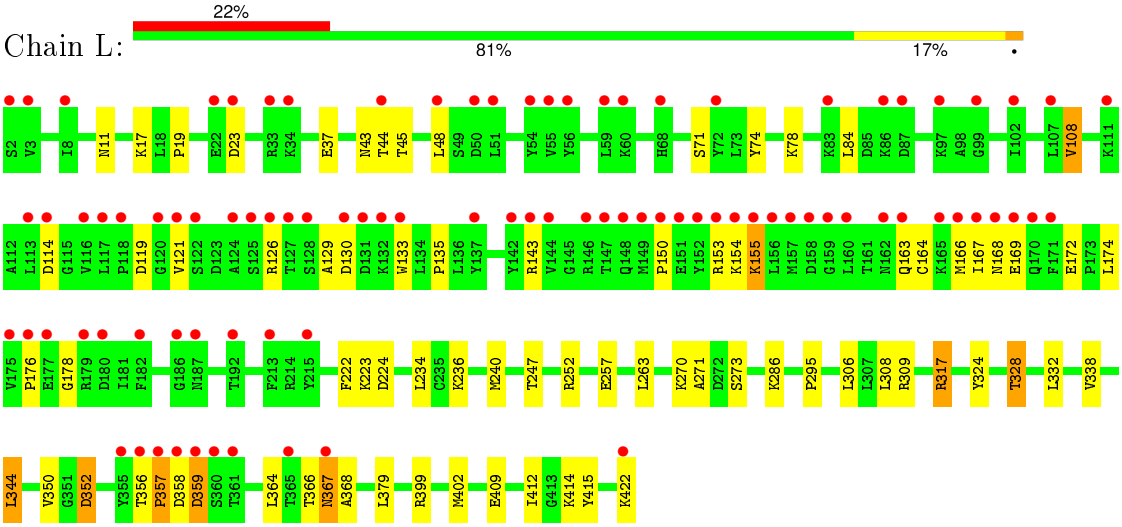
• Molecule 2: Nucleoprotein

Chain K:



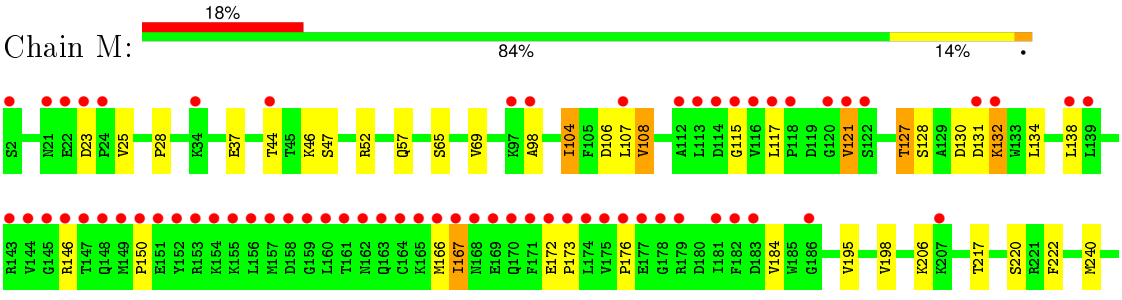
• Molecule 2: Nucleoprotein

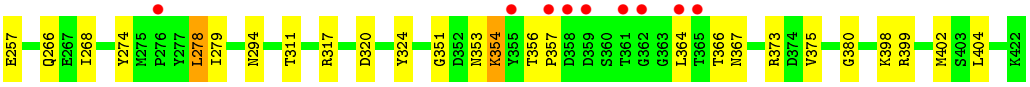
Chain L:



• Molecule 2: Nucleoprotein

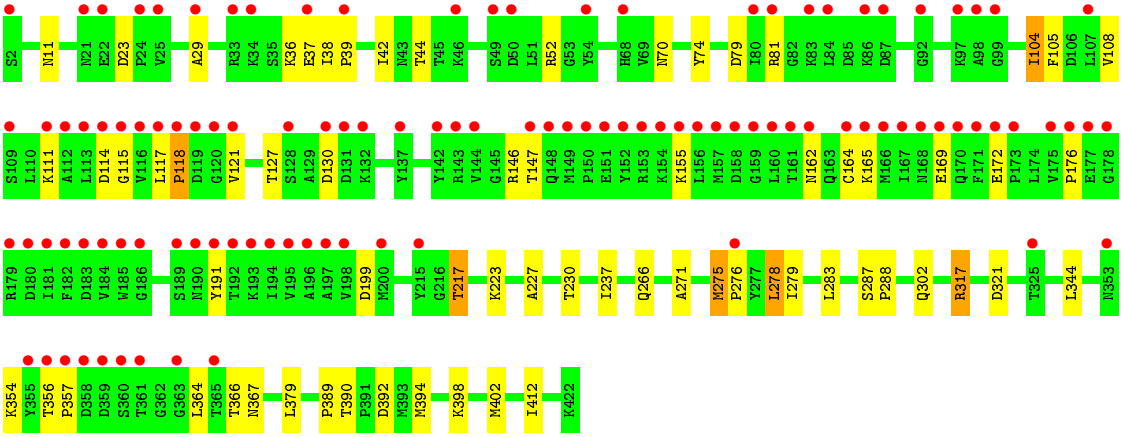
Chain M:





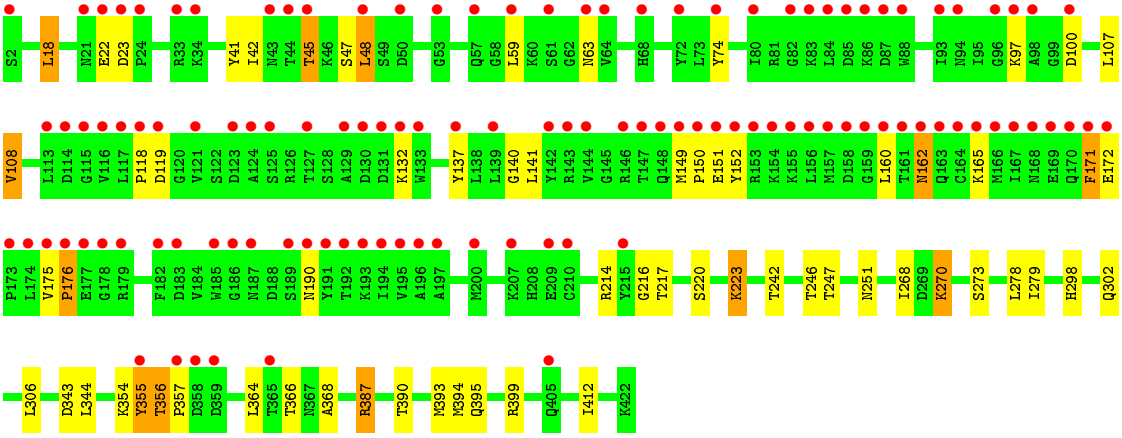
• Molecule 2: Nucleoprotein

Chain N:



• Molecule 2: Nucleoprotein

Chain O:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 77602 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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
2:L:317:ARG:NE	2:L:317:ARG:H	1.89	0.70
1:A:261:VAL:HG21	2:K:376:VAL:HG12	1.72	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:L:317:ARG:HE	2:L:317:ARG:H	1.50	0.58
2:K:342:ALA:HB1	2:K:344:LEU:HD23	1.84	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:N:398:LYS:O	2:N:402:MET:HB2	2.07	0.54
2:K:350:VAL:HG23	2:O:247:THR:HG21	1.90	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)
2:M:240:MET:CE	2:M:373:ARG:HD3	2.40	0.51
1:B:201:SER:HB2	1:B:222:ASP:HB2	1.91	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:O:387:ARG:HG2	2:O:387:ARG:HH11	1.76	0.51
2:L:223:LYS:O	2:L:224:ASP:HB2	2.10	0.51
2:N:389:PRO:HB2	2:N:394:MET:HE1	1.93	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
1:E:234:VAL:HG12	1:E:251:ARG:HH21	1.75	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:M:130:ASP:C	2:M:132:LYS:N	2.67	0.48
2:L:257:GLU:OE2	2:L:295:PRO:HD2	2.14	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:O:42:ILE:HD13	2:O:74:TYR:HB2	1.96	0.47
2:N:147:THR:HG21	2:N:155:LYS:HG3	1.97	0.47
2:M:44:THR:HG23	2:M:46:LYS:HE2	1.97	0.47
2:K:232:GLY:HA2	2:O:18:LEU:HD21	1.97	0.47
2:N:164:CYS:HB3	2:N:169:GLU:HG2	1.97	0.47
1:D:201:SER:HA	1:D:221:LEU:HB2	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
2:K:368:ALA:HB1	2:K:369:PRO:HD2	1.98	0.45
1:C:209:PRO:HB3	1:C:214:LEU:HB3	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:306:LEU:HD22	2:L:412:ILE:HD12	2.00	0.44
2:L:37:GLU:HB2	2:L:108:VAL:HG21	1.99	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:M:364:LEU:O	2:M:366:THR:HG22	2.18	0.44
2:M:320:ASP:HA	2:M:324:TYR:HH	1.82	0.44
2:L:143:ARG:HH21	2:L:155:LYS:HE2	1.82	0.44
2:N:162:ASN:HA	2:N:165:LYS:HE3	2.00	0.44
2:N:104:ILE:HG22	2:N:105:PHE:H	1.83	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: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
2:L:130:ASP:O	2:L:135:PRO:HD3	2.17	0.43
2:K:28:PRO:HD2	2:K:266:GLN:OE1	2.19	0.43
2:L:126:ARG:HH21	2:L:129:ALA:HB2	1.83	0.43
2:K:175:VAL:HB	2:K:176:PRO:HD3	2.01	0.43
1:A:235:GLY:HA3	2:L:364:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:79:ASP:HB2	2:N:81:ARG:HG3	2.00	0.43
1:D:193:ALA:N	1:D:199:SER:HG	2.17	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
2:O:278:LEU:HG	2:O:279:ILE:HD12	2.00	0.42
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:M:366:THR:HG23	2:M:367:ASN:N	2.31	0.42
2:M:195:VAL:HG13	2:M:217:THR:HG22	2.00	0.42
2:O:137:TYR:O	2:O:141:LEU:HG	2.19	0.42
2:M:52:ARG:HD3	2:M:130:ASP:OD2	2.20	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: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
2:K:390:THR:H	2:K:393:MET:HE2	1.85	0.42
1:B:220:SER:HB3	1:B:223:GLU:HG2	2.01	0.42
2:L:23:ASP:HB3	2:L:286:LYS:HE3	2.02	0.42
2:O:387:ARG:CB	2:O:387:ARG:HH11	2.32	0.42
2:M:257:GLU:HB3	2:M:294:ASN:HD22	1.85	0.42
2:K:19:PRO:HB3	2:L:222:PHE:CZ	2.55	0.42
2:N:278:LEU:HD13	2:N:279:ILE:HG12	2.02	0.41
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: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
2:N:38:ILE:HA	2:N:39:PRO:HD3	1.86	0.41
1:E:201:SER:HA	1:E:221:LEU:HB2	2.02	0.41
2:N:287:SER:HA	2:N:288:PRO:HD3	1.86	0.41
2:K:330:ALA:HB2	2:L:344:LEU:HD21	2.03	0.41
2:L:19:PRO:HB3	2:M:222:PHE:CZ	2.56	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:28:PRO:HD2	2:M:266:GLN:OE1	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:K:224:ASP:CG	2:K:279:ILE:HG21	2.41	0.41
2:O:175:VAL:HB	2:O:176:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:227:ALA:HA	2:N:230:THR:HG22	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:42:ILE:HD13	2:N:74:TYR:HB2	2.04	0.40
2:N:356:THR:N	2:N:357:PRO:HD3	2.36	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
2:O:355:TYR:HB2	2:O:357:PRO:HD3	2.04	0.40
1:C:214:LEU:HD23	1:C:215:GLN:H	1.86	0.40
1:B:204:SER:HB3	1:B:220:SER:HB2	2.03	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%)	14 35
1	B	71/87 (82%)	59 (83%)	11 (16%)	1 (1%)	14 35
1	C	71/87 (82%)	60 (84%)	10 (14%)	1 (1%)	14 35
1	D	71/87 (82%)	58 (82%)	11 (16%)	2 (3%)	6 15
1	E	71/87 (82%)	64 (90%)	7 (10%)	0	100 100
2	K	419/421 (100%)	377 (90%)	29 (7%)	13 (3%)	5 12
2	L	419/421 (100%)	373 (89%)	35 (8%)	11 (3%)	7 16
2	M	419/421 (100%)	372 (89%)	37 (9%)	10 (2%)	7 19
2	N	419/421 (100%)	376 (90%)	36 (9%)	7 (2%)	11 29
2	O	419/421 (100%)	369 (88%)	37 (9%)	13 (3%)	5 12
All	All	2450/2540 (96%)	2170 (89%)	221 (9%)	59 (2%)	7 19

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 (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	64/75 (85%)	63 (98%)	1 (2%)	70	91
1	B	64/75 (85%)	61 (95%)	3 (5%)	32	63
1	C	64/75 (85%)	59 (92%)	5 (8%)	16	35
1	D	64/75 (85%)	61 (95%)	3 (5%)	32	63
1	E	64/75 (85%)	61 (95%)	3 (5%)	32	63
2	K	362/362 (100%)	341 (94%)	21 (6%)	25	52
2	L	362/362 (100%)	339 (94%)	23 (6%)	22	47
2	M	362/362 (100%)	346 (96%)	16 (4%)	35	65
2	N	362/362 (100%)	349 (96%)	13 (4%)	42	73
2	O	362/362 (100%)	343 (95%)	19 (5%)	29	58
All	All	2130/2185 (98%)	2023 (95%)	107 (5%)	30	60

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	0.55	0
3	TAR	K	424	-	3,9,9	0.56	0	6,12,12	0.90	0
3	TAR	K	425	-	3,9,9	0.57	0	6,12,12	0.86	0
3	TAR	K	426	-	3,9,9	0.46	0	6,12,12	0.84	0
3	TAR	M	1	-	3,9,9	0.47	0	6,12,12	1.03	0
3	TAR	O	423	-	3,9,9	0.49	0	6,12,12	0.93	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, 95^{th} 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%)	1.65	19 (26%)	1	1	59, 84, 88, 89	0
1	B	71/87 (81%)	5.67	64 (90%)	0	0	137, 145, 147, 147	0
1	C	71/87 (81%)	1.87	23 (32%)	1	0	71, 87, 92, 92	0
1	D	71/87 (81%)	4.36	55 (77%)	0	0	107, 126, 127, 127	0
1	E	71/87 (81%)	4.47	58 (81%)	0	0	119, 133, 135, 135	0
2	K	421/421 (100%)	1.12	71 (16%)	2	2	31, 49, 111, 120	0
2	L	421/421 (100%)	1.35	92 (21%)	1	1	33, 62, 132, 139	0
2	M	421/421 (100%)	1.26	75 (17%)	2	1	31, 53, 116, 126	0
2	N	421/421 (100%)	1.58	108 (25%)	1	1	36, 66, 139, 145	0
2	O	421/421 (100%)	1.54	116 (27%)	1	1	34, 62, 135, 139	0
All	All	2460/2540 (96%)	1.69	681 (27%)	1	1	31, 64, 137, 147	0

All (681) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	ASN	18.9
1	D	252	TYR	17.9
2	O	148	GLN	17.8
1	B	252	TYR	17.3
2	O	157	MET	15.5
2	O	162	ASN	15.4
1	D	253	LYS	15.1
1	B	228	ARG	15.1
1	D	194	VAL	14.9
2	N	150	PRO	14.6
2	M	162	ASN	13.4
1	E	198	TRP	13.0
2	M	167	ILE	12.9

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Mol	Chain	Res	Type	RSRZ
2	L	149	MET	12.8
2	M	178	GLY	12.7
2	O	149	MET	12.5
1	C	194	VAL	12.3
1	E	193	ALA	12.2
1	B	229	GLY	12.2
1	B	201	SER	12.1
1	E	253	LYS	12.0
2	M	149	MET	11.9
2	N	154	LYS	11.6
1	B	198	TRP	11.5
2	N	153	ARG	11.2
2	L	131	ASP	11.2
1	B	193	ALA	11.1
1	B	223	GLU	11.1
2	N	152	TYR	10.8
1	E	239	ARG	10.7
2	N	180	ASP	10.5
1	B	253	LYS	10.4
2	M	163	GLN	10.3
2	L	150	PRO	10.1
2	N	169	GLU	10.0
2	O	147	THR	10.0
2	K	117	LEU	10.0
1	B	194	VAL	10.0
2	K	166	MET	10.0
1	E	196	ASP	9.9
1	B	261	VAL	9.8
2	K	177	GLU	9.8
1	E	227	SER	9.8
1	B	200	LEU	9.7
2	N	151	GLU	9.7
1	B	222	ASP	9.7
1	B	195	SER	9.6
1	B	237	ASN	9.5
2	N	2	SER	9.5
2	O	176	PRO	9.5
1	D	234	VAL	9.4
2	K	149	MET	9.3
2	L	144	VAL	9.3
2	M	151	GLU	9.3
2	L	147	THR	9.2

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Mol	Chain	Res	Type	RSRZ
1	E	234	VAL	9.2
2	K	167	ILE	9.2
2	N	149	MET	9.2
2	O	151	GLU	9.2
1	E	195	SER	9.1
2	K	168	ASN	9.0
2	M	152	TYR	9.0
2	L	160	LEU	8.9
1	E	214	LEU	8.9
2	K	176	PRO	8.9
2	N	155	LYS	8.9
2	K	178	GLY	8.8
2	M	150	PRO	8.8
2	M	357	PRO	8.8
2	N	117	LEU	8.8
2	O	150	PRO	8.8
2	O	358	ASP	8.8
2	N	160	LEU	8.8
2	O	357	PRO	8.7
2	L	171	PHE	8.7
2	O	168	ASN	8.7
2	N	186	GLY	8.7
2	K	154	LYS	8.6
2	L	170	GLN	8.6
2	K	165	LYS	8.5
2	M	131	ASP	8.4
1	E	194	VAL	8.4
2	M	2	SER	8.3
2	N	148	GLN	8.2
2	N	168	ASN	8.2
1	E	235	GLY	8.2
2	M	159	GLY	8.2
2	M	176	PRO	8.2
1	D	226	SER	8.1
2	O	365	THR	8.1
2	L	166	MET	8.1
2	L	151	GLU	8.0
2	L	152	TYR	8.0
1	E	197	VAL	8.0
1	E	252	TYR	8.0
2	O	152	TYR	7.9
1	B	227	SER	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	252	TYR	7.9
2	L	153	ARG	7.9
1	E	215	GLN	7.8
1	B	212	ALA	7.8
1	B	238	GLY	7.8
2	K	364	LEU	7.8
2	M	164	CYS	7.8
2	O	131	ASP	7.7
2	N	159	GLY	7.7
1	B	230	GLU	7.7
2	K	175	VAL	7.6
1	D	213	SER	7.6
2	L	132	LYS	7.6
2	M	154	LYS	7.6
2	L	177	GLU	7.6
1	E	233	SER	7.4
2	M	153	ARG	7.4
2	L	358	ASP	7.4
1	D	211	LYS	7.4
2	N	165	LYS	7.4
2	L	182	PHE	7.4
2	N	176	PRO	7.4
1	B	199	SER	7.3
2	N	182	PHE	7.3
2	N	177	GLU	7.2
2	K	150	PRO	7.2
2	K	171	PHE	7.2
2	N	158	ASP	7.2
2	N	147	THR	7.0
2	N	161	THR	7.0
2	O	144	VAL	7.0
1	A	194	VAL	7.0
2	K	147	THR	7.0
1	B	221	LEU	7.0
2	L	154	LYS	6.9
1	A	212	ALA	6.9
2	M	148	GLN	6.9
1	C	253	LYS	6.9
1	E	222	ASP	6.9
2	M	157	MET	6.8
1	B	233	SER	6.8
2	N	357	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
2	M	118	PRO	6.8
1	B	231	PHE	6.8
1	C	193	ALA	6.7
2	M	145	GLY	6.7
2	M	170	GLN	6.7
2	N	178	GLY	6.7
2	K	148	GLN	6.7
1	D	210	LYS	6.7
1	E	229	GLY	6.7
1	D	195	SER	6.6
1	E	208	GLN	6.6
1	A	226	SER	6.6
1	B	213	SER	6.5
1	D	212	ALA	6.5
1	B	214	LEU	6.5
2	N	81	ARG	6.5
2	M	161	THR	6.5
2	K	179	ARG	6.5
2	O	118	PRO	6.4
2	O	173	PRO	6.4
1	D	220	SER	6.4
2	O	175	VAL	6.4
1	B	217	LEU	6.4
2	L	157	MET	6.3
1	D	230	GLU	6.3
2	K	151	GLU	6.3
2	L	159	GLY	6.3
2	K	361	THR	6.2
2	M	175	VAL	6.2
2	M	168	ASN	6.2
2	O	130	ASP	6.2
2	N	167	ILE	6.2
2	K	120	GLY	6.1
2	O	160	LEU	6.1
2	O	167	ILE	6.1
1	D	258	GLN	6.1
2	M	364	LEU	6.1
1	D	229	GLY	6.1
2	O	45	THR	6.1
2	K	119	ASP	6.1
2	K	144	VAL	6.0
2	M	358	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
2	O	156	LEU	6.0
2	K	114	ASP	6.0
2	M	166	MET	6.0
2	L	148	GLN	6.0
1	B	258	GLN	6.0
2	N	175	VAL	5.9
2	N	68	HIS	5.9
1	C	252	TYR	5.9
2	L	2	SER	5.9
2	M	120	GLY	5.9
1	B	218	THR	5.8
2	O	171	PHE	5.8
2	K	170	GLN	5.8
2	N	114	ASP	5.8
1	D	236	GLY	5.8
2	O	163	GLN	5.8
2	M	165	LYS	5.7
2	L	56	TYR	5.7
1	B	197	VAL	5.7
1	E	216	PRO	5.7
2	K	363	GLY	5.6
1	E	261	VAL	5.6
2	M	144	VAL	5.6
2	K	116	VAL	5.6
2	K	159	GLY	5.6
2	N	120	GLY	5.5
2	K	365	THR	5.5
2	O	153	ARG	5.5
2	L	168	ASN	5.5
2	N	131	ASP	5.5
2	N	118	PRO	5.4
2	N	181	ILE	5.4
1	A	193	ALA	5.4
1	E	199	SER	5.4
2	N	164	CYS	5.4
1	B	254	LYS	5.4
2	K	355	TYR	5.4
1	D	260	ARG	5.3
1	B	241	SER	5.3
1	D	222	ASP	5.3
2	O	68	HIS	5.3
2	M	114	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	232	ILE	5.2
1	E	220	SER	5.2
2	M	22	GLU	5.2
1	C	208	GLN	5.2
2	K	143	ARG	5.2
1	D	196	ASP	5.2
2	K	153	ARG	5.2
2	L	113	LEU	5.2
2	L	155	LYS	5.2
1	B	263	TYR	5.1
2	O	177	GLU	5.1
2	M	147	THR	5.1
2	M	365	THR	5.1
1	B	239	ARG	5.1
2	L	127	THR	5.1
1	B	251	ARG	5.1
2	N	83	LYS	5.1
2	N	137	TYR	5.1
2	L	117	LEU	5.1
1	B	234	VAL	5.0
2	N	361	THR	5.0
2	N	98	ALA	5.0
2	M	169	GLU	5.0
2	O	125	SER	5.0
2	O	169	GLU	5.0
2	N	50	ASP	4.9
2	N	113	LEU	4.9
2	O	174	LEU	4.9
2	M	171	PHE	4.9
2	O	161	THR	4.9
2	M	160	LEU	4.9
1	E	212	ALA	4.9
2	L	121	VAL	4.9
1	C	213	SER	4.9
1	D	250	LEU	4.9
1	B	211	LYS	4.8
2	L	107	LEU	4.8
2	O	215	TYR	4.8
2	L	365	THR	4.8
2	O	143	ARG	4.8
1	C	212	ALA	4.8
2	L	124	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	251	ARG	4.8
2	L	162	ASN	4.8
2	O	183	ASP	4.7
2	K	113	LEU	4.7
1	A	213	SER	4.7
1	E	230	GLU	4.7
1	D	264	SER	4.7
2	K	360	SER	4.7
2	M	177	GLU	4.7
2	O	97	LYS	4.7
2	M	174	LEU	4.7
2	N	183	ASP	4.7
2	K	161	THR	4.6
2	L	34	LYS	4.6
2	M	155	LYS	4.6
2	L	125	SER	4.6
1	D	202	LYS	4.6
1	B	260	ARG	4.6
2	K	164	CYS	4.5
2	K	169	GLU	4.5
2	O	83	LYS	4.5
1	B	242	HIS	4.5
1	D	238	GLY	4.5
2	N	171	PHE	4.5
1	B	264	SER	4.4
1	D	228	ARG	4.4
2	L	175	VAL	4.4
2	M	182	PHE	4.4
1	B	208	GLN	4.4
2	M	143	ARG	4.4
2	N	34	LYS	4.4
2	O	146	ARG	4.3
1	B	206	THR	4.3
1	E	209	PRO	4.3
2	K	155	LYS	4.3
2	L	130	ASP	4.3
1	D	208	GLN	4.3
2	O	115	GLY	4.3
2	K	162	ASN	4.3
2	L	114	ASP	4.3
2	K	146	ARG	4.2
2	O	154	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	357	PRO	4.2
1	D	214	LEU	4.2
1	E	217	LEU	4.2
2	L	176	PRO	4.2
2	O	159	GLY	4.2
2	O	57	GLN	4.2
1	B	257	ASN	4.2
2	O	2	SER	4.1
1	D	261	VAL	4.1
1	D	198	TRP	4.1
2	O	96	GLY	4.1
1	C	234	VAL	4.1
2	N	87	ASP	4.1
1	B	265	LEU	4.0
2	M	158	ASP	4.0
1	E	231	PHE	4.0
2	O	93	ILE	4.0
1	C	220	SER	4.0
1	E	225	PHE	4.0
1	E	219	ILE	4.0
1	E	226	SER	4.0
2	O	179	ARG	4.0
1	B	247	LEU	4.0
1	B	226	SER	4.0
2	M	23	ASP	4.0
1	C	251	ARG	4.0
2	M	113	LEU	4.0
2	N	144	VAL	4.0
1	B	232	ILE	4.0
2	K	183	ASP	4.0
1	D	227	SER	3.9
1	B	224	LEU	3.9
1	E	251	ARG	3.9
2	O	127	THR	3.9
1	B	256	TYR	3.9
1	B	236	GLY	3.9
1	E	228	ARG	3.9
1	C	214	LEU	3.9
2	L	359	ASP	3.9
2	L	143	ARG	3.8
2	M	21	ASN	3.8
2	N	162	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	O	63	ASN	3.8
1	E	262	LYS	3.8
2	L	169	GLU	3.8
1	C	211	LYS	3.8
1	D	241	SER	3.8
2	L	120	GLY	3.8
1	E	245	ALA	3.8
2	O	53	GLY	3.8
2	K	115	GLY	3.8
2	M	361	THR	3.8
2	M	98	ALA	3.8
2	K	157	MET	3.8
2	N	143	ARG	3.8
1	B	216	PRO	3.8
2	L	116	VAL	3.8
2	N	179	ARG	3.8
2	K	359	ASP	3.7
2	N	358	ASP	3.7
1	B	255	LEU	3.7
2	N	107	LEU	3.7
1	D	193	ALA	3.7
1	E	210	LYS	3.7
2	N	86	LYS	3.7
2	N	359	ASP	3.7
2	N	37	GLU	3.7
2	N	109	SER	3.7
2	N	360	SER	3.6
1	A	253	LYS	3.6
1	E	258	GLN	3.6
2	K	131	ASP	3.6
1	C	229	GLY	3.6
1	D	233	SER	3.6
2	M	117	LEU	3.6
2	O	117	LEU	3.6
2	O	197	ALA	3.6
2	M	116	VAL	3.6
1	D	243	LYS	3.6
2	O	22	GLU	3.6
2	O	207	LYS	3.6
2	N	356	THR	3.5
2	O	114	ASP	3.5
2	L	118	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	O	182	PHE	3.5
2	K	118	PRO	3.5
1	B	196	ASP	3.5
2	K	152	TYR	3.5
2	L	355	TYR	3.5
2	L	111	LYS	3.5
2	N	195	VAL	3.5
1	C	227	SER	3.4
2	L	126	ARG	3.4
2	L	186	GLY	3.4
1	A	228	ARG	3.4
2	L	367	ASN	3.4
1	B	225	PHE	3.4
2	M	156	LEU	3.4
2	O	48	LEU	3.4
1	D	263	TYR	3.4
2	O	170	GLN	3.4
1	D	224	LEU	3.4
2	N	156	LEU	3.4
2	L	33	ARG	3.4
1	B	259	ALA	3.4
2	L	133	TRP	3.4
1	E	221	LEU	3.4
2	M	146	ARG	3.4
2	L	167	ILE	3.4
2	K	358	ASP	3.4
2	M	121	VAL	3.4
2	K	160	LEU	3.4
2	O	34	LYS	3.3
2	L	146	ARG	3.3
2	N	365	THR	3.3
2	L	361	THR	3.3
1	D	239	ARG	3.3
2	L	97	LYS	3.3
2	N	173	PRO	3.3
2	O	132	LYS	3.3
2	O	164	CYS	3.3
2	N	166	MET	3.3
2	N	33	ARG	3.3
2	O	119	ASP	3.3
2	O	133	TRP	3.3
1	C	228	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	202	LYS	3.3
2	L	360	SER	3.3
1	D	232	ILE	3.3
1	D	254	LYS	3.2
1	B	209	PRO	3.2
2	K	121	VAL	3.2
1	D	262	LYS	3.2
2	N	39	PRO	3.2
2	N	157	MET	3.2
1	B	207	PHE	3.2
1	E	254	LYS	3.2
2	L	68	HIS	3.2
2	N	80	ILE	3.2
2	K	23	ASP	3.2
2	O	113	LEU	3.2
2	K	362	GLY	3.2
2	N	363	GLY	3.1
2	O	74	TYR	3.1
2	M	34	LYS	3.1
2	N	21	ASN	3.1
2	M	107	LEU	3.1
2	M	172	GLU	3.1
1	A	229	GLY	3.1
2	N	115	GLY	3.1
2	O	121	VAL	3.1
2	M	179	ARG	3.1
1	E	243	LYS	3.1
2	O	196	ALA	3.1
1	D	265	LEU	3.1
2	L	60	LYS	3.1
2	N	121	VAL	3.1
2	N	193	LYS	3.1
1	D	215	GLN	3.1
2	N	325	THR	3.1
2	K	34	LYS	3.1
1	E	264	SER	3.1
2	N	132	LYS	3.1
2	O	186	GLY	3.1
2	N	112	ALA	3.0
2	N	196	ALA	3.0
2	O	44	THR	3.0
1	A	220	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	N	128	SER	3.0
1	B	235	GLY	3.0
1	A	231	PHE	3.0
2	K	86	LYS	3.0
2	L	158	ASP	3.0
1	B	248	LEU	3.0
2	M	186	GLY	3.0
2	N	197	ALA	3.0
2	N	49	SER	3.0
2	M	362	GLY	3.0
2	N	353	ASN	3.0
2	O	137	TYR	3.0
2	O	355	TYR	3.0
1	E	236	GLY	3.0
1	E	237	ASN	3.0
1	D	256	TYR	2.9
2	O	192	THR	2.9
2	O	21	ASN	2.9
1	C	260	ARG	2.9
2	N	22	GLU	2.9
2	L	180	ASP	2.9
2	K	357	PRO	2.9
2	O	178	GLY	2.9
2	O	124	ALA	2.9
1	B	262	LYS	2.9
1	E	207	PHE	2.9
2	O	209	GLU	2.9
2	L	3	VAL	2.9
1	D	207	PHE	2.9
2	O	193	LYS	2.9
1	B	244	GLU	2.9
1	D	235	GLY	2.9
2	L	99	GLY	2.9
2	O	33	ARG	2.9
2	M	97	LYS	2.9
2	L	55	VAL	2.9
2	O	50	ASP	2.9
2	O	158	ASP	2.9
2	O	129	ALA	2.9
1	E	244	GLU	2.8
2	L	50	ASP	2.8
2	K	22	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	265	LEU	2.8
2	N	130	ASP	2.8
2	N	184	VAL	2.8
2	L	165	LYS	2.8
1	C	198	TRP	2.8
2	N	200	MET	2.8
1	A	234	VAL	2.8
2	N	172	GLU	2.8
2	O	80	ILE	2.8
2	M	24	PRO	2.8
2	M	132	LYS	2.7
2	O	123	ASP	2.7
2	N	185	TRP	2.7
1	A	260	ARG	2.7
2	O	86	LYS	2.7
2	L	142	TYR	2.7
1	D	223	GLU	2.7
2	N	29	ALA	2.7
2	L	156	LEU	2.7
2	O	195	VAL	2.7
2	O	23	ASP	2.7
1	B	204	SER	2.7
1	D	199	SER	2.7
2	M	181	ILE	2.7
2	N	111	LYS	2.7
2	K	172	GLU	2.7
2	N	54	TYR	2.7
1	D	225	PHE	2.7
1	E	218	THR	2.7
2	L	128	SER	2.7
2	K	156	LEU	2.7
2	M	359	ASP	2.7
1	A	214	LEU	2.6
2	L	48	LEU	2.6
2	N	99	GLY	2.6
1	D	204	SER	2.6
2	K	173	PRO	2.6
2	O	87	ASP	2.6
2	L	102	ILE	2.6
2	N	142	TYR	2.6
1	E	206	THR	2.6
2	K	85	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	359	ASP	2.6
1	D	203	THR	2.6
1	E	256	TYR	2.6
2	L	54	TYR	2.6
1	E	257	ASN	2.6
2	O	43	ASN	2.6
2	K	158	ASP	2.6
1	D	244	GLU	2.6
1	E	242	HIS	2.6
2	K	106	ASP	2.6
2	L	83	LYS	2.6
2	O	194	ILE	2.6
1	A	251	ARG	2.5
2	O	59	LEU	2.5
1	B	203	THR	2.5
1	E	260	ARG	2.5
2	O	200	MET	2.5
2	M	355	TYR	2.5
1	A	195	SER	2.5
1	D	197	VAL	2.5
2	K	350	VAL	2.5
2	N	191	TYR	2.5
2	L	22	GLU	2.5
2	L	215	TYR	2.5
2	O	142	TYR	2.5
2	M	112	ALA	2.5
1	D	231	PHE	2.5
2	M	139	LEU	2.4
1	D	242	HIS	2.4
2	O	116	VAL	2.4
2	L	213	PHE	2.4
2	N	276	PRO	2.4
2	N	119	ASP	2.4
1	D	200	LEU	2.4
2	O	405	GLN	2.4
2	N	92	GLY	2.4
2	L	187	ASN	2.4
1	B	210	LYS	2.4
2	O	185	TRP	2.4
2	K	108	VAL	2.4
2	N	194	ILE	2.4
2	N	192	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	O	165	LYS	2.4
2	K	174	LEU	2.4
2	N	84	LEU	2.4
2	O	84	LEU	2.4
2	M	44	THR	2.4
1	C	239	ARG	2.3
2	M	115	GLY	2.3
2	N	215	TYR	2.3
2	O	191	TYR	2.3
2	O	64	VAL	2.3
2	O	100	ASP	2.3
2	O	98	ALA	2.3
2	K	184	VAL	2.3
2	O	61	SER	2.3
1	E	238	GLY	2.3
2	L	163	GLN	2.3
2	O	24	PRO	2.3
2	N	189	SER	2.3
2	O	166	MET	2.3
1	A	235	GLY	2.3
1	C	210	LYS	2.3
2	N	24	PRO	2.2
2	L	356	THR	2.2
2	K	182	PHE	2.2
2	O	139	LEU	2.2
2	K	370	PRO	2.2
2	O	210	CYS	2.2
2	N	170	GLN	2.2
2	O	94	ASN	2.2
2	L	86	LYS	2.2
2	L	179	ARG	2.2
2	L	422	LYS	2.2
1	E	200	LEU	2.2
1	E	224	LEU	2.2
2	N	355	TYR	2.2
2	M	122	SER	2.2
1	C	237	ASN	2.2
2	N	97	LYS	2.2
2	K	408	ARG	2.2
2	L	192	THR	2.2
1	E	248	LEU	2.2
2	M	183	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	122	SER	2.2
1	E	241	SER	2.1
2	O	88	TRP	2.1
2	K	163	GLN	2.1
2	L	137	TYR	2.1
2	L	23	ASP	2.1
2	O	187	ASN	2.1
2	O	155	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	M	173	PRO	2.1
2	N	46	LYS	2.1
1	A	208	GLN	2.1
2	O	72	TYR	2.1
2	O	85	ASP	2.1
1	A	210	LYS	2.1
1	C	238	GLY	2.1
2	M	138	LEU	2.1
2	O	172	GLU	2.1
2	N	116	VAL	2.1
2	L	87	ASP	2.1
2	O	189	SER	2.1
2	L	44	THR	2.1
2	N	190	ASN	2.1
2	K	145	GLY	2.1
2	K	308	LEU	2.0
2	O	190	ASN	2.0
2	N	25	VAL	2.0
2	L	72	TYR	2.0
1	E	250	LEU	2.0
1	E	265	LEU	2.0
2	M	207	LYS	2.0
2	M	276	PRO	2.0
1	C	235	GLY	2.0
2	O	82	GLY	2.0
2	N	198	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, 95^{th} 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	5.66	120,120,120,120	0
3	TAR	O	423	10/10	0.73	0.41	4.61	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	1.31	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.