



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 02:20 PM EDT

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

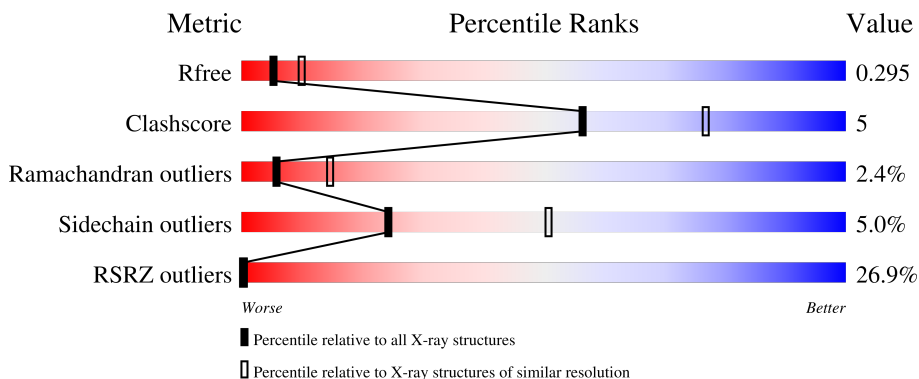
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	87	 22% (red), 74% (green), 9% (yellow), 16% (grey)
1	B	87	 74% (green), 10% (yellow), 16% (grey)
1	C	87	 25% (red), 69% (green), 13% (yellow), 16% (grey)
1	D	87	 64% (red), 72% (green), 9% (yellow), 16% (grey)
1	E	87	 66% (red), 75% (green), 9% (yellow), 16% (grey)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	421	
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	-	-	-
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
			Total	C	N	O	Se			
1	A	73	576	368	100	106	2	0	0	0
1	B	73	576	368	100	106	2	0	0	0
1	C	73	576	368	100	106	2	0	0	0
1	D	73	576	368	100	106	2	0	0	0
1	E	73	576	368	100	106	2	0	0	0

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	182	MET	-	expression tag	UNP P04880

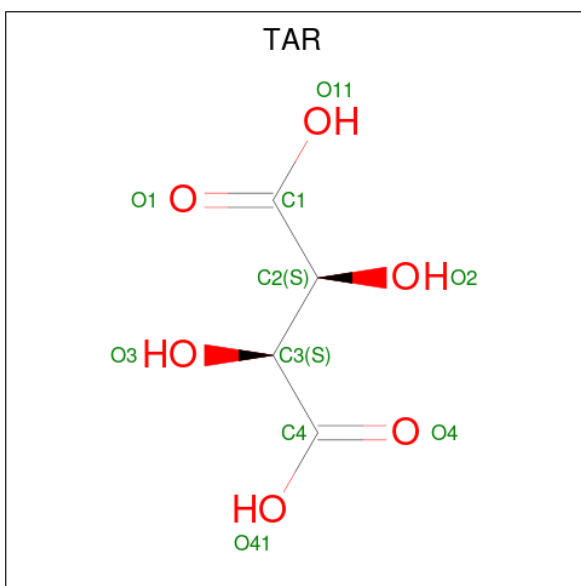
- Molecule 2 is a protein called Nucleoprotein.

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 mutation	UNP Q77E03
L	290	TRP	SER	engineered mutation	UNP Q77E03
M	290	TRP	SER	engineered mutation	UNP Q77E03
N	290	TRP	SER	engineered mutation	UNP Q77E03
O	290	TRP	SER	engineered mutation	UNP Q77E03

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

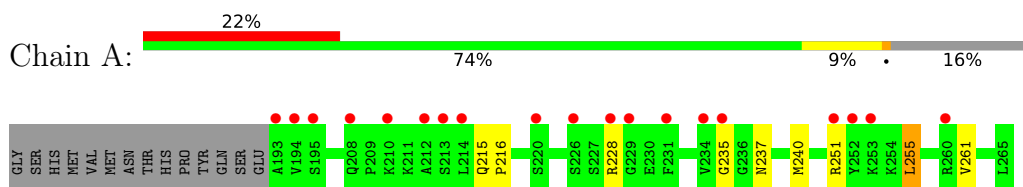


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	M	1	Total	C	O	0	0
			10	4	6		
3	O	1	Total	C	O	0	0
			10	4	6		

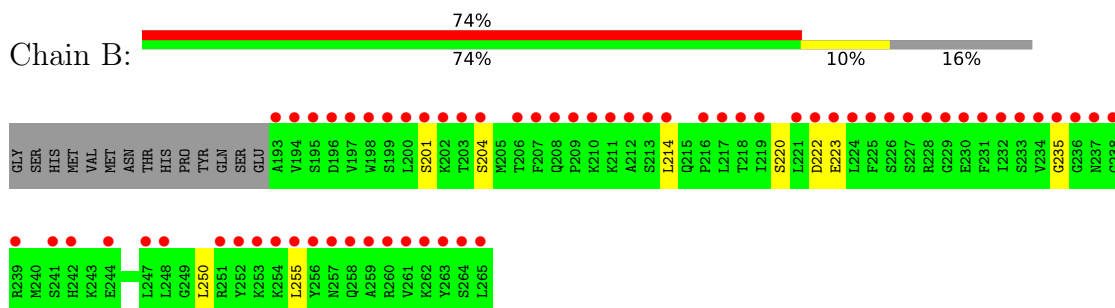
3 Residue-property plots [i](#)

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.

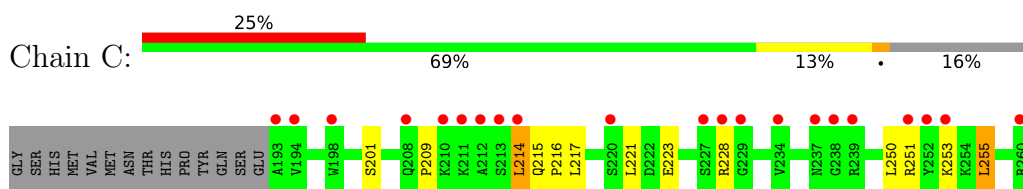
- Molecule 1: Phosphoprotein



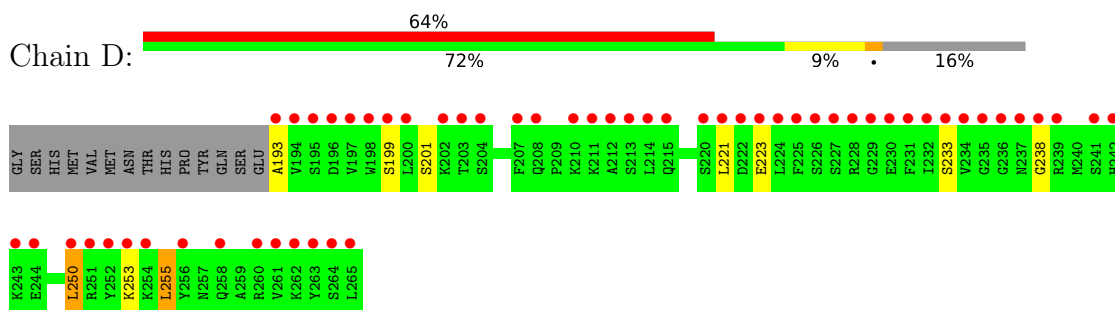
- Molecule 1: Phosphoprotein



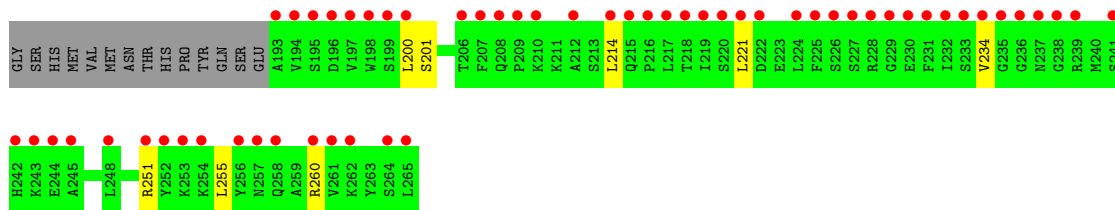
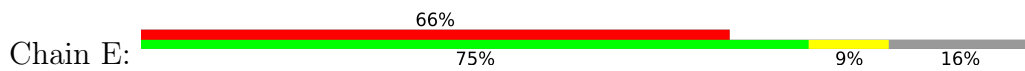
- Molecule 1: Phosphoprotein



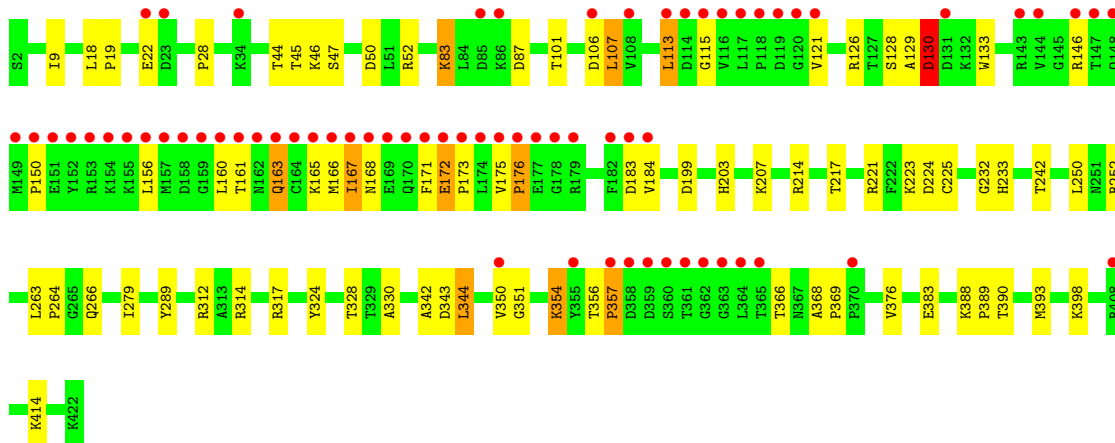
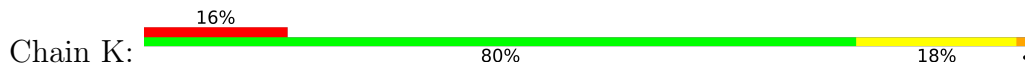
- Molecule 1: Phosphoprotein



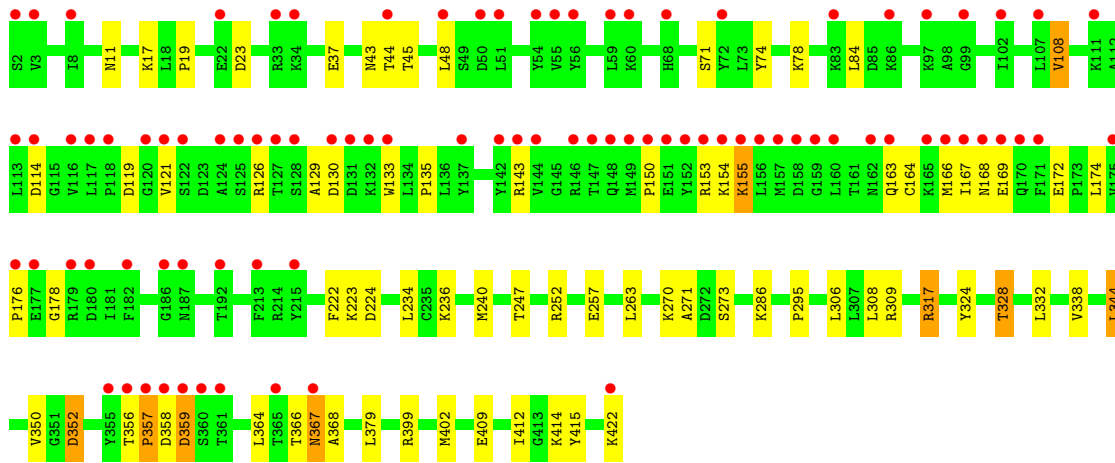
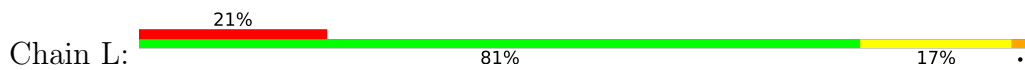
- Molecule 1: Phosphoprotein



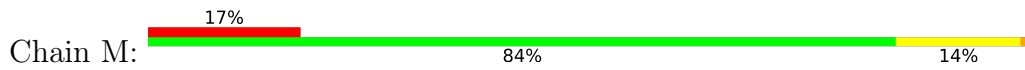
• Molecule 2: Nucleoprotein

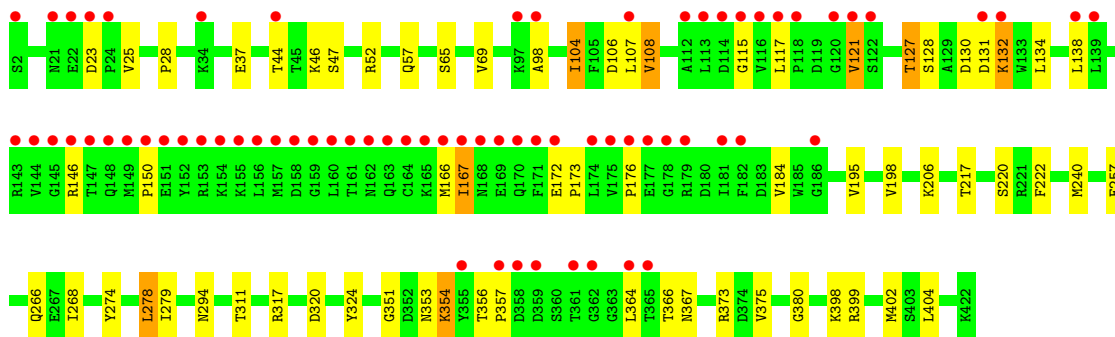


• Molecule 2: Nucleoprotein

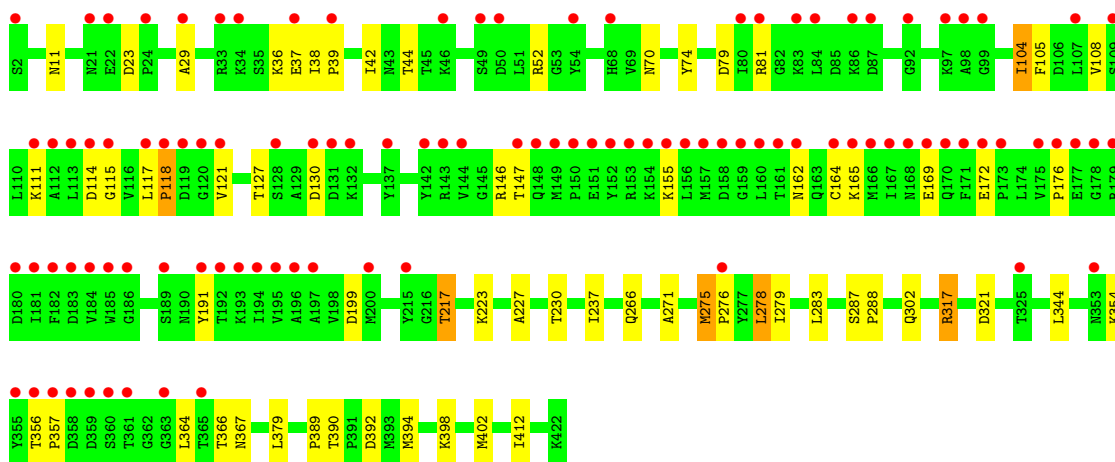
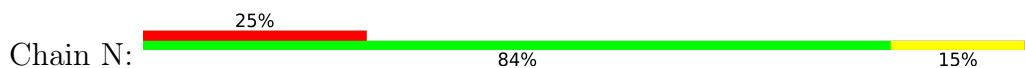


• Molecule 2: Nucleoprotein

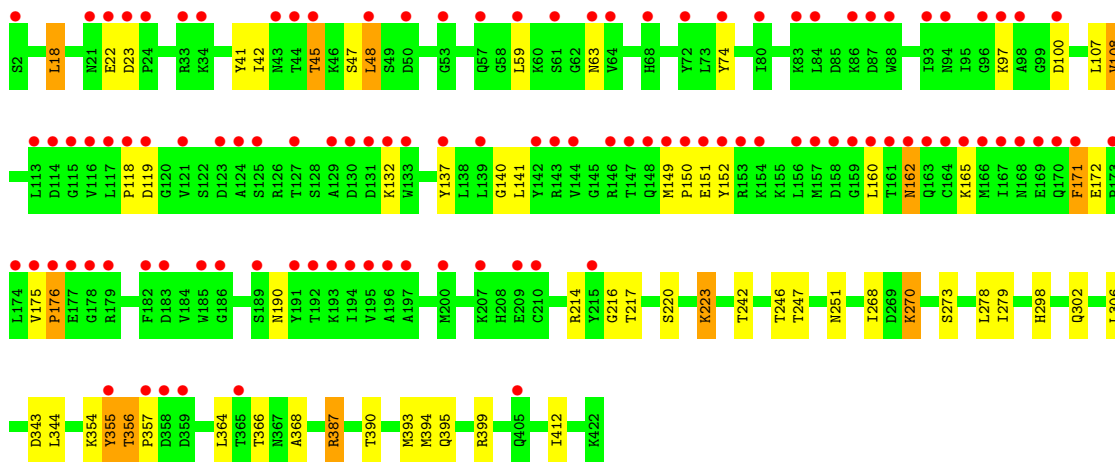
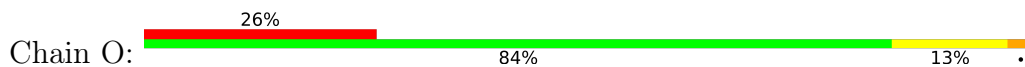




• Molecule 2: Nucleoprotein



• 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)	Xtrriage
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 (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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

Continued on next page...

Continued from previous page...

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:HG2	1:A:251:ARG:HH21	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

Continued on next page...

Continued from previous page...

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:9:ILE:HD13	2:L:252:ARG:HH22	1.64	0.61
2:K:172:GLU:N	2:K:173:PRO:CD	2.63	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:H	2:L:317:ARG:HE	1.50	0.58
2:L:366:THR:C	2:L:368:ALA:H	2.07	0.58
2:O:387:ARG:CG	2:O:387:ARG:HH11	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:HG2	1:A:251:ARG:NH2	2.22	0.55
2:K:106:ASP:OD1	2:K:107:LEU:N	2.39	0.55
2:K:366:THR:HG23	2:K:366:THR:O	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:H	2:K:113:LEU:HD13	1.74	0.52

Continued on next page...

Continued from previous page...

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:HH11	2:O:387:ARG:HG2	1.76	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
1:E:234:VAL:HG12	1:E:251:ARG:HH21	1.75	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:HG2	2:O:387:ARG:NH1	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:K:232:GLY:HA2	2:O:18:LEU:HD21	1.97	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: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

Continued on next page...

Continued from previous page...

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:CG	2:O:387:ARG:NH1	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

Continued on next page...

Continued from previous page...

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:74:TYR:O	2:L:78:LYS:HB2	2.19	0.42
2:L:366:THR:C	2:L:368:ALA:N	2.73	0.42
2:M:52:ARG:HD3	2:M:130:ASP:OD2	2.20	0.42
2:N:317:ARG:H	2:N:317:ARG:HG2	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:HH11	2:O:387:ARG:CB	2.32	0.42
1:C:215:GLN:HA	1:C:216:PRO:HD3	1.95	0.41
2:K:314:ARG:H	2:K:314:ARG:HG2	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: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:N:227:ALA:HA	2:N:230:THR:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

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: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
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%)	11	28
1	B	71/87 (82%)	59 (83%)	11 (16%)	1 (1%)	11	28
1	C	71/87 (82%)	60 (84%)	10 (14%)	1 (1%)	11	28
1	D	71/87 (82%)	58 (82%)	11 (16%)	2 (3%)	5	11
1	E	71/87 (82%)	64 (90%)	7 (10%)	0	100	100
2	K	419/421 (100%)	377 (90%)	29 (7%)	13 (3%)	4	9
2	L	419/421 (100%)	373 (89%)	35 (8%)	11 (3%)	5	13
2	M	419/421 (100%)	372 (89%)	37 (9%)	10 (2%)	6	15
2	N	419/421 (100%)	376 (90%)	36 (9%)	7 (2%)	9	23
2	O	419/421 (100%)	369 (88%)	37 (9%)	13 (3%)	4	9
All	All	2450/2540 (96%)	2170 (89%)	221 (9%)	59 (2%)	6	15

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

Continued on next page...

Continued from previous page...

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%)	62 85
1	B	64/75 (85%)	61 (95%)	3 (5%)	26 54
1	C	64/75 (85%)	59 (92%)	5 (8%)	12 29
1	D	64/75 (85%)	61 (95%)	3 (5%)	26 54
1	E	64/75 (85%)	61 (95%)	3 (5%)	26 54
2	K	362/362 (100%)	341 (94%)	21 (6%)	20 43
2	L	362/362 (100%)	339 (94%)	23 (6%)	17 39
2	M	362/362 (100%)	346 (96%)	16 (4%)	28 56
2	N	362/362 (100%)	349 (96%)	13 (4%)	35 64
2	O	362/362 (100%)	343 (95%)	19 (5%)	23 49
All	All	2130/2185 (98%)	2023 (95%)	107 (5%)	24 51

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Sometimes 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

Continued on next page...

Continued from previous page...

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 [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](#)

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	426	-	9,9,9	1.10	0	12,12,12	0.98	1 (8%)
3	TAR	O	423	-	9,9,9	1.15	0	12,12,12	0.96	0
3	TAR	K	425	-	9,9,9	1.17	0	12,12,12	0.97	1 (8%)
3	TAR	K	423	-	9,9,9	1.08	0	12,12,12	1.04	0
3	TAR	K	424	-	9,9,9	1.13	0	12,12,12	0.97	0
3	TAR	M	1	-	9,9,9	1.21	0	12,12,12	0.87	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	426	-	1/1/4/4	5/12/12/12	-
3	TAR	O	423	-	1/1/4/4	5/12/12/12	-
3	TAR	K	425	-	1/1/4/4	9/12/12/12	-
3	TAR	K	423	-	1/1/4/4	10/12/12/12	-
3	TAR	K	424	-	1/1/4/4	7/12/12/12	-
3	TAR	M	1	-	1/1/4/4	7/12/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	425	TAR	O41-C4-C3	2.14	119.06	113.27
3	K	426	TAR	O41-C4-C3	2.01	118.70	113.27

All (6) chirality outliers are listed below:

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

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	423	TAR	O1-C1-C2-O2
3	K	423	TAR	O11-C1-C2-O2
3	K	426	TAR	O1-C1-C2-O2
3	K	426	TAR	O11-C1-C2-O2
3	K	426	TAR	O3-C3-C4-O4
3	K	426	TAR	O3-C3-C4-O41
3	K	423	TAR	O2-C2-C3-O3
3	K	423	TAR	O3-C3-C4-O4
3	K	423	TAR	O3-C3-C4-O41
3	K	424	TAR	O3-C3-C4-O4
3	K	424	TAR	O3-C3-C4-O41
3	K	425	TAR	O3-C3-C4-O4
3	K	425	TAR	O3-C3-C4-O41
3	O	423	TAR	O3-C3-C4-O4
3	O	423	TAR	O3-C3-C4-O41
3	K	423	TAR	C2-C3-C4-O4
3	K	423	TAR	C2-C3-C4-O41
3	K	423	TAR	C1-C2-C3-O3
3	K	424	TAR	O2-C2-C3-O3
3	K	425	TAR	O11-C1-C2-O2
3	M	1	TAR	O1-C1-C2-O2
3	M	1	TAR	O11-C1-C2-O2
3	M	1	TAR	O3-C3-C4-O4
3	O	423	TAR	O1-C1-C2-O2
3	O	423	TAR	O11-C1-C2-O2
3	K	423	TAR	O2-C2-C3-C4
3	K	425	TAR	O1-C1-C2-O2
3	M	1	TAR	O3-C3-C4-O41
3	K	424	TAR	C1-C2-C3-O3
3	K	426	TAR	O2-C2-C3-O3
3	K	424	TAR	O2-C2-C3-C4
3	K	423	TAR	C1-C2-C3-C4
3	K	424	TAR	C1-C2-C3-C4
3	K	425	TAR	C2-C3-C4-O4
3	K	425	TAR	C2-C3-C4-O41
3	K	425	TAR	O2-C2-C3-O3
3	M	1	TAR	O2-C2-C3-O3
3	O	423	TAR	O2-C2-C3-O3
3	M	1	TAR	C2-C3-C4-O4
3	K	425	TAR	O1-C1-C2-C3
3	M	1	TAR	C2-C3-C4-O41
3	K	424	TAR	C2-C3-C4-O41
3	K	425	TAR	O11-C1-C2-C3

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%) 0 0	59, 84, 88, 89	0
1	B	71/87 (81%)	5.57	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%)	4.28	56 (78%) 0 0	107, 126, 127, 127	0
1	E	71/87 (81%)	4.39	57 (80%) 0 0	119, 133, 135, 135	0
2	K	421/421 (100%)	1.08	69 (16%) 1 1	31, 49, 111, 120	0
2	L	421/421 (100%)	1.30	90 (21%) 0 0	33, 62, 132, 139	0
2	M	421/421 (100%)	1.21	71 (16%) 1 1	31, 53, 116, 126	0
2	N	421/421 (100%)	1.53	104 (24%) 0 0	36, 66, 139, 145	0
2	O	421/421 (100%)	1.49	110 (26%) 0 0	34, 62, 135, 139	0
All	All	2460/2540 (96%)	1.64	662 (26%) 0 0	31, 64, 137, 147	0

All (662) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	ASN	18.8
1	D	252	TYR	17.5
1	B	252	TYR	16.7
2	O	148	GLN	16.7
2	O	157	MET	15.0
2	O	162	ASN	15.0
1	D	194	VAL	14.8
1	D	253	LYS	14.8
1	B	228	ARG	14.8
2	N	150	PRO	14.6
2	M	167	ILE	13.2
2	M	162	ASN	13.2
1	E	198	TRP	12.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	178	GLY	12.9
1	C	194	VAL	12.3
2	L	149	MET	12.3
1	E	193	ALA	12.2
1	B	201	SER	12.0
2	O	149	MET	11.9
1	E	253	LYS	11.8
1	B	229	GLY	11.8
2	M	149	MET	11.4
1	B	198	TRP	11.4
2	N	154	LYS	11.2
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	10.8
1	E	239	ARG	10.6
1	B	253	LYS	10.2
2	M	163	GLN	10.1
2	N	180	ASP	10.1
1	B	194	VAL	10.1
2	L	150	PRO	10.0
2	N	169	GLU	9.9
2	K	117	LEU	9.9
1	B	195	SER	9.9
2	O	147	THR	9.8
1	B	237	ASN	9.8
2	K	177	GLU	9.7
2	K	166	MET	9.7
1	B	261	VAL	9.6
1	E	227	SER	9.5
1	E	196	ASP	9.5
1	B	200	LEU	9.5
2	L	144	VAL	9.4
2	N	151	GLU	9.4
1	B	222	ASP	9.4
2	N	2	SER	9.4
2	O	176	PRO	9.4
1	E	234	VAL	9.3
1	D	234	VAL	9.3
2	K	167	ILE	9.2
2	K	168	ASN	9.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	147	THR	9.1
1	E	195	SER	9.1
2	N	149	MET	9.1
2	K	149	MET	9.0
1	E	214	LEU	9.0
2	M	151	GLU	9.0
2	L	160	LEU	9.0
2	K	176	PRO	9.0
2	N	160	LEU	8.9
2	O	151	GLU	8.8
2	M	357	PRO	8.8
2	O	150	PRO	8.7
2	K	178	GLY	8.7
2	O	357	PRO	8.7
2	M	150	PRO	8.6
2	N	155	LYS	8.6
2	O	358	ASP	8.6
2	N	117	LEU	8.6
2	M	152	TYR	8.6
2	K	154	LYS	8.5
2	L	171	PHE	8.4
2	O	168	ASN	8.4
2	M	176	PRO	8.4
2	L	170	GLN	8.3
2	N	168	ASN	8.3
2	M	131	ASP	8.3
2	N	186	GLY	8.2
1	E	194	VAL	8.2
2	N	148	GLN	8.2
2	K	165	LYS	8.2
2	M	2	SER	8.2
2	M	159	GLY	8.1
1	D	226	SER	8.0
1	E	235	GLY	8.0
2	O	365	THR	8.0
1	B	227	SER	7.9
2	O	152	TYR	7.9
1	E	252	TYR	7.9
2	N	159	GLY	7.9
2	L	152	TYR	7.9
1	B	238	GLY	7.8
2	L	151	GLU	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	153	ARG	7.8
1	A	252	TYR	7.7
2	K	364	LEU	7.7
1	E	197	VAL	7.7
1	E	215	GLN	7.7
2	O	131	ASP	7.6
2	L	166	MET	7.6
2	K	175	VAL	7.5
1	B	212	ALA	7.5
2	L	132	LYS	7.5
2	M	164	CYS	7.5
2	N	176	PRO	7.5
1	B	230	GLU	7.5
1	D	213	SER	7.5
2	L	182	PHE	7.4
2	M	154	LYS	7.4
2	L	177	GLU	7.4
2	L	358	ASP	7.3
1	D	211	LYS	7.2
1	E	233	SER	7.2
2	N	182	PHE	7.2
2	N	177	GLU	7.2
2	O	144	VAL	7.2
2	M	153	ARG	7.2
2	K	150	PRO	7.1
2	N	158	ASP	7.1
1	B	199	SER	7.1
2	K	171	PHE	7.0
1	A	194	VAL	7.0
2	N	165	LYS	7.0
2	N	147	THR	7.0
2	K	147	THR	6.9
2	N	161	THR	6.9
1	B	221	LEU	6.8
2	M	148	GLN	6.8
2	N	357	PRO	6.8
1	A	212	ALA	6.8
1	E	222	ASP	6.8
1	B	231	PHE	6.8
1	C	193	ALA	6.7
1	D	210	LYS	6.7
2	M	145	GLY	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	118	PRO	6.6
1	B	214	LEU	6.6
2	M	157	MET	6.6
2	L	154	LYS	6.6
1	E	229	GLY	6.6
1	C	253	LYS	6.6
2	M	170	GLN	6.6
1	B	233	SER	6.5
1	D	220	SER	6.5
2	K	148	GLN	6.5
2	N	178	GLY	6.5
1	B	213	SER	6.5
1	D	195	SER	6.5
2	N	81	ARG	6.5
1	A	226	SER	6.4
2	M	161	THR	6.4
1	E	208	GLN	6.4
1	D	230	GLU	6.3
2	K	179	ARG	6.3
2	O	118	PRO	6.3
2	M	168	ASN	6.2
2	O	175	VAL	6.2
1	D	212	ALA	6.2
2	L	159	GLY	6.2
2	O	130	ASP	6.2
2	K	361	THR	6.2
2	O	160	LEU	6.2
2	O	173	PRO	6.2
2	M	175	VAL	6.2
2	K	151	GLU	6.1
1	B	217	LEU	6.1
2	N	167	ILE	6.1
2	L	157	MET	6.1
1	D	229	GLY	6.1
2	K	144	VAL	6.0
2	O	156	LEU	6.0
1	D	258	GLN	6.0
2	K	120	GLY	6.0
2	O	167	ILE	6.0
1	B	258	GLN	5.9
2	N	175	VAL	5.9
2	N	68	HIS	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	119	ASP	5.8
2	O	45	THR	5.8
1	C	252	TYR	5.8
2	M	358	ASP	5.8
2	M	364	LEU	5.8
2	M	166	MET	5.8
2	L	2	SER	5.8
2	K	114	ASP	5.8
1	B	218	THR	5.8
2	M	120	GLY	5.7
1	D	236	GLY	5.7
2	L	148	GLN	5.7
2	O	171	PHE	5.7
2	M	144	VAL	5.7
2	L	56	TYR	5.6
2	K	170	GLN	5.6
2	K	363	GLY	5.6
2	O	153	ARG	5.6
2	N	114	ASP	5.5
1	E	261	VAL	5.5
2	K	159	GLY	5.5
2	O	163	GLN	5.5
1	A	193	ALA	5.5
1	B	197	VAL	5.4
2	M	165	LYS	5.4
2	N	131	ASP	5.4
2	N	120	GLY	5.4
2	K	116	VAL	5.4
2	N	181	ILE	5.4
2	L	168	ASN	5.4
2	K	365	THR	5.4
1	E	216	PRO	5.3
1	B	254	LYS	5.3
2	N	118	PRO	5.3
1	E	220	SER	5.2
1	E	199	SER	5.2
2	K	143	ARG	5.2
2	O	68	HIS	5.2
2	N	164	CYS	5.2
2	K	153	ARG	5.1
2	O	169	GLU	5.1
2	K	355	TYR	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	114	ASP	5.1
2	N	137	TYR	5.1
1	B	241	SER	5.1
1	B	239	ARG	5.1
1	E	232	ILE	5.1
1	B	251	ARG	5.0
1	D	260	ARG	5.0
1	D	222	ASP	5.0
2	M	147	THR	5.0
2	M	169	GLU	5.0
1	C	208	GLN	5.0
1	B	234	VAL	5.0
2	L	155	LYS	5.0
2	M	22	GLU	5.0
2	L	127	THR	5.0
2	O	177	GLU	5.0
2	L	113	LEU	5.0
1	B	263	TYR	5.0
2	L	117	LEU	4.9
1	D	196	ASP	4.9
2	O	161	THR	4.9
2	M	365	THR	4.9
2	N	83	LYS	4.9
2	M	160	LEU	4.9
2	L	121	VAL	4.9
1	C	213	SER	4.9
2	N	361	THR	4.9
1	E	212	ALA	4.8
1	D	250	LEU	4.8
2	N	98	ALA	4.8
2	N	50	ASP	4.8
2	L	107	LEU	4.8
1	D	264	SER	4.8
2	M	171	PHE	4.8
2	M	177	GLU	4.8
2	O	215	TYR	4.8
2	O	125	SER	4.8
2	L	162	ASN	4.8
2	N	113	LEU	4.7
2	K	113	LEU	4.7
2	O	143	ARG	4.7
2	L	124	ALA	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	213	SER	4.7
2	K	360	SER	4.7
1	B	211	LYS	4.7
1	E	230	GLU	4.7
1	D	251	ARG	4.6
1	D	202	LYS	4.6
1	C	212	ALA	4.6
2	O	174	LEU	4.6
2	L	365	THR	4.6
2	K	169	GLU	4.6
2	M	174	LEU	4.6
2	O	183	ASP	4.5
2	L	34	LYS	4.5
2	K	161	THR	4.5
2	O	97	LYS	4.5
2	M	155	LYS	4.5
2	K	164	CYS	4.5
2	L	125	SER	4.5
2	O	83	LYS	4.5
2	O	146	ARG	4.5
2	L	175	VAL	4.5
2	N	183	ASP	4.4
1	B	260	ARG	4.4
1	D	228	ARG	4.4
2	M	143	ARG	4.3
1	B	264	SER	4.3
1	B	208	GLN	4.3
2	O	115	GLY	4.3
2	N	34	LYS	4.3
1	D	214	LEU	4.3
2	M	182	PHE	4.3
2	K	155	LYS	4.3
1	E	209	PRO	4.2
2	L	130	ASP	4.2
1	B	206	THR	4.2
2	K	146	ARG	4.2
1	B	242	HIS	4.2
1	D	238	GLY	4.2
2	N	171	PHE	4.2
1	D	208	GLN	4.2
2	L	357	PRO	4.1
2	K	162	ASN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	57	GLN	4.1
2	L	176	PRO	4.1
2	O	159	GLY	4.1
2	O	2	SER	4.1
1	B	257	ASN	4.1
2	O	154	LYS	4.1
1	D	198	TRP	4.1
1	B	247	LEU	4.0
1	E	225	PHE	4.0
1	C	234	VAL	4.0
1	E	231	PHE	4.0
2	O	93	ILE	4.0
1	D	261	VAL	4.0
1	E	217	LEU	4.0
2	L	114	ASP	4.0
1	B	226	SER	4.0
1	C	220	SER	4.0
2	N	87	ASP	4.0
2	M	158	ASP	3.9
2	N	144	VAL	3.9
1	E	219	ILE	3.9
1	B	236	GLY	3.9
1	B	265	LEU	3.9
1	E	226	SER	3.9
1	D	227	SER	3.9
1	B	256	TYR	3.9
1	C	251	ARG	3.9
1	C	214	LEU	3.9
1	E	262	LYS	3.9
2	O	96	GLY	3.9
2	O	127	THR	3.9
2	L	143	ARG	3.8
2	O	179	ARG	3.8
1	B	232	ILE	3.8
2	M	113	LEU	3.8
2	M	23	ASP	3.8
1	E	228	ARG	3.8
1	E	251	ARG	3.8
2	O	63	ASN	3.8
1	E	245	ALA	3.8
2	K	183	ASP	3.8
2	N	109	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	224	LEU	3.7
2	M	21	ASN	3.7
2	L	169	GLU	3.7
2	N	143	ARG	3.7
1	B	255	LEU	3.7
2	N	107	LEU	3.7
2	K	359	ASP	3.7
2	L	359	ASP	3.7
2	N	358	ASP	3.7
1	D	193	ALA	3.7
2	M	361	THR	3.7
2	O	53	GLY	3.7
2	N	37	GLU	3.7
2	N	162	ASN	3.7
2	L	120	GLY	3.7
2	L	116	VAL	3.7
1	C	211	LYS	3.7
2	K	157	MET	3.7
1	E	258	GLN	3.6
2	N	359	ASP	3.6
2	N	179	ARG	3.6
2	N	86	LYS	3.6
2	K	115	GLY	3.6
2	M	98	ALA	3.6
1	D	241	SER	3.6
2	N	360	SER	3.6
1	E	210	LYS	3.6
1	B	216	PRO	3.6
2	K	131	ASP	3.5
1	D	233	SER	3.5
1	A	253	LYS	3.5
2	O	197	ALA	3.5
2	M	121	VAL	3.5
2	O	182	PHE	3.5
1	E	221	LEU	3.5
2	M	117	LEU	3.5
2	M	156	LEU	3.5
2	N	156	LEU	3.5
2	N	356	THR	3.5
1	C	229	GLY	3.4
2	O	117	LEU	3.4
1	D	243	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	146	ARG	3.4
2	K	152	TYR	3.4
2	M	116	VAL	3.4
2	L	133	TRP	3.4
2	L	126	ARG	3.4
2	O	207	LYS	3.4
2	K	118	PRO	3.4
1	D	224	LEU	3.4
2	K	160	LEU	3.4
2	N	195	VAL	3.4
2	O	48	LEU	3.4
2	L	361	THR	3.4
2	O	22	GLU	3.4
1	B	196	ASP	3.4
2	L	33	ARG	3.4
2	L	146	ARG	3.4
1	C	227	SER	3.3
2	L	118	PRO	3.3
1	B	202	LYS	3.3
1	D	263	TYR	3.3
2	L	355	TYR	3.3
2	O	114	ASP	3.3
1	D	232	ILE	3.3
2	L	167	ILE	3.3
2	L	367	ASN	3.3
1	B	225	PHE	3.3
1	A	228	ARG	3.3
1	B	259	ALA	3.3
2	K	358	ASP	3.3
2	L	111	LYS	3.3
2	O	170	GLN	3.3
2	L	186	GLY	3.3
1	C	228	ARG	3.2
2	N	33	ARG	3.2
2	O	34	LYS	3.2
2	O	133	TRP	3.2
2	L	97	LYS	3.2
2	L	360	SER	3.2
2	N	365	THR	3.2
2	O	132	LYS	3.2
1	D	262	LYS	3.2
2	N	173	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	80	ILE	3.2
2	K	362	GLY	3.1
1	B	209	PRO	3.1
1	D	239	ARG	3.1
2	N	157	MET	3.1
2	N	166	MET	3.1
2	O	164	CYS	3.1
2	N	21	ASN	3.1
1	E	264	SER	3.1
2	L	68	HIS	3.1
2	K	121	VAL	3.1
2	O	119	ASP	3.1
1	E	254	LYS	3.1
2	N	132	LYS	3.1
2	O	121	VAL	3.1
2	M	107	LEU	3.1
1	E	243	LYS	3.1
2	N	115	GLY	3.0
2	N	121	VAL	3.0
1	D	254	LYS	3.0
2	K	34	LYS	3.0
1	D	215	GLN	3.0
2	O	74	TYR	3.0
1	B	207	PHE	3.0
2	N	49	SER	3.0
2	N	193	LYS	3.0
2	K	23	ASP	3.0
2	N	39	PRO	3.0
1	A	229	GLY	3.0
2	M	179	ARG	3.0
2	N	325	THR	3.0
1	D	265	LEU	3.0
2	O	196	ALA	3.0
2	M	34	LYS	3.0
1	A	220	SER	3.0
2	N	363	GLY	3.0
2	O	113	LEU	3.0
2	N	196	ALA	3.0
1	A	231	PHE	3.0
2	K	86	LYS	3.0
2	N	128	SER	3.0
1	B	248	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	235	GLY	3.0
2	O	192	THR	2.9
2	N	112	ALA	2.9
2	L	60	LYS	2.9
2	O	44	THR	2.9
2	M	172	GLU	2.9
1	C	260	ARG	2.9
1	E	236	GLY	2.9
2	M	186	GLY	2.9
2	K	357	PRO	2.9
2	O	33	ARG	2.9
2	N	22	GLU	2.9
2	O	137	TYR	2.9
2	N	197	ALA	2.9
2	L	158	ASP	2.9
2	L	99	GLY	2.9
1	E	237	ASN	2.9
2	O	21	ASN	2.9
2	O	178	GLY	2.9
2	O	129	ALA	2.9
2	O	355	TYR	2.9
2	O	186	GLY	2.8
2	M	362	GLY	2.8
1	E	207	PHE	2.8
2	O	193	LYS	2.8
1	D	235	GLY	2.8
1	D	199	SER	2.8
2	O	158	ASP	2.8
2	N	353	ASN	2.8
2	L	55	VAL	2.8
2	O	209	GLU	2.8
1	D	256	TYR	2.8
1	B	262	LYS	2.8
1	B	244	GLU	2.8
1	C	198	TRP	2.8
1	E	244	GLU	2.8
2	K	22	GLU	2.7
2	N	130	ASP	2.7
2	O	50	ASP	2.7
1	C	265	LEU	2.7
1	A	234	VAL	2.7
1	D	207	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	97	LYS	2.7
1	B	204	SER	2.7
2	L	3	VAL	2.7
2	L	156	LEU	2.7
1	D	203	THR	2.7
1	D	204	SER	2.7
2	L	50	ASP	2.7
2	N	29	ALA	2.7
1	A	260	ARG	2.7
2	O	80	ILE	2.7
2	L	180	ASP	2.7
2	M	132	LYS	2.7
1	D	225	PHE	2.7
2	N	185	TRP	2.7
2	M	24	PRO	2.7
2	O	195	VAL	2.7
2	N	200	MET	2.7
2	K	156	LEU	2.7
2	L	165	LYS	2.7
2	N	111	LYS	2.7
2	O	123	ASP	2.7
2	O	124	ALA	2.6
2	N	184	VAL	2.6
2	O	86	LYS	2.6
2	L	128	SER	2.6
2	M	181	ILE	2.6
2	N	54	TYR	2.6
2	L	48	LEU	2.6
1	E	218	THR	2.6
1	D	223	GLU	2.6
2	K	172	GLU	2.6
1	A	214	LEU	2.6
2	O	23	ASP	2.6
2	L	142	TYR	2.6
2	N	172	GLU	2.6
2	L	102	ILE	2.5
2	O	194	ILE	2.5
1	E	256	TYR	2.5
2	K	158	ASP	2.5
2	M	359	ASP	2.5
2	N	99	GLY	2.5
1	E	257	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	173	PRO	2.5
2	O	43	ASN	2.5
2	N	142	TYR	2.5
2	K	350	VAL	2.5
1	D	244	GLU	2.5
2	L	215	TYR	2.5
2	O	359	ASP	2.5
1	E	260	ARG	2.5
2	O	59	LEU	2.5
2	L	83	LYS	2.5
1	A	251	ARG	2.5
2	K	85	ASP	2.5
2	O	87	ASP	2.5
1	E	206	THR	2.5
2	K	106	ASP	2.5
1	D	231	PHE	2.5
1	B	203	THR	2.4
2	L	54	TYR	2.4
2	N	191	TYR	2.4
1	A	195	SER	2.4
1	E	242	HIS	2.4
2	M	112	ALA	2.4
2	N	92	GLY	2.4
2	M	355	TYR	2.4
2	O	142	TYR	2.4
2	L	22	GLU	2.4
2	M	139	LEU	2.4
2	O	200	MET	2.4
2	N	276	PRO	2.4
1	D	197	VAL	2.4
1	D	200	LEU	2.4
1	B	210	LYS	2.4
2	L	213	PHE	2.4
2	N	194	ILE	2.3
2	O	116	VAL	2.3
2	O	185	TRP	2.3
1	D	242	HIS	2.3
2	K	174	LEU	2.3
2	N	192	THR	2.3
2	K	108	VAL	2.3
1	C	239	ARG	2.3
1	E	238	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	215	TYR	2.3
2	O	84	LEU	2.3
2	O	191	TYR	2.3
2	O	405	GLN	2.3
2	O	24	PRO	2.3
2	O	64	VAL	2.3
2	M	44	THR	2.3
1	C	210	LYS	2.3
2	O	165	LYS	2.3
2	M	115	GLY	2.2
2	L	187	ASN	2.2
2	N	189	SER	2.2
2	O	61	SER	2.2
2	K	184	VAL	2.2
2	M	122	SER	2.2
2	N	24	PRO	2.2
1	A	235	GLY	2.2
2	N	84	LEU	2.2
2	N	119	ASP	2.2
2	O	100	ASP	2.2
1	E	248	LEU	2.2
2	O	139	LEU	2.2
2	O	98	ALA	2.2
1	E	224	LEU	2.2
2	K	370	PRO	2.2
2	L	163	GLN	2.2
2	L	179	ARG	2.2
2	L	122	SER	2.1
2	L	192	THR	2.1
2	L	356	THR	2.1
1	C	237	ASN	2.1
2	O	94	ASN	2.1
2	L	86	LYS	2.1
2	L	44	THR	2.1
2	K	182	PHE	2.1
2	K	408	ARG	2.1
1	A	210	LYS	2.1
2	L	8	ILE	2.1
2	N	170	GLN	2.1
2	O	88	TRP	2.1
2	O	166	MET	2.1
2	O	210	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	137	TYR	2.1
2	L	422	LYS	2.1
2	L	51	LEU	2.1
2	N	355	TYR	2.1
2	O	72	TYR	2.1
1	E	241	SER	2.1
1	E	200	LEU	2.1
1	E	265	LEU	2.1
2	M	138	LEU	2.1
2	N	46	LYS	2.1
2	K	163	GLN	2.0
2	N	97	LYS	2.0
1	B	219	ILE	2.0
2	L	72	TYR	2.0
1	C	238	GLY	2.0
1	A	208	GLN	2.0
1	D	221	LEU	2.0
2	O	189	SER	2.0
2	L	59	LEU	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](#)

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. 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	B-factors(Å ²)	Q<0.9
3	TAR	K	423	10/10	0.55	0.51	120,120,120,120	0
3	TAR	K	425	10/10	0.65	0.38	67,69,70,71	0
3	TAR	K	424	10/10	0.71	0.31	92,93,93,93	0
3	TAR	O	423	10/10	0.73	0.42	108,108,108,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TAR	K	426	10/10	0.75	0.32	87,88,88,88	0
3	TAR	M	1	10/10	0.80	0.31	117,118,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.