Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 12:53 PM EDT

PDB ID	:	5H9F
Title	:	Crystal structure of E. coli Cascade bound to a PAM-containing dsDNA target at 2.45 angstrom resolution.
Authors	:	Hayes, R.P.; Xiao, Y.; Ding, F.; van Erp, P.B.G.; Rajashankar, K.; Bailey, S.; Wiedenheft, B.; Ke, A.
Deposited on	:	2015-12-28
Resolution	:	2.45 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:

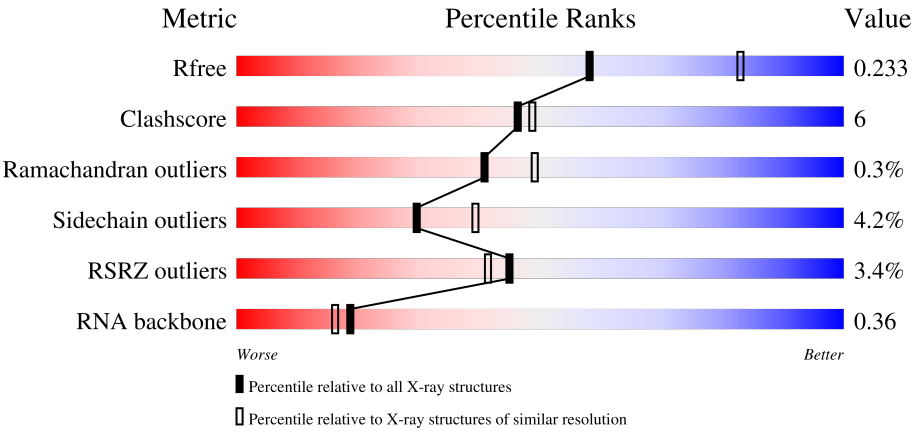
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.45 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.



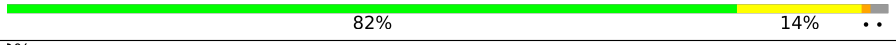
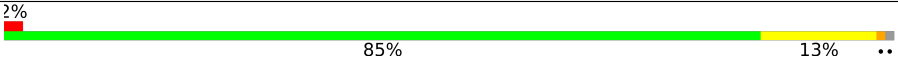
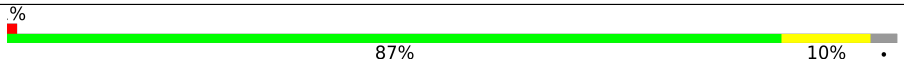
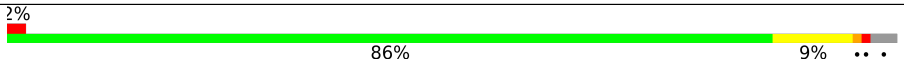
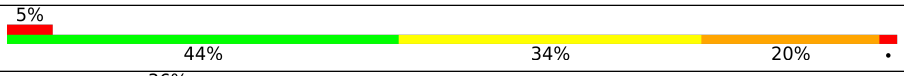
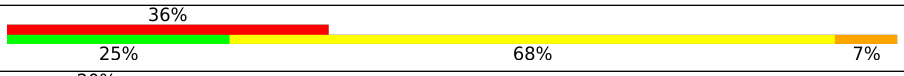
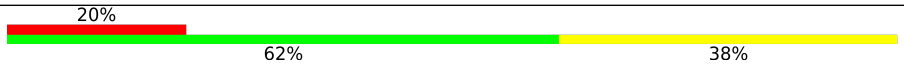
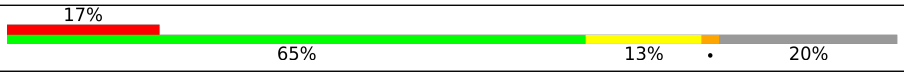
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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 <=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	502	82% 13%
2	B	165	5% 73% 19% 7%
2	C	165	84% 6% 9%
3	D	363	6% 65% 20% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	363	
3	F	363	
3	G	363	
3	H	363	
3	I	363	
4	J	224	
5	L	61	
6	M	28	
7	N	50	
8	K	199	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28930 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 CRISPR system Cascade subunit CasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3746	2389	663	675	19			

- Molecule 2 is a protein called CRISPR system Cascade subunit CasB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1246	782	239	218	7			
2	C	150	Total	C	N	O	S	0	0	0
			1223	770	231	215	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P76632
B	-3	PRO	-	expression tag	UNP P76632
B	-2	GLY	-	expression tag	UNP P76632
B	-1	TYR	-	expression tag	UNP P76632
B	0	GLN	-	expression tag	UNP P76632
C	-4	GLY	-	expression tag	UNP P76632
C	-3	PRO	-	expression tag	UNP P76632
C	-2	GLY	-	expression tag	UNP P76632
C	-1	TYR	-	expression tag	UNP P76632
C	0	GLN	-	expression tag	UNP P76632

- Molecule 3 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	318	Total	C	N	O	S	0	0	0
			2399	1503	431	450	15			
3	E	354	Total	C	N	O	S	0	0	0
			2694	1685	479	515	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	361	Total	C	N	O	S	0	0	0
			2755	1721	490	529	15			
3	G	354	Total	C	N	O	S	0	0	0
			2713	1698	484	516	15			
3	H	352	Total	C	N	O	S	0	0	0
			2691	1681	479	516	15			
3	I	351	Total	C	N	O	S	0	0	0
			2686	1680	476	515	15			

- Molecule 4 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	219	Total	C	N	O	S	0	0	0
			1731	1097	308	317	9			

- Molecule 5 is a RNA chain called crRNA (61-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	61	Total	C	N	O	P	0	0	0
			1300	580	233	426	61			

- Molecule 6 is a DNA chain called DNA (28-MER) Non-target.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	28	Total	C	N	O	P	0	0	0
			572	276	90	178	28			

- Molecule 7 is a DNA chain called DNA (50-MER) Target.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	50	Total	C	N	O	P	0	0	0
			1025	486	195	294	50			

- Molecule 8 is a protein called CRISPR system Cascade subunit CasE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	159	Total	C	N	O	S	0	0	0
			1098	704	182	205	7			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Zn 1 1	0	0

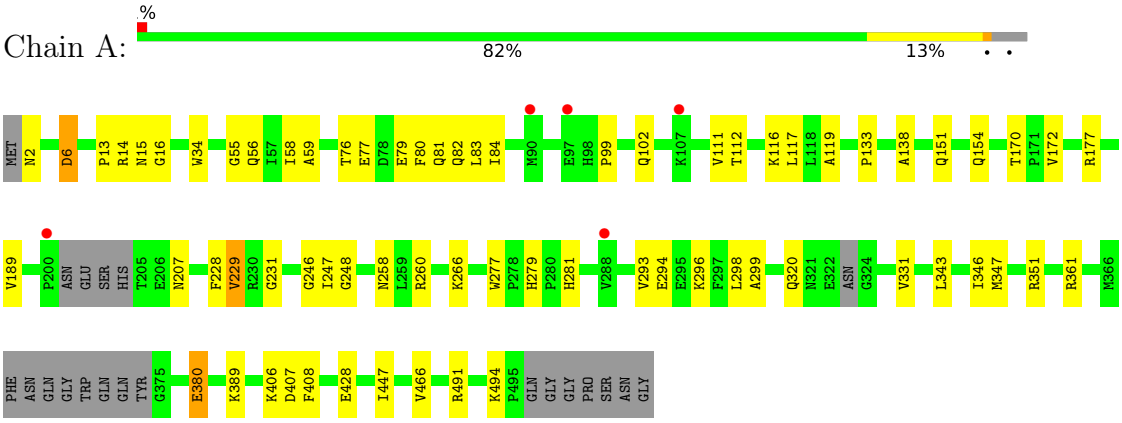
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	133	Total O 133 133	0	0
10	B	22	Total O 22 22	0	0
10	C	63	Total O 63 63	0	0
10	D	32	Total O 32 32	0	0
10	E	95	Total O 95 95	0	0
10	F	99	Total O 99 99	0	0
10	G	144	Total O 144 144	0	0
10	H	130	Total O 130 130	0	0
10	I	128	Total O 128 128	0	0
10	J	69	Total O 69 69	0	0
10	L	67	Total O 67 67	0	0
10	M	13	Total O 13 13	0	0
10	N	49	Total O 49 49	0	0
10	K	6	Total O 6 6	0	0

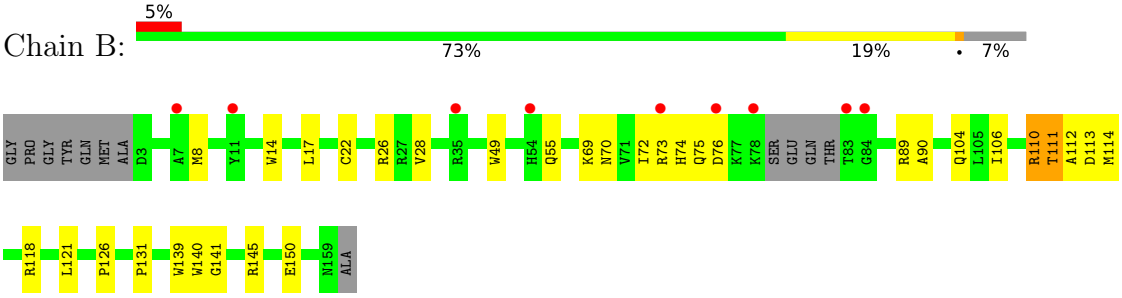
3 Residue-property plots (i)

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.

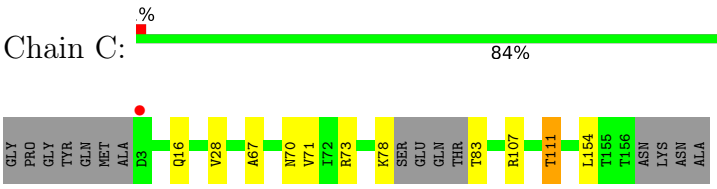
• Molecule 1: CRISPR system Cascade subunit CasA



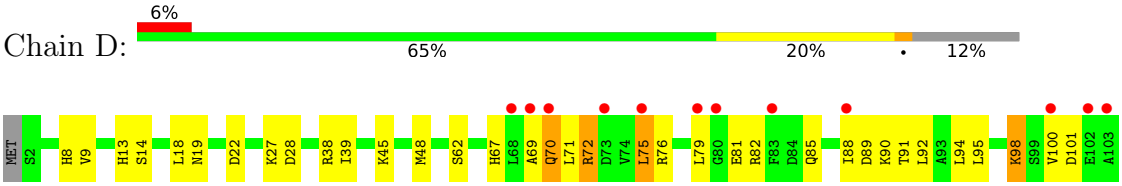
• Molecule 2: CRISPR system Cascade subunit CasB

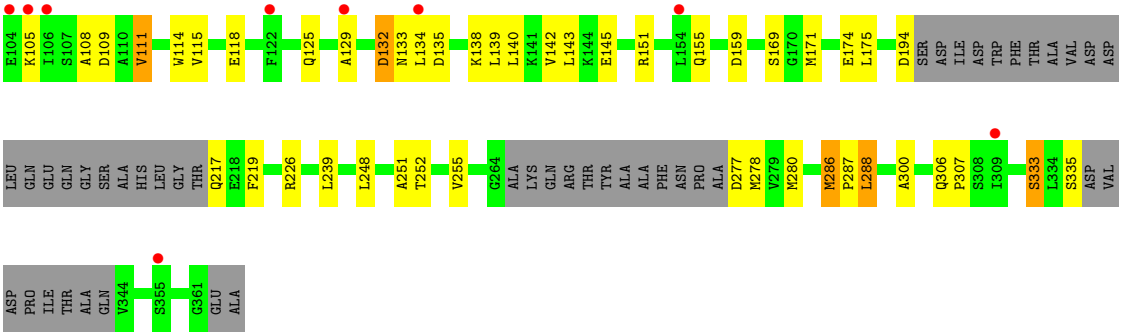


• Molecule 2: CRISPR system Cascade subunit CasB



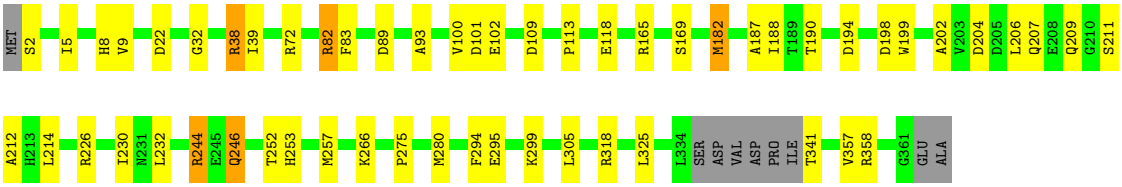
• Molecule 3: CRISPR system Cascade subunit CasC





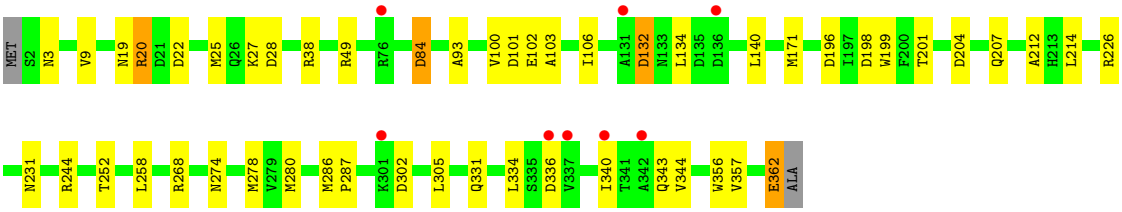
• Molecule 3: CRISPR system Cascade subunit CasC

Chain E:



• Molecule 3: CRISPR system Cascade subunit CasC

Chain F:

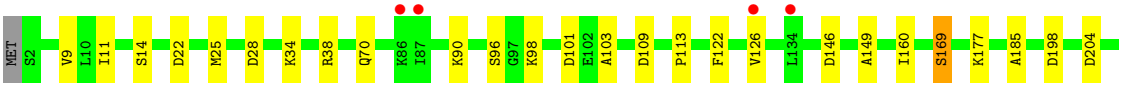


• Molecule 3: CRISPR system Cascade subunit CasC

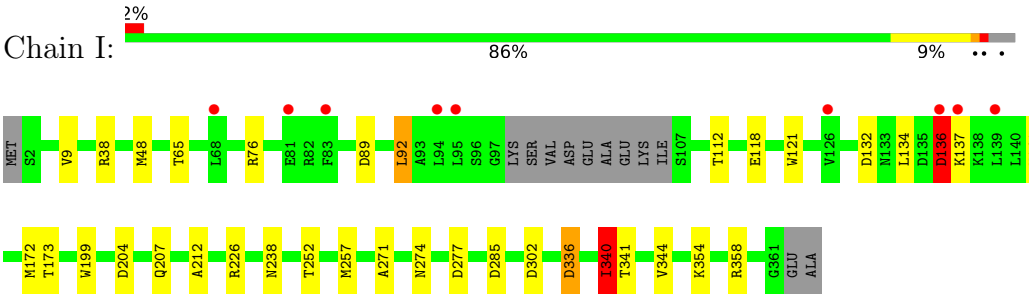
Chain G:

• Molecule 3: CRISPR system Cascade subunit CasC

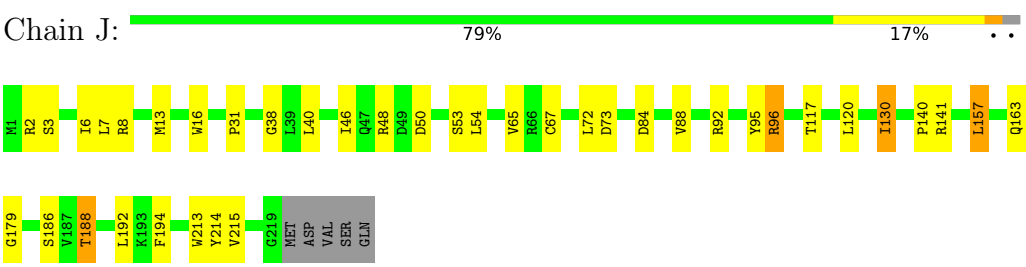
Chain H:



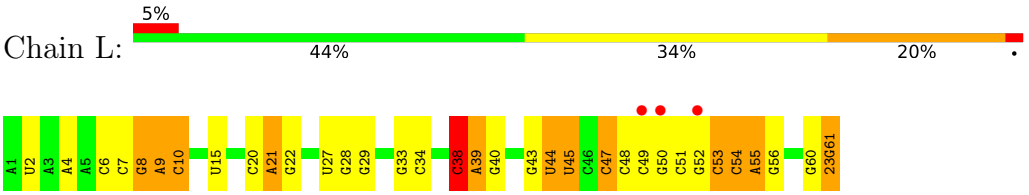
• Molecule 3: CRISPR system Cascade subunit CasC



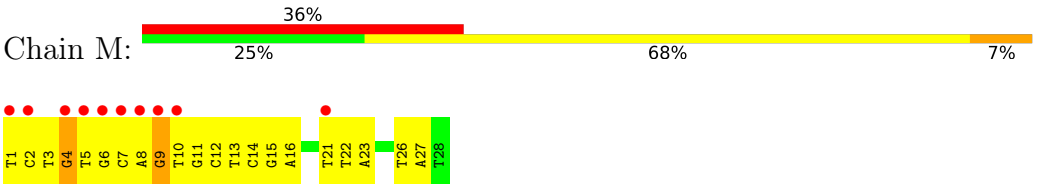
• Molecule 4: CRISPR system Cascade subunit CasD



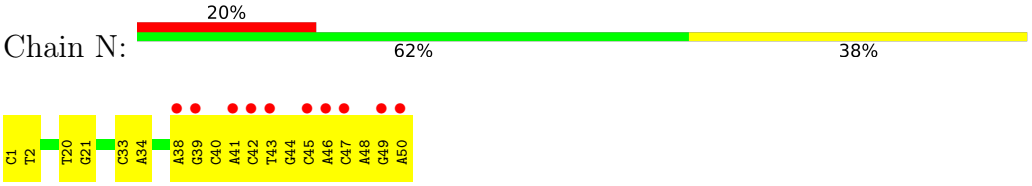
• Molecule 5: crRNA (61-MER)



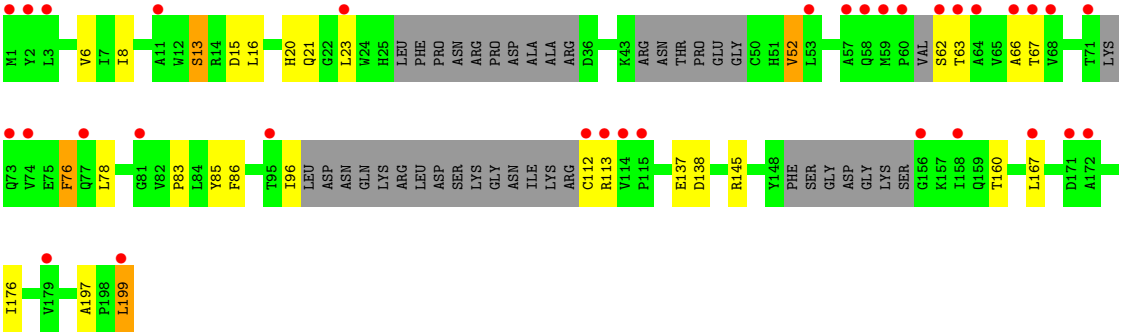
• Molecule 6: DNA (28-MER) Non-target



• Molecule 7: DNA (50-MER) Target



• Molecule 8: CRISPR system Cascade subunit CasE


M1 Y2 L3 V6 I7 I8 A11 W12 S13 R14 D15 L16 H20 Q21 G22 L23 W24 H25 LEU PHE PRO ASN ARG PRO ASP ALA ALA ARG D36 K43 ARG ASN THR PRO GLU GLY C50 H51 V52 L53 A57 Q58 M59 P60 VAL S62 T63 A64 V65 A66 T67 V68 T71 LYS
Q73 V74 E75 F76 Q77 L78 G81 V82 P83 L84 Y85 P86 T95 I96 LEU ASP ASN GLN LYS ARG LEU ASP SER LYS GLY ASN ILE LYS ARG C112 R113 V114 P115 E137 D138 R145 Y148 PHE SER GLY ASP GLY LYS SER G156 K157 I158 Q159 T160 L167 D171 A172
I176 V179 A197 P198 L199

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.98Å 150.06Å 400.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 2.45 49.87 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.87-2.45) 92.9 (49.87-2.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.206 , 0.233 0.208 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28930	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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, 0.333 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: ZN, 23G

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	0.28	0/3830	0.42	0/5200
2	B	0.42	0/1270	0.43	0/1717
2	C	0.28	0/1247	0.41	0/1686
3	D	0.26	0/2433	0.41	0/3286
3	E	0.27	0/2737	0.39	0/3702
3	F	0.29	0/2800	0.42	0/3790
3	G	0.29	0/2756	0.41	0/3721
3	H	0.29	0/2734	0.41	0/3697
3	I	0.33	0/2730	0.44	0/3693
4	J	0.37	0/1773	0.50	1/2407 (0.0%)
5	L	0.51	1/1423 (0.1%)	0.95	7/2216 (0.3%)
6	M	0.73	0/637	1.20	3/982 (0.3%)
7	N	0.76	0/1151	0.92	0/1773
8	K	0.23	0/1112	0.42	0/1521
All	All	0.36	1/28633 (0.0%)	0.53	11/39391 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	44	U	O3'-P	-6.49	1.53	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	38	C	C2-N1-C1'	7.80	127.38	118.80
6	M	4	DG	O4'-C1'-N9	7.80	113.46	108.00
6	M	4	DG	OP1-P-O3'	7.72	122.18	105.20
5	L	38	C	N1-C2-O2	6.75	122.95	118.90
5	L	38	C	N3-C2-O2	-6.02	117.68	121.90
5	L	8	G	O4'-C1'-N9	5.91	112.93	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	38	C	C6-N1-C2	-5.86	117.96	120.30
4	J	188	THR	N-CA-C	5.36	125.48	111.00
5	L	20	C	C2-N1-C1'	5.21	124.53	118.80
5	L	38	C	C6-N1-C1'	-5.14	114.63	120.80
6	M	9	DG	O4'-C1'-N9	5.04	111.53	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3746	0	3735	37	0
2	B	1246	0	1235	17	0
2	C	1223	0	1214	4	0
3	D	2399	0	2350	49	0
3	E	2694	0	2629	32	0
3	F	2755	0	2692	31	0
3	G	2713	0	2674	24	0
3	H	2691	0	2627	25	0
3	I	2686	0	2630	28	0
4	J	1731	0	1723	29	0
5	L	1300	0	659	39	0
6	M	572	0	323	30	0
7	N	1025	0	560	23	0
8	K	1098	0	1010	14	0
9	A	1	0	0	0	0
10	A	133	0	0	6	0
10	B	22	0	0	2	0
10	C	63	0	0	0	0
10	D	32	0	0	0	0
10	E	95	0	0	1	0
10	F	99	0	0	3	0
10	G	144	0	0	4	0
10	H	130	0	0	4	0
10	I	128	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	69	0	0	1	0
10	K	6	0	0	1	0
10	L	67	0	0	1	0
10	M	13	0	0	0	0
10	N	49	0	0	0	0
All	All	28930	0	26061	336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (336) 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)
5:L:52:G:N7	5:L:55:A:N6	1.88	1.20
5:L:50:G:C6	5:L:51:C:N4	2.13	1.17
3:H:28:ASP:O	3:H:38:ARG:NH1	1.92	1.03
5:L:52:G:C8	5:L:55:A:N6	2.29	0.98
3:D:72:ARG:NH1	3:D:101:ASP:O	1.98	0.95
3:F:20:ARG:NH1	5:L:29:G:OP2	2.01	0.93
3:D:28:ASP:O	3:D:38:ARG:NH1	2.02	0.93
5:L:44:U:O2'	5:L:45:U:OP2	1.86	0.92
6:M:14:DC:H2"	6:M:15:DG:H5'	1.48	0.92
1:A:296:LYS:NZ	6:M:21:DT:OP2	2.04	0.89
1:A:116:LYS:NZ	10:A:701:HOH:O	2.06	0.86
5:L:60:G:C3'	5:L:61:23G:H5'	2.05	0.86
7:N:38:DA:H2'	7:N:39:DG:C8	2.15	0.82
3:I:137:LYS:NZ	7:N:46:DA:OP2	2.12	0.82
1:A:246:GLY:O	1:A:260:ARG:NH1	2.12	0.81
6:M:7:DC:H42	7:N:44:DG:H1	1.26	0.80
5:L:60:G:H3'	5:L:61:23G:H5'	1.63	0.80
3:G:93:ALA:HB2	3:G:100:VAL:HG22	1.64	0.80
3:G:82:ARG:NH1	10:G:402:HOH:O	2.14	0.79
3:D:27:LYS:NZ	5:L:39:A:OP1	2.15	0.79
2:B:26:ARG:HH21	2:B:69:LYS:HB2	1.48	0.79
6:M:9:DG:H4'	6:M:10:DT:OP1	1.83	0.77
3:E:93:ALA:HB2	3:E:100:VAL:HG22	1.67	0.77
6:M:9:DG:OP2	6:M:9:DG:H3'	1.84	0.76
2:C:70:ASN:O	2:C:73:ARG:NH1	2.19	0.75
5:L:50:G:C5	5:L:51:C:N4	2.55	0.75
4:J:92:ARG:NH1	5:L:6:C:O2	2.21	0.73
2:B:139:TRP:O	2:B:141:GLY:N	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:10:DT:H3	7:N:41:DA:H61	1.36	0.72
10:I:523:HOH:O	4:J:13:MET:SD	2.47	0.71
6:M:6:DG:O6	7:N:45:DC:N4	2.16	0.70
3:F:84:ASP:OD1	3:F:84:ASP:N	2.24	0.70
1:A:320:GLN:NE2	10:A:704:HOH:O	2.23	0.69
3:D:109:ASP:OD2	3:D:169:SER:OG	2.07	0.69
3:E:318:ARG:NH2	3:F:336:ASP:OD1	2.26	0.69
3:H:90:LYS:NZ	10:H:401:HOH:O	2.13	0.69
3:F:28:ASP:O	3:F:38:ARG:NH1	2.26	0.68
1:A:428:GLU:OE2	10:A:702:HOH:O	2.10	0.68
4:J:50:ASP:OD2	4:J:53:SER:OG	2.12	0.68
6:M:10:DT:H2"	6:M:11:DG:C8	2.28	0.68
3:G:351:GLU:OE2	10:G:401:HOH:O	2.12	0.68
6:M:3:DT:H2"	6:M:4:DG:C8	2.29	0.67
6:M:14:DC:C2'	6:M:15:DG:H5'	2.22	0.66
3:F:93:ALA:HB2	3:F:100:VAL:HG22	1.78	0.66
3:F:196:ASP:OD2	10:F:401:HOH:O	2.14	0.65
10:A:707:HOH:O	6:M:23:DA:N1	2.30	0.65
1:A:99:PRO:HB2	1:A:102:GLN:HB2	1.80	0.64
2:C:67:ALA:HB3	2:C:71:VAL:HG21	1.79	0.63
3:E:72:ARG:NH1	3:E:101:ASP:O	2.31	0.63
5:L:61:23G:OP1	10:L:102:HOH:O	2.15	0.63
6:M:9:DG:O6	7:N:42:DC:N4	2.28	0.63
1:A:2:ASN:N	1:A:6:ASP:OD2	2.31	0.63
5:L:50:G:H2'	5:L:51:C:C6	2.33	0.63
3:D:278:MET:HG2	3:D:333:SER:HB2	1.79	0.62
3:I:38:ARG:NH2	4:J:84:ASP:OD1	2.31	0.62
3:F:204:ASP:HB2	3:F:212:ALA:HB2	1.82	0.62
7:N:49:DG:H2"	7:N:50:DA:OP2	1.98	0.62
3:F:38:ARG:NH2	3:G:198:ASP:OD1	2.34	0.61
2:B:89:ARG:NH2	10:B:203:HOH:O	2.33	0.61
4:J:72:LEU:O	4:J:73:ASP:HB2	1.99	0.61
3:G:204:ASP:HB2	3:G:212:ALA:HB2	1.81	0.61
7:N:45:DC:H2"	7:N:46:DA:C8	2.35	0.61
6:M:11:DG:H2"	6:M:12:DC:H5"	1.82	0.61
5:L:51:C:H2'	5:L:52:G:O4'	2.00	0.60
3:I:252:THR:HG23	3:I:354:LYS:HB3	1.82	0.60
3:E:9:VAL:HB	3:E:226:ARG:HB2	1.82	0.60
6:M:4:DG:H2"	6:M:5:DT:OP1	2.01	0.60
3:E:8:HIS:HB2	3:E:280:MET:HB3	1.84	0.60
4:J:3:SER:HB3	4:J:130:ILE:HD13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLU:HG2	1:A:447:ILE:HD13	1.84	0.59
3:G:155:GLN:HG2	3:G:239:LEU:HD22	1.83	0.59
4:J:8:ARG:NH2	4:J:117:THR:OG1	2.36	0.59
5:L:52:G:HO2'	5:L:53:C:H5	1.47	0.59
4:J:7:LEU:HG	4:J:157:LEU:HD22	1.84	0.59
3:H:204:ASP:HB3	3:H:207:GLN:HB3	1.85	0.59
4:J:3:SER:OG	4:J:163:GLN:OE1	2.21	0.59
3:E:39:ILE:HB	3:E:187:ALA:HB3	1.85	0.58
3:D:62:SER:OG	3:D:159:ASP:OD2	2.14	0.58
3:I:76:ARG:HH11	3:I:89:ASP:CG	2.07	0.58
3:I:76:ARG:NH1	3:I:89:ASP:OD2	2.36	0.58
3:I:118:GLU:OE2	3:I:173:THR:OG1	2.15	0.57
1:A:361:ARG:NH2	10:A:713:HOH:O	2.35	0.57
2:B:110:ARG:O	2:B:112:ALA:N	2.27	0.57
5:L:50:G:C6	5:L:51:C:C4	2.91	0.57
1:A:331:VAL:HG13	1:A:343:LEU:HD21	1.87	0.57
6:M:6:DG:H2'	6:M:7:DC:O4'	2.04	0.57
3:G:204:ASP:HB3	3:G:207:GLN:HB3	1.86	0.57
6:M:10:DT:H3	7:N:41:DA:N6	2.02	0.57
3:H:98:LYS:NZ	3:H:109:ASP:OD1	2.36	0.57
2:B:74:HIS:NE2	2:B:75:GLN:O	2.37	0.57
3:D:18:LEU:HD13	3:D:39:ILE:HD11	1.87	0.56
3:F:204:ASP:HB3	3:F:207:GLN:HG2	1.87	0.56
3:I:112:THR:HG23	3:I:238:ASN:HA	1.87	0.56
3:D:79:LEU:HD12	3:D:88:ILE:HD11	1.87	0.56
3:I:136:ASP:OD1	3:I:136:ASP:N	2.38	0.56
3:G:38:ARG:NH2	3:H:198:ASP:OD1	2.33	0.56
6:M:10:DT:H2"	6:M:11:DG:H8	1.71	0.56
3:G:9:VAL:HB	3:G:226:ARG:HB2	1.88	0.55
3:F:22:ASP:HB3	3:G:199:TRP:CE2	2.42	0.55
1:A:112:THR:OG1	1:A:266:LYS:NZ	2.38	0.54
3:H:315:TYR:OH	10:H:402:HOH:O	2.17	0.54
3:E:182:MET:HB2	3:E:230:ILE:HD13	1.88	0.54
4:J:48:ARG:NH1	5:L:2:U:OP2	2.34	0.54
3:F:226:ARG:NH1	3:F:258:LEU:O	2.39	0.54
5:L:47:C:H42	5:L:60:G:H1	1.55	0.54
3:D:129:ALA:HB2	3:D:139:LEU:HD13	1.90	0.54
5:L:53:C:H5"	5:L:54:C:C5	2.42	0.54
3:F:9:VAL:HB	3:F:226:ARG:HB2	1.90	0.53
3:D:140:LEU:HD13	3:D:171:MET:HG3	1.90	0.53
3:F:286:MET:HG3	3:F:287:PRO:HD2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:296:LYS:HG3	3:I:302:ASP:HB3	1.90	0.53
3:D:69:ALA:O	3:D:72:ARG:HG3	2.08	0.52
7:N:46:DA:H2"	7:N:47:DC:O4'	2.10	0.52
6:M:7:DC:H3'	6:M:8:DA:C8	2.45	0.52
6:M:8:DA:H1'	6:M:9:DG:H5'	1.90	0.52
1:A:13:PRO:HG2	1:A:16:GLY:HA3	1.89	0.52
3:D:38:ARG:NH2	3:E:198:ASP:OD1	2.39	0.52
1:A:247:ILE:HG13	1:A:258:ASN:HA	1.92	0.52
3:G:27:LYS:NZ	5:L:21:A:OP1	2.30	0.52
3:H:9:VAL:HB	3:H:226:ARG:HB2	1.91	0.52
4:J:6:ILE:HG13	4:J:174:TYR:CE1	2.44	0.52
3:E:252:THR:HG21	3:E:358:ARG:HG3	1.90	0.51
1:A:177:ARG:HB2	1:A:346:ILE:HG13	1.92	0.51
3:I:204:ASP:HB2	3:I:212:ALA:HB2	1.92	0.51
5:L:52:G:O2'	5:L:53:C:H5	1.94	0.51
5:L:38:C:N4	5:L:40:G:O2'	2.43	0.51
5:L:50:G:C4	5:L:51:C:C5	2.98	0.51
8:K:8:ILE:O	8:K:13:SER:OG	2.28	0.51
3:D:95:LEU:HD23	3:D:114:TRP:HZ3	1.76	0.51
3:D:76:ARG:NH2	3:D:89:ASP:OD2	2.44	0.51
3:H:34:LYS:NZ	10:H:405:HOH:O	2.33	0.51
2:B:106:ILE:HA	2:B:145:ARG:HH11	1.75	0.50
3:D:76:ARG:HG2	3:D:88:ILE:HG21	1.94	0.50
3:D:155:GLN:HG3	3:D:239:LEU:HD22	1.92	0.50
3:G:46:ARG:NH1	3:G:50:LYS:HE3	2.26	0.50
3:E:204:ASP:HB2	3:E:212:ALA:HB2	1.93	0.50
5:L:54:C:H4'	5:L:55:A:O5'	2.12	0.50
3:I:9:VAL:HB	3:I:226:ARG:HB2	1.92	0.50
1:A:491:ARG:NH2	6:M:27:DA:OP1	2.41	0.50
7:N:48:DA:H2"	7:N:49:DG:OP2	2.12	0.50
5:L:38:C:N4	5:L:40:G:HO2'	2.09	0.49
6:M:12:DC:H2"	6:M:13:DT:OP1	2.12	0.49
3:F:344:VAL:O	10:F:402:HOH:O	2.20	0.49
2:C:107:ARG:HB3	3:H:25:MET:HE1	1.94	0.49
4:J:194:PHE:HB3	4:J:213:TRP:HB2	1.94	0.49
5:L:9:A:O2'	5:L:10:C:H5"	2.11	0.49
3:F:49:ARG:HD3	10:F:406:HOH:O	2.13	0.49
5:L:50:G:N1	5:L:51:C:N4	2.59	0.49
3:E:252:THR:HG22	3:E:357:VAL:HB	1.95	0.49
6:M:1:DT:H2"	6:M:2:DC:O4'	2.13	0.49
6:M:21:DT:H2"	6:M:22:DT:OP2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLN:CG	2:B:76:ASP:N	2.76	0.48
3:D:151:ARG:NH2	3:D:175:LEU:O	2.46	0.48
8:K:83:PRO:HG2	8:K:199:LEU:HD11	1.95	0.48
2:B:14:TRP:HE1	2:B:69:LYS:HA	1.79	0.48
1:A:117:LEU:HD23	1:A:151:GLN:HG3	1.95	0.48
3:E:199:TRP:CZ2	3:E:214:LEU:HD23	2.49	0.48
5:L:50:G:C2	5:L:51:C:C4	3.01	0.48
3:D:67:HIS:CE1	3:E:207:GLN:HE21	2.31	0.48
3:F:19:ASN:OD1	3:F:27:LYS:HD2	2.14	0.48
3:I:340:ILE:HD12	3:I:344:VAL:HG21	1.96	0.48
3:D:132:ASP:OD1	3:D:132:ASP:N	2.47	0.48
3:E:246:GLN:O	3:E:246:GLN:NE2	2.47	0.48
8:K:76:PHE:HB2	8:K:78:LEU:HD13	1.94	0.48
1:A:77:GLU:O	1:A:81:GLN:HG2	2.14	0.48
3:H:101:ASP:OD1	3:H:103:ALA:N	2.42	0.47
5:L:50:G:O6	5:L:51:C:N4	2.44	0.47
1:A:247:ILE:HD12	1:A:247:ILE:H	1.78	0.47
3:G:2:SER:HB2	3:G:283:PHE:HB3	1.96	0.47
3:H:122:PHE:O	3:H:126:VAL:HG23	2.15	0.47
1:A:138:ALA:HB1	1:A:260:ARG:HE	1.79	0.47
3:I:358:ARG:NH2	10:I:410:HOH:O	2.42	0.47
5:L:38:C:O2	5:L:39:A:H4'	2.15	0.47
1:A:228:PHE:HA	1:A:277:TRP:HZ2	1.79	0.47
1:A:248:GLY:N	1:A:260:ARG:NH1	2.63	0.47
3:D:89:ASP:HB3	3:D:100:VAL:HG11	1.97	0.47
3:D:288:LEU:HD21	3:E:275:PRO:HG3	1.95	0.47
8:K:86:PHE:CD1	8:K:167:LEU:HG	2.49	0.47
8:K:85:TYR:CE2	8:K:199:LEU:HB3	2.50	0.47
5:L:50:G:C5	5:L:51:C:C4	3.02	0.47
6:M:4:DG:O5'	6:M:4:DG:H8	1.97	0.47
7:N:44:DG:H2"	7:N:45:DC:H5'	1.97	0.47
3:E:82:ARG:HD2	3:E:83:PHE:CZ	2.50	0.47
1:A:133:PRO:HB3	4:J:95:TYR:CD1	2.50	0.47
4:J:40:LEU:HD11	4:J:120:LEU:HD11	1.97	0.47
3:D:71:LEU:O	3:D:75:LEU:HG	2.15	0.46
3:H:70:GLN:N	3:H:70:GLN:OE1	2.48	0.46
3:H:185:ALA:HB2	3:I:271:ALA:HB3	1.97	0.46
1:A:13:PRO:HD3	1:A:34:TRP:HZ3	1.81	0.46
3:E:253:HIS:O	3:E:257:MET:HG3	2.16	0.46
7:N:1:DC:H2'	7:N:2:DT:C6	2.50	0.46
3:G:89:ASP:O	3:G:100:VAL:HG21	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:67:HIS:CE1	3:E:204:ASP:OD2	2.69	0.46
7:N:42:DC:H2"	7:N:43:DT:H5'	1.98	0.46
3:D:125:GLN:HG2	3:D:143:LEU:HD21	1.98	0.46
3:I:137:LYS:O	3:I:141:LYS:N	2.48	0.46
3:F:252:THR:HG22	3:F:357:VAL:HB	1.98	0.46
3:I:136:ASP:HB2	3:I:137:LYS:H	1.46	0.46
5:L:44:U:HO2'	5:L:45:U:P	2.27	0.46
8:K:78:LEU:HD22	8:K:176:ILE:HD11	1.97	0.46
3:D:85:GLN:O	3:D:88:ILE:HG22	2.16	0.46
8:K:85:TYR:N	8:K:197:ALA:O	2.49	0.46
3:H:204:ASP:HB2	3:H:212:ALA:HB2	1.98	0.45
3:I:165:ARG:HH11	4:J:92:ARG:NH1	2.14	0.45
4:J:192:LEU:HB3	4:J:215:VAL:HB	1.98	0.45
8:K:15:ASP:OD1	8:K:16:LEU:N	2.46	0.45
3:D:91:THR:O	3:D:95:LEU:HB2	2.17	0.45
3:F:356:TRP:CD1	3:F:362:GLU:HB2	2.51	0.45
3:E:89:ASP:O	3:E:100:VAL:HG21	2.16	0.45
3:H:96:SER:O	3:H:169:SER:OG	2.34	0.45
7:N:39:DG:H2"	7:N:40:DC:H5"	1.97	0.45
7:N:46:DA:H2"	7:N:47:DC:C6	2.52	0.45
2:C:154:LEU:HD22	6:M:26:DT:C2	2.51	0.45
3:G:45:LYS:HD2	3:G:184:ILE:HG21	1.98	0.45
3:D:115:VAL:HG12	3:D:118:GLU:H	1.80	0.45
3:E:32:GLY:HA2	3:E:295:GLU:OE2	2.15	0.45
4:J:2:ARG:NH1	10:J:304:HOH:O	2.49	0.45
4:J:38:GLY:HA3	5:L:2:U:O4'	2.16	0.45
5:L:50:G:N1	5:L:51:C:C4	2.85	0.45
1:A:231:GLY:HA3	1:A:277:TRP:CZ2	2.51	0.45
2:B:113:ASP:OD1	2:B:114:MET:N	2.49	0.45
3:I:76:ARG:HD2	3:I:89:ASP:OD1	2.17	0.45
1:A:59:ALA:HB2	1:A:83:LEU:HD13	1.99	0.45
3:D:300:ALA:HB2	3:D:307:PRO:HG2	1.98	0.45
3:G:19:ASN:OD1	3:G:27:LYS:HD2	2.16	0.45
3:H:113:PRO:HB2	3:H:160:ILE:HD11	1.99	0.45
5:L:53:C:H5"	5:L:54:C:H5	1.81	0.45
2:B:75:GLN:CG	2:B:76:ASP:H	2.30	0.45
3:D:8:HIS:HB2	3:D:280:MET:HB3	1.99	0.45
3:D:98:LYS:HD3	3:D:108:ALA:HA	1.99	0.45
7:N:20:DT:H72	7:N:21:DG:N1	2.31	0.45
3:I:204:ASP:HB3	3:I:207:GLN:HB3	1.98	0.45
3:E:22:ASP:HB3	3:F:199:TRP:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:22:ASP:OD1	3:H:22:ASP:N	2.50	0.44
3:H:318:ARG:NH1	10:H:411:HOH:O	2.49	0.44
3:D:45:LYS:HA	3:D:48:MET:HE2	1.98	0.44
3:D:138:LYS:O	3:D:142:VAL:HG23	2.17	0.44
1:A:56:GLN:HA	1:A:189:VAL:HG13	2.00	0.44
3:D:88:ILE:HD12	3:D:88:ILE:HA	1.90	0.44
4:J:186:SER:HB3	4:J:214:TYR:CE1	2.53	0.44
3:E:109:ASP:OD2	3:E:169:SER:OG	2.18	0.44
4:J:50:ASP:O	4:J:54:LEU:HB2	2.18	0.44
3:E:118:GLU:OE1	10:E:401:HOH:O	2.21	0.44
3:D:135:ASP:O	3:D:138:LYS:N	2.48	0.44
3:E:38:ARG:NH2	3:F:198:ASP:OD1	2.51	0.44
7:N:42:DC:H1'	7:N:43:DT:H5'	2.00	0.44
8:K:145:ARG:O	10:K:201:HOH:O	2.21	0.44
3:D:70:GLN:H	3:D:70:GLN:HG2	1.39	0.43
3:D:251:ALA:O	3:D:255:VAL:HG23	2.18	0.43
4:J:48:ARG:NH1	5:L:2:U:P	2.91	0.43
6:M:3:DT:C4	7:N:47:DC:N4	2.86	0.43
1:A:154:GLN:O	1:A:170:THR:HA	2.19	0.43
3:D:174:GLU:OE2	3:D:174:GLU:N	2.51	0.43
8:K:63:THR:OG1	8:K:66:ALA:N	2.50	0.43
3:F:278:MET:CE	3:F:331:GLN:HE21	2.31	0.43
2:B:104:GLN:HA	3:F:25:MET:HE1	2.00	0.43
3:D:14:SER:OG	8:K:138:ASP:OD1	2.35	0.43
3:D:306:GLN:HB2	3:D:307:PRO:HD3	2.00	0.43
3:I:336:ASP:OD1	3:I:336:ASP:N	2.50	0.43
8:K:6:VAL:HB	8:K:52:VAL:HG12	1.99	0.43
3:E:82:ARG:HD2	3:E:83:PHE:CE2	2.53	0.43
2:B:8:MET:HG2	2:B:131:PRO:HG3	2.01	0.42
3:H:146:ASP:OD2	3:H:149:ALA:HB2	2.19	0.42
1:A:80:PHE:CE2	1:A:84:ILE:HD13	2.53	0.42
3:F:132:ASP:OD1	3:F:132:ASP:N	2.52	0.42
3:F:199:TRP:CZ2	3:F:214:LEU:HD23	2.54	0.42
7:N:41:DA:H2"	7:N:42:DC:OP1	2.19	0.42
3:I:121:TRP:CE2	3:I:172:MET:HG2	2.54	0.42
4:J:31:PRO:HD2	4:J:65:VAL:HG11	2.02	0.42
5:L:52:G:O2'	5:L:53:C:C5	2.70	0.42
3:F:3:ASN:ND2	3:F:231:ASN:OD1	2.52	0.42
6:M:4:DG:C2'	6:M:5:DT:OP1	2.67	0.42
3:D:9:VAL:HB	3:D:226:ARG:HB2	2.01	0.42
4:J:186:SER:HB3	4:J:214:TYR:CD1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:22:DT:H2"	6:M:23:DA:O5'	2.19	0.42
3:I:92:LEU:HD12	3:I:92:LEU:HA	1.80	0.42
3:F:134:LEU:HD12	3:F:134:LEU:H	1.85	0.42
3:G:64:ARG:HD3	10:G:459:HOH:O	2.19	0.42
5:L:49:C:H2'	5:L:50:G:C8	2.55	0.42
2:B:49:TRP:CZ3	2:B:55:GLN:HB2	2.55	0.41
3:I:146:ASP:OD2	4:J:96:ARG:NH2	2.53	0.41
7:N:48:DA:H1'	7:N:49:DG:O4'	2.21	0.41
8:K:20:HIS:ND1	8:K:21:GLN:HG3	2.35	0.41
1:A:207:ASN:OD1	1:A:229:VAL:HG13	2.20	0.41
3:F:140:LEU:HD13	3:F:171:MET:HE2	2.01	0.41
3:G:177:LYS:HB2	3:G:177:LYS:NZ	2.35	0.41
3:H:306:GLN:HB2	3:H:307:PRO:HD3	2.02	0.41
3:I:48:MET:HG2	3:I:257:MET:HB3	2.02	0.41
1:A:76:THR:OG1	1:A:79:GLU:HG3	2.19	0.41
1:A:172:VAL:HG23	1:A:299:ALA:HA	2.02	0.41
1:A:279:HIS:CE1	1:A:281:HIS:HB2	2.56	0.41
3:D:286:MET:HA	3:D:287:PRO:HD3	1.96	0.41
4:J:46:ILE:HG21	4:J:54:LEU:HD13	2.01	0.41
7:N:33:DC:H2'	7:N:34:DA:O4'	2.20	0.41
3:D:22:ASP:HB3	3:E:199:TRP:CD2	2.56	0.41
3:D:72:ARG:O	3:D:76:ARG:HG3	2.20	0.41
3:E:101:ASP:OD1	3:E:101:ASP:N	2.52	0.41
3:E:113:PRO:HG2	3:E:165:ARG:HD3	2.02	0.41
3:E:232:LEU:HD13	3:E:244:ARG:HE	1.85	0.41
3:G:82:ARG:NH2	10:G:413:HOH:O	2.43	0.41
7:N:46:DA:H2"	7:N:47:DC:H6	1.85	0.41
1:A:55:GLY:HA2	1:A:58:ILE:HG12	2.01	0.41
3:D:219:PHE:CE2	8:K:137:GLU:HB3	2.55	0.41
3:F:22:ASP:HB3	3:G:199:TRP:CD2	2.55	0.41
1:A:406:LYS:HB3	1:A:408:PHE:HD1	1.86	0.41
2:B:17:LEU:HD23	2:B:22:CYS:HB3	2.02	0.41
1:A:14:ARG:NH1	1:A:15:ASN:OD1	2.52	0.41
3:D:90:LYS:HG3	3:D:94:LEU:HD23	2.02	0.41
3:D:248:LEU:O	3:D:252:THR:HG23	2.21	0.41
3:G:100:VAL:O	3:G:100:VAL:HG23	2.21	0.41
3:I:118:GLU:OE1	3:I:172:MET:N	2.50	0.41
2:B:150:GLU:OE2	10:B:201:HOH:O	2.22	0.41
3:D:111:VAL:HG21	3:E:202:ALA:HB1	2.03	0.41
3:G:185:ALA:HB2	3:H:271:ALA:HB3	2.02	0.41
3:I:277:ASP:OD1	10:I:401:HOH:O	2.22	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:67:CYS:O	4:J:179:GLY:HA3	2.21	0.41
4:J:88:VAL:HG22	5:L:7:C:H1'	2.02	0.41
6:M:15:DG:H2"	6:M:16:DA:C8	2.56	0.41
2:B:90:ALA:HB1	2:B:126:PRO:HB2	2.03	0.41
6:M:22:DT:H4'	6:M:23:DA:OP1	2.20	0.41
3:F:103:ALA:HB3	3:F:106:ILE:HD11	2.02	0.40
3:G:347:MET:HA	3:G:348:PRO:HD3	1.89	0.40
1:A:151:GLN:NE2	10:A:703:HOH:O	2.20	0.40
1:A:494:LYS:HG3	1:A:494:LYS:O	2.22	0.40
3:D:171:MET:HG2	3:D:175:LEU:HD12	2.02	0.40
3:E:299:LYS:NZ	3:F:302:ASP:OD1	2.54	0.40
3:H:11:ILE:HD11	3:H:274:ASN:O	2.21	0.40
2:B:72:ILE:HD11	2:B:121:LEU:HD13	2.03	0.40
3:F:101:ASP:HB2	3:F:102:GLU:H	1.68	0.40
3:D:75:LEU:HD11	3:D:92:LEU:HD22	2.04	0.40
3:E:190:THR:HG23	3:E:294:PHE:CD1	2.57	0.40
3:G:296:LYS:HG3	3:H:302:ASP:HB3	2.03	0.40
3:H:22:ASP:HB3	3:I:199:TRP:CE2	2.56	0.40
3:I:285:ASP:O	4:J:140:PRO:HD2	2.21	0.40
4:J:16:TRP:CG	4:J:31:PRO:HA	2.56	0.40
5:L:53:C:O5'	5:L:53:C:H6	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	473/502 (94%)	455 (96%)	17 (4%)	1 (0%)	47	57
2	B	149/165 (90%)	144 (97%)	3 (2%)	2 (1%)	12	11
2	C	146/165 (88%)	143 (98%)	2 (1%)	1 (1%)	22	25
3	D	310/363 (85%)	293 (94%)	16 (5%)	1 (0%)	41	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	350/363 (96%)	338 (97%)	11 (3%)	1 (0%)	41 49
3	F	359/363 (99%)	345 (96%)	14 (4%)	0	100 100
3	G	350/363 (96%)	343 (98%)	7 (2%)	0	100 100
3	H	348/363 (96%)	339 (97%)	9 (3%)	0	100 100
3	I	347/363 (96%)	338 (97%)	7 (2%)	2 (1%)	25 29
4	J	217/224 (97%)	215 (99%)	2 (1%)	0	100 100
8	K	145/199 (73%)	137 (94%)	8 (6%)	0	100 100
All	All	3194/3433 (93%)	3090 (97%)	96 (3%)	8 (0%)	41 49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	111	THR
2	B	140	TRP
3	I	136	ASP
3	D	133	ASN
3	E	209	GLN
1	A	119	ALA
2	C	111	THR
3	I	340	ILE

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	403/426 (95%)	390 (97%)	13 (3%)	39 50
2	B	129/141 (92%)	123 (95%)	6 (5%)	26 34
2	C	127/141 (90%)	122 (96%)	5 (4%)	32 42
3	D	246/298 (83%)	226 (92%)	20 (8%)	11 13
3	E	278/298 (93%)	262 (94%)	16 (6%)	20 25
3	F	287/298 (96%)	274 (96%)	13 (4%)	27 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	G	283/298 (95%)	276 (98%)	7 (2%)	47 60
3	H	280/298 (94%)	276 (99%)	4 (1%)	67 77
3	I	281/298 (94%)	272 (97%)	9 (3%)	39 50
4	J	186/192 (97%)	180 (97%)	6 (3%)	39 50
8	K	102/170 (60%)	91 (89%)	11 (11%)	6 6
All	All	2602/2858 (91%)	2492 (96%)	110 (4%)	30 39

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	82	GLN
1	A	111	VAL
1	A	229	VAL
1	A	293	VAL
1	A	294	GLU
1	A	298	LEU
1	A	347	MET
1	A	351	ARG
1	A	380	GLU
1	A	389	LYS
1	A	407	ASP
1	A	466	VAL
2	B	28	VAL
2	B	70	ASN
2	B	73	ARG
2	B	110	ARG
2	B	111	THR
2	B	118	ARG
2	C	16	GLN
2	C	28	VAL
2	C	78	LYS
2	C	83	THR
2	C	111	THR
3	D	13	HIS
3	D	19	ASN
3	D	70	GLN
3	D	72	ARG
3	D	75	LEU
3	D	81	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	82	ARG
3	D	98	LYS
3	D	105	LYS
3	D	111	VAL
3	D	132	ASP
3	D	134	LEU
3	D	145	GLU
3	D	194	ASP
3	D	217	GLN
3	D	277	ASP
3	D	286	MET
3	D	288	LEU
3	D	333	SER
3	D	335	SER
3	E	2	SER
3	E	5	ILE
3	E	38	ARG
3	E	82	ARG
3	E	102	GLU
3	E	182	MET
3	E	188	ILE
3	E	194	ASP
3	E	206	LEU
3	E	211	SER
3	E	244	ARG
3	E	246	GLN
3	E	266	LYS
3	E	305	LEU
3	E	325	LEU
3	E	341	THR
3	F	20	ARG
3	F	84	ASP
3	F	132	ASP
3	F	201	THR
3	F	244	ARG
3	F	268	ARG
3	F	274	ASN
3	F	280	MET
3	F	305	LEU
3	F	334	LEU
3	F	340	ILE
3	F	343	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	362	GLU
3	G	87	ILE
3	G	274	ASN
3	G	277	ASP
3	G	317	ASP
3	G	343	GLN
3	G	347	MET
3	G	359	ASN
3	H	14	SER
3	H	169	SER
3	H	177	LYS
3	H	282	ASN
3	I	65	THR
3	I	92	LEU
3	I	132	ASP
3	I	134	LEU
3	I	136	ASP
3	I	274	ASN
3	I	336	ASP
3	I	340	ILE
3	I	341	THR
4	J	96	ARG
4	J	130	ILE
4	J	141	ARG
4	J	157	LEU
4	J	165	SER
4	J	188	THR
8	K	13	SER
8	K	23	LEU
8	K	52	VAL
8	K	62	SER
8	K	67	THR
8	K	76	PHE
8	K	96	ILE
8	K	112	CYS
8	K	113	ARG
8	K	160	THR
8	K	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	19	ASN
3	D	234	GLN
3	E	207	GLN
3	F	331	GLN
3	F	343	GLN
3	F	346	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	59/61 (96%)	21 (35%)	1 (1%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L	4	A
5	L	8	G
5	L	9	A
5	L	10	C
5	L	15	U
5	L	21	A
5	L	22	G
5	L	27	U
5	L	28	G
5	L	33	G
5	L	34	C
5	L	38	C
5	L	39	A
5	L	43	G
5	L	45	U
5	L	47	C
5	L	48	C
5	L	53	C
5	L	54	C
5	L	55	A
5	L	56	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L	54	C

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
5	23G	L	61	5	19,29,30	1.26	1 (5%)	20,45,48	1.46	5 (25%)

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
5	23G	L	61	5	-	1/3/35/36	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	61	23G	C6-N1	-3.77	1.32	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	61	23G	C5-C6-N1	2.77	118.84	113.95
5	L	61	23G	C8-N7-C5	2.72	108.18	102.99
5	L	61	23G	C2-N1-C6	-2.34	120.78	125.10
5	L	61	23G	OC1-PC-OC2	2.24	117.13	109.89
5	L	61	23G	O6-C6-N1	-2.21	118.04	120.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	61	23G	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	61	23G	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	481/502 (95%)	-0.08	5 (1%) 82 83	19, 48, 84, 110	0
2	B	153/165 (92%)	0.38	9 (5%) 22 19	33, 59, 87, 100	0
2	C	150/165 (90%)	-0.19	1 (0%) 87 88	19, 32, 56, 84	0
3	D	318/363 (87%)	0.37	21 (6%) 18 14	44, 67, 120, 164	0
3	E	354/363 (97%)	-0.07	0 100 100	33, 49, 75, 101	0
3	F	361/363 (99%)	0.00	8 (2%) 62 58	22, 44, 74, 147	0
3	G	354/363 (97%)	-0.16	1 (0%) 94 94	19, 32, 55, 73	0
3	H	352/363 (96%)	-0.04	4 (1%) 80 80	16, 33, 79, 112	0
3	I	351/363 (96%)	-0.01	9 (2%) 56 52	18, 39, 89, 131	0
4	J	219/224 (97%)	-0.28	0 100 100	20, 37, 63, 77	0
5	L	60/61 (98%)	0.12	3 (5%) 28 26	20, 36, 130, 134	0
6	M	28/28 (100%)	1.74	10 (35%) 0 0	52, 110, 264, 267	0
7	N	50/50 (100%)	0.33	10 (20%) 1 0	22, 43, 257, 281	0
8	K	159/199 (79%)	1.06	33 (20%) 1 0	67, 93, 108, 125	0
All	All	3390/3572 (94%)	0.06	114 (3%) 45 41	16, 45, 99, 281	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	M	9	DG	8.2
8	K	158	ILE	6.8
3	I	137	LYS	5.6
6	M	8	DA	5.6
6	M	10	DT	5.6
3	D	69	ALA	5.2
8	K	199	LEU	5.2
8	K	60	PRO	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	M	7	DC	4.9
8	K	1	MET	4.8
7	N	42	DC	4.7
3	D	100	VAL	4.6
6	M	6	DG	4.6
6	M	4	DG	4.4
3	D	75	LEU	4.2
8	K	57	ALA	4.2
8	K	59	MET	4.2
8	K	112	CYS	4.2
7	N	45	DC	4.1
1	A	288	VAL	3.9
3	D	105	LYS	3.8
2	C	3	ASP	3.7
7	N	49	DG	3.7
3	D	88	ILE	3.6
3	D	104	GLU	3.6
7	N	46	DA	3.5
8	K	156	GLY	3.5
3	D	106	ILE	3.4
3	F	340	ILE	3.4
2	B	83	THR	3.4
3	F	131	ALA	3.4
3	F	336	ASP	3.4
6	M	1	DT	3.4
6	M	2	DC	3.4
8	K	68	VAL	3.3
2	B	7	ALA	3.3
8	K	2	TYR	3.3
1	A	90	MET	3.2
8	K	74	VAL	3.2
7	N	41	DA	3.2
8	K	71	THR	3.1
6	M	21	DT	3.1
7	N	47	DC	3.1
3	D	129	ALA	3.0
8	K	114	VAL	3.0
8	K	95	THR	3.0
8	K	3	LEU	2.9
3	I	95	LEU	2.8
8	K	63	THR	2.8
8	K	81	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	K	67	THR	2.7
3	F	337	VAL	2.7
3	F	342	ALA	2.7
7	N	50	DA	2.7
3	D	70	GLN	2.6
8	K	23	LEU	2.6
3	G	343	GLN	2.6
3	D	79	LEU	2.6
2	B	78	LYS	2.6
2	B	84	GLY	2.6
2	B	73	ARG	2.6
8	K	171	ASP	2.6
8	K	73	GLN	2.6
5	L	49	C	2.6
3	D	83	PHE	2.5
3	I	139	LEU	2.5
8	K	167	LEU	2.5
1	A	107	LYS	2.5
3	D	134	LEU	2.5
8	K	172	ALA	2.5
2	B	76	ASP	2.4
3	I	126	VAL	2.4
7	N	39	DG	2.4
3	H	87	ILE	2.4
3	D	102	GLU	2.4
3	D	68	LEU	2.4
3	D	122	PHE	2.3
8	K	11	ALA	2.3
3	F	136	ASP	2.3
7	N	43	DT	2.3
3	I	81	GLU	2.3
3	D	80	GLY	2.3
8	K	64	ALA	2.3
3	H	126	VAL	2.3
8	K	113	ARG	2.3
8	K	53	LEU	2.3
1	A	200	PRO	2.2
8	K	179	VAL	2.2
8	K	66	ALA	2.2
3	D	73	ASP	2.2
3	H	86	LYS	2.2
3	F	76	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	54	HIS	2.2
3	D	309	ILE	2.2
1	A	97	GLU	2.2
2	B	35	ARG	2.2
8	K	62	SER	2.1
7	N	38	DA	2.1
3	I	83	PHE	2.1
3	I	68	LEU	2.1
3	D	355	SER	2.1
3	I	94	LEU	2.1
3	F	301	LYS	2.1
3	D	103	ALA	2.1
6	M	5	DT	2.1
8	K	115	PRO	2.1
8	K	58	GLN	2.1
8	K	77	GLN	2.1
2	B	11	TYR	2.0
5	L	52	G	2.0
3	D	154	LEU	2.0
3	H	134	LEU	2.0
3	I	136	ASP	2.0
5	L	50	G	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	B-factors(Å^2)	Q<0.9
5	23G	L	61	26/27	0.73	0.17	98,123,163,171	0

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, 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	B-factors(Å^2)	Q<0.9
9	ZN	A	601	1/1	0.97	0.10	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.