Full wwPDB X-ray Structure Validation Report (i)

Mar 28, 2016 – 03:02 PM EDT

PDB ID	:	5F9H
Title	:	Crystal structure of RIG-I helicase-RD in complex with 24-mer 5' triphosphate hairpin RNA
Authors	:	Wang, C.; Marcotrigiano, J.; Miller, M.; Jiang, F.
Deposited on	:	2015-12-09
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

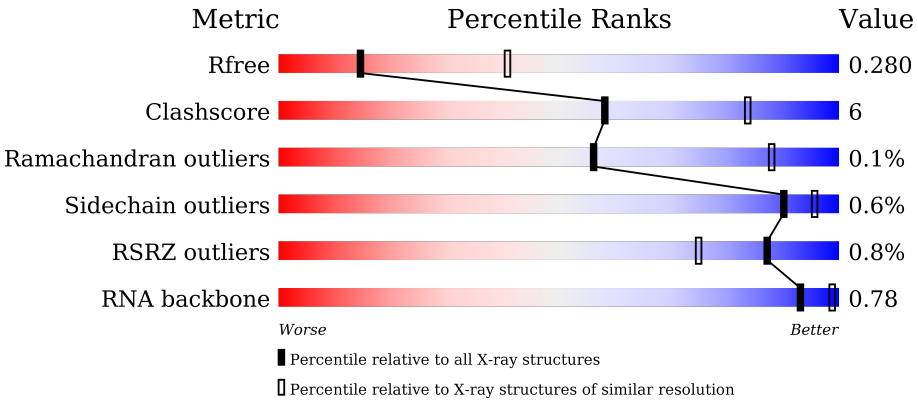
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 3.10 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.



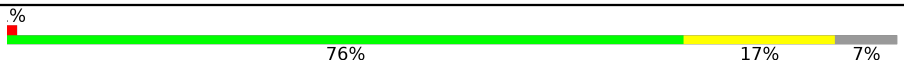
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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	695	.% 80% 13% 7%
1	C	695	2% 83% 10% 7%
1	E	695	74% 17% • 8%
1	G	695	77% 16% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	695	
1	K	695	
2	B	23	
2	D	23	
2	F	23	
2	H	23	
2	J	23	
2	L	23	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33602 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	646	Total	C	N	O	S	0	0	0
			5119	3272	865	951	31			
1	C	647	Total	C	N	O	S	0	0	0
			5083	3249	854	949	31			
1	E	638	Total	C	N	O	S	0	0	0
			5047	3234	847	935	31			
1	G	653	Total	C	N	O	S	0	0	0
			5168	3307	877	953	31			
1	I	644	Total	C	N	O	S	0	0	0
			5039	3229	846	932	32			
1	K	637	Total	C	N	O	S	0	0	0
			5024	3217	845	932	30			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	SER	-	expression tag	UNP O95786
C	231	SER	-	expression tag	UNP O95786
E	231	SER	-	expression tag	UNP O95786
G	231	SER	-	expression tag	UNP O95786
I	231	SER	-	expression tag	UNP O95786
K	231	SER	-	expression tag	UNP O95786

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			
2	D	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			
2	F	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			
2	J	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			
2	L	23	Total	C	N	O	P	0	0	0
			486	219	83	161	23			

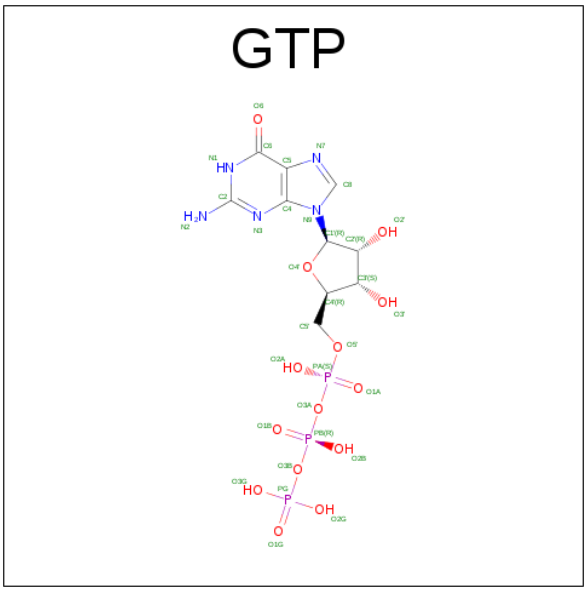
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Mg	0	0
			2	2		
4	I	1	Total	Mg	0	0
			1	1		
4	A	3	Total	Mg	0	0
			3	3		
4	K	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



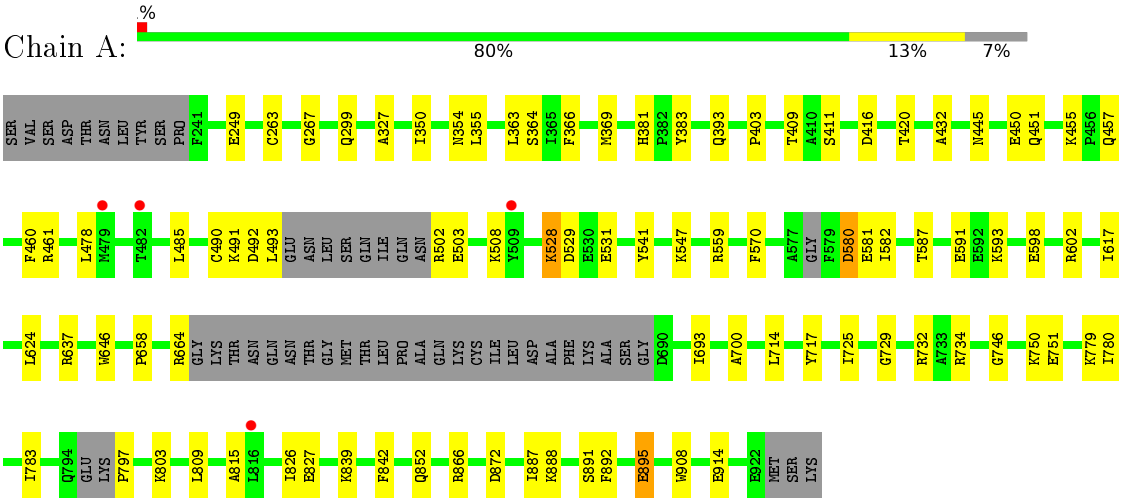
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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.

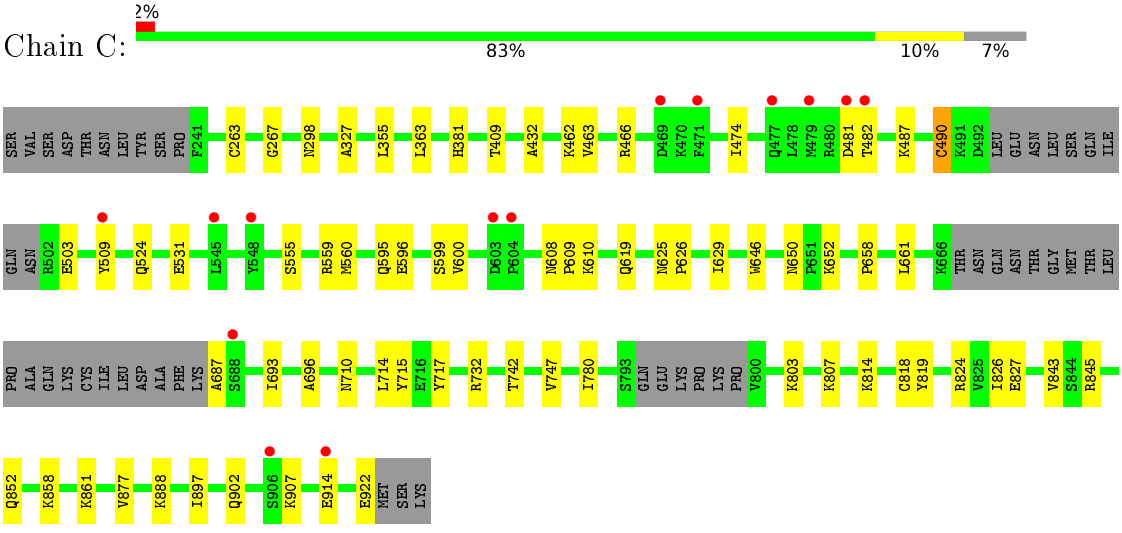
- Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain A:



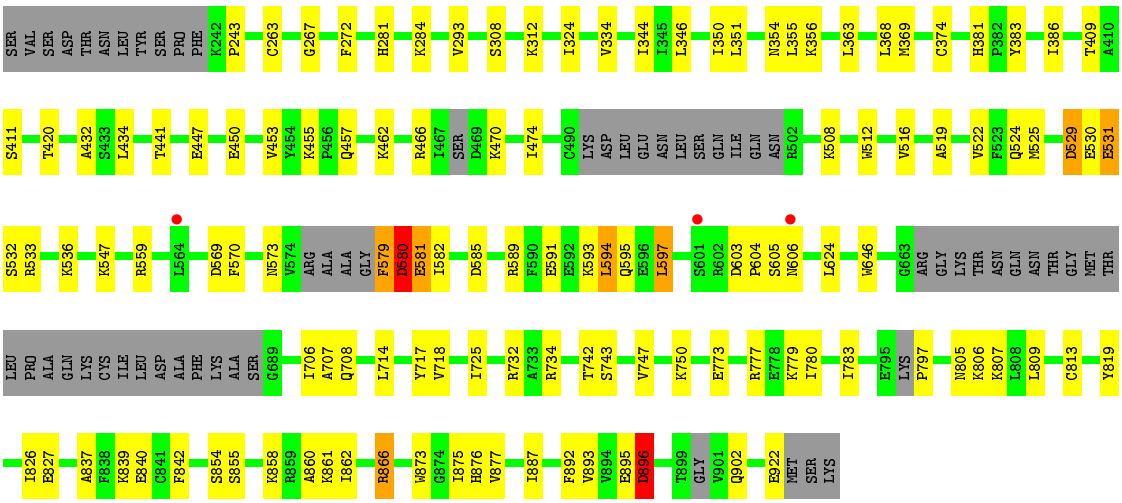
- Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain C:



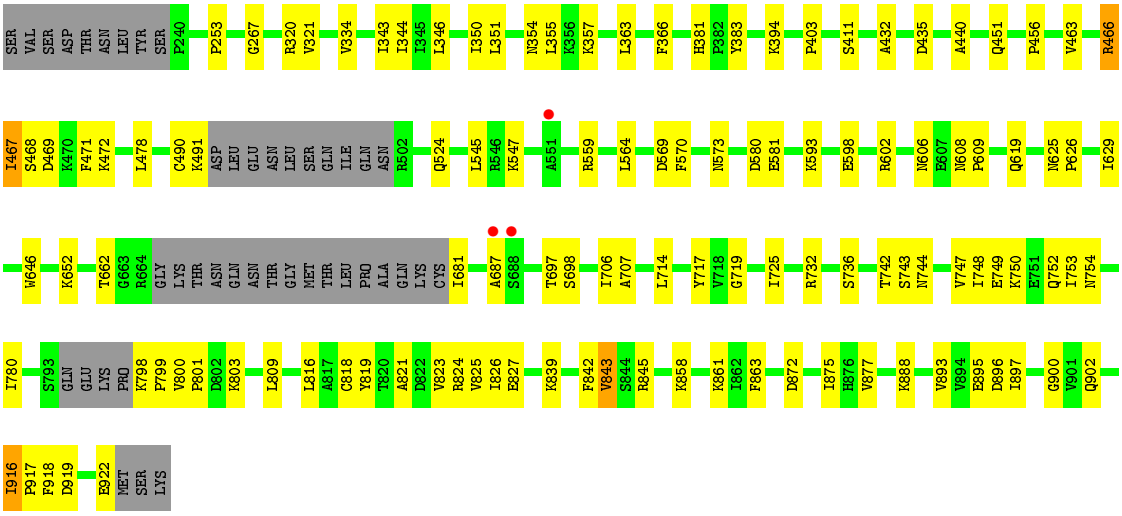
- Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain E:



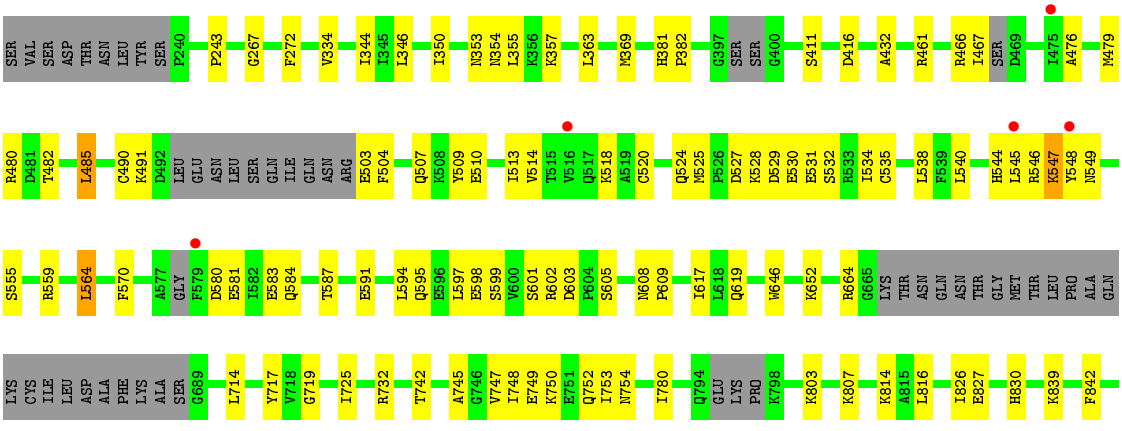
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

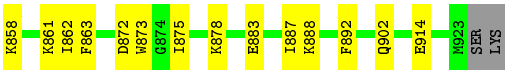
Chain G:



• Molecule 1: Probable ATP-dependent RNA helicase DDX58

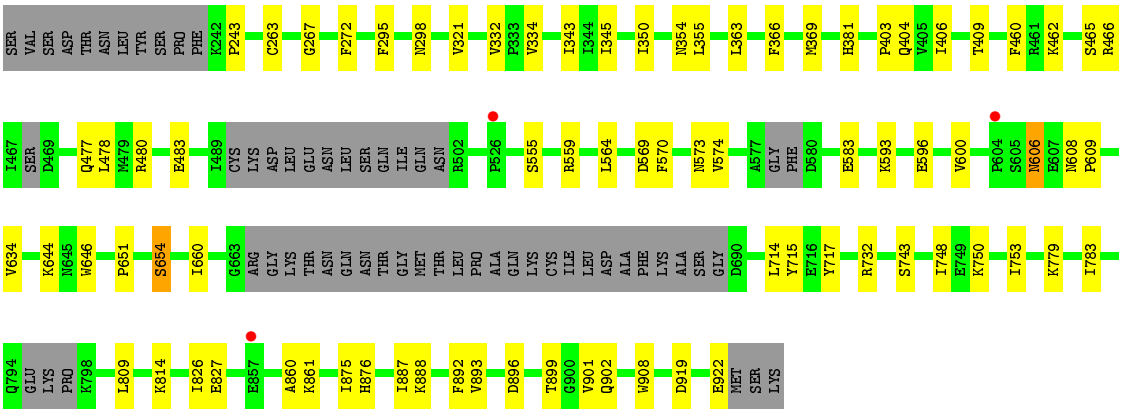
Chain I:





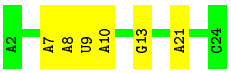
• Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain K:



• Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*AP*UP*AP*UP*UP*C)-3')

Chain B:

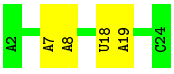


• Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*AP*UP*AP*UP*UP*C)-3')

Chain D:

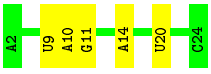
• Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*AP*UP*AP*UP*UP*C)-3')

Chain F:



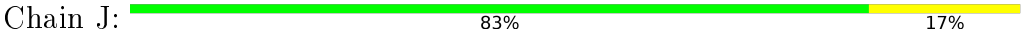
• Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*AP*UP*AP*UP*UP*C)-3')

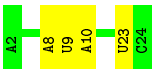
Chain H:



• Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')

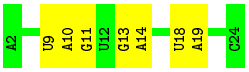
Chain J:





• Molecule 2: RNA (5'-R(P*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.18Å 174.81Å 309.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.44 – 3.10 49.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.44-3.10) 93.2 (49.44-3.10)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.213 , 0.266 0.231 , 0.280	Depositor DCC
R_{free} test set	5111 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 109351 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	33602	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.25% 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: GTP, ZN, MG

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	0.24	0/5220	0.42	1/7052 (0.0%)
1	C	0.24	0/5184	0.42	0/7008
1	E	0.31	1/5148 (0.0%)	0.52	8/6957 (0.1%)
1	G	0.23	0/5273	0.41	0/7124
1	I	0.27	0/5138	0.45	1/6943 (0.0%)
1	K	0.23	0/5125	0.41	0/6930
2	B	0.16	0/543	0.67	0/842
2	D	0.17	0/543	0.66	0/842
2	F	0.15	0/543	0.65	0/842
2	H	0.16	0/543	0.68	0/842
2	J	0.16	0/543	0.67	0/842
2	L	0.14	0/543	0.66	0/842
All	All	0.25	1/34346 (0.0%)	0.47	10/47066 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	4
1	G	0	1
1	K	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	896	ASP	CB-CG	-5.07	1.41	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	580	ASP	CB-CG-OD1	12.46	129.51	118.30
1	E	597	LEU	CA-CB-CG	6.16	129.46	115.30
1	E	580	ASP	N-CA-C	6.15	127.61	111.00
1	A	797	PRO	N-CA-CB	5.93	110.42	103.30
1	E	797	PRO	N-CA-CB	5.92	110.40	103.30
1	E	896	ASP	N-CA-C	5.87	126.84	111.00
1	E	896	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	E	580	ASP	OD1-CG-OD2	-5.44	112.96	123.30
1	E	581	GLU	N-CA-C	5.43	125.66	111.00
1	I	564	LEU	CA-CB-CG	5.39	127.69	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	ASP	Peptide
1	E	579	PHE	Peptide
1	E	580	ASP	Peptide
1	E	593	LYS	Peptide
1	E	896	ASP	Peptide
1	G	466	ARG	Peptide
1	K	606	ASN	Peptide

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	5119	0	5077	55	0
1	C	5083	0	5012	41	0
1	E	5047	0	4975	84	0
1	G	5168	0	5132	74	0
1	I	5039	0	4966	78	0
1	K	5024	0	4950	48	0
2	B	486	0	244	4	0
2	D	486	0	244	1	0
2	F	486	0	244	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	486	0	244	3	0
2	J	486	0	244	4	0
2	L	486	0	244	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	A	3	0	0	0	0
4	E	1	0	0	0	0
4	G	2	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	B	32	0	11	1	0
5	D	32	0	11	2	0
5	F	32	0	11	0	0
5	H	32	0	11	2	0
5	J	32	0	11	4	0
5	L	32	0	11	1	0
All	All	33602	0	31642	383	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 (383) 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:E:525:MET:HE2	1:E:531:GLU:HB3	1.63	0.81
1:E:594:LEU:O	1:E:597:LEU:HB2	1.80	0.81
1:K:466:ARG:NH2	1:K:555:SER:O	2.16	0.78
1:G:267:GLY:HA3	1:G:732:ARG:HD3	1.66	0.78
1:A:478:LEU:HD11	1:A:593:LYS:HG3	1.67	0.77
1:I:591:GLU:HA	1:I:594:LEU:HB2	1.69	0.74
1:G:826:ILE:HG22	1:G:827:GLU:HG3	1.69	0.73
1:K:267:GLY:HA3	1:K:732:ARG:HD3	1.69	0.72
1:E:895:GLU:HG3	1:E:902:GLN:CG	2.19	0.72
1:C:803:LYS:NZ	1:C:914:GLU:OE1	2.18	0.72
1:E:806:LYS:HA	1:E:896:ASP:OD1	1.90	0.72
1:A:267:GLY:HA3	1:A:732:ARG:HD3	1.72	0.70
1:C:267:GLY:HA3	1:C:732:ARG:HD3	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:895:GLU:HG3	1:E:902:GLN:HG2	1.76	0.68
1:C:327:ALA:HA	1:C:852:GLN:HE22	1.58	0.68
1:G:478:LEU:HD11	1:G:593:LYS:HG3	1.76	0.67
1:A:432:ALA:HA	1:A:780:ILE:HG23	1.76	0.67
1:I:490:CYS:SG	1:I:491:LYS:N	2.63	0.66
1:G:843:VAL:HG22	1:G:863:PHE:HB2	1.77	0.66
1:I:564:LEU:HD21	1:I:598:GLU:HA	1.77	0.66
1:K:600:VAL:O	1:K:606:ASN:ND2	2.29	0.65
1:I:267:GLY:HA3	1:I:732:ARG:HD3	1.80	0.64
1:E:559:ARG:HD3	1:E:646:TRP:HD1	1.62	0.64
1:E:594:LEU:HG	1:E:595:GLN:N	2.13	0.64
1:I:355:LEU:HD11	1:I:363:LEU:HD21	1.80	0.63
1:A:355:LEU:HD11	1:A:363:LEU:HD21	1.81	0.63
1:E:524:GLN:OE1	1:E:525:MET:N	2.28	0.63
1:E:861:LYS:HD2	1:E:875:ILE:HG22	1.81	0.62
1:C:596:GLU:O	1:C:600:VAL:HG23	1.98	0.62
1:I:888:LYS:HB3	5:J:101:GTP:H5'	1.81	0.61
1:I:466:ARG:NH2	1:I:555:SER:O	2.33	0.61
1:I:531:GLU:HA	1:I:534:ILE:HG12	1.80	0.61
1:G:559:ARG:HD3	1:G:646:TRP:HD1	1.66	0.61
1:G:821:ALA:O	1:G:824:ARG:NH2	2.34	0.60
1:I:580:ASP:OD1	1:I:581:GLU:N	2.34	0.60
2:J:9:U:H2'	2:J:10:A:C8	2.36	0.60
1:E:243:PRO:HB3	1:E:272:PHE:HE2	1.67	0.60
1:C:559:ARG:HD3	1:C:646:TRP:HD1	1.67	0.60
1:C:462:LYS:NZ	1:C:463:VAL:O	2.26	0.60
1:E:714:LEU:HB3	1:E:717:TYR:HB3	1.84	0.59
1:A:490:CYS:SG	1:A:491:LYS:N	2.75	0.59
1:A:451:GLN:NE2	1:E:447:GLU:OE1	2.35	0.59
1:A:637:ARG:HH12	1:A:664:ARG:HD2	1.68	0.59
1:A:826:ILE:HG22	1:A:827:GLU:HG3	1.84	0.59
1:G:466:ARG:NH2	1:G:606:ASN:O	2.36	0.58
1:G:748:ILE:O	1:G:752:GLN:HG2	2.03	0.58
1:A:327:ALA:HA	1:A:852:GLN:HE22	1.69	0.58
1:G:861:LYS:NZ	5:H:101:GTP:O1B	2.23	0.58
1:I:587:THR:O	1:I:591:GLU:HG3	2.02	0.58
1:K:651:PRO:O	1:K:654:SER:OG	2.22	0.58
1:E:308:SER:OG	1:E:312:LYS:NZ	2.36	0.58
1:E:569:ASP:O	1:E:573:ASN:ND2	2.36	0.58
1:I:540:LEU:HD13	1:I:583:GLU:HG3	1.86	0.58
1:C:355:LEU:HD11	1:C:363:LEU:HD21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ALA:HA	1:C:780:ILE:HG23	1.86	0.57
1:G:471:PHE:HE1	1:G:564:LEU:HG	1.70	0.57
1:I:479:MET:HE2	1:I:548:TYR:HB3	1.87	0.57
1:E:355:LEU:HD11	1:E:363:LEU:HD21	1.87	0.57
1:I:598:GLU:O	1:I:601:SER:HB2	2.05	0.57
1:G:824:ARG:HG2	1:G:918:PHE:HA	1.86	0.56
1:I:719:GLY:O	1:I:754:ASN:ND2	2.37	0.56
1:K:596:GLU:O	1:K:600:VAL:HG23	2.05	0.56
1:K:644:LYS:HD2	1:K:660:ILE:HD11	1.88	0.56
1:C:481:ASP:OD1	1:C:482:THR:N	2.38	0.56
1:E:381:HIS:HD1	1:E:383:TYR:H	1.52	0.56
1:I:714:LEU:HB3	1:I:717:TYR:HB3	1.86	0.56
1:E:842:PHE:HB2	1:E:862:ILE:HG23	1.87	0.55
1:K:477:GLN:HA	1:K:480:ARG:CG	2.36	0.55
1:K:896:ASP:HB3	1:K:899:THR:HG22	1.88	0.55
1:A:559:ARG:HD3	1:A:646:TRP:HD1	1.70	0.55
1:E:267:GLY:HA3	1:E:732:ARG:HD3	1.88	0.55
1:I:664:ARG:NH2	2:J:23:U:OP2	2.40	0.55
1:A:420:THR:HG21	1:E:624:LEU:HD11	1.88	0.55
1:C:845:ARG:HH21	1:G:843:VAL:HG12	1.72	0.55
1:K:714:LEU:HB3	1:K:717:TYR:HB3	1.87	0.55
1:C:714:LEU:HB3	1:C:717:TYR:HB3	1.88	0.55
1:E:742:THR:HG21	1:E:747:VAL:HB	1.87	0.55
1:E:525:MET:HE2	1:E:531:GLU:CB	2.36	0.55
1:I:803:LYS:HG2	1:I:914:GLU:HB2	1.90	0.54
1:C:861:LYS:NZ	5:D:101:GTP:O1B	2.38	0.54
1:A:457:GLN:OE1	1:E:455:LYS:NZ	2.40	0.54
1:A:502:ARG:NE	1:A:503:GLU:OE2	2.36	0.54
1:I:830:HIS:HE1	5:J:101:GTP:HN22	1.56	0.54
1:K:809:LEU:HB2	1:K:893:VAL:HG13	1.89	0.54
1:A:528:LYS:O	1:A:531:GLU:HB2	2.07	0.54
1:G:355:LEU:HD11	1:G:363:LEU:HD21	1.89	0.54
1:A:714:LEU:HB3	1:A:717:TYR:HB3	1.90	0.54
1:G:321:VAL:HG22	1:G:343:ILE:HB	1.90	0.54
1:K:355:LEU:HD11	1:K:363:LEU:HD21	1.90	0.54
1:C:845:ARG:NH2	1:G:843:VAL:HG12	2.23	0.53
1:G:823:VAL:O	1:G:916:ILE:HD11	2.08	0.53
1:I:559:ARG:HD3	1:I:646:TRP:HD1	1.73	0.53
1:G:432:ALA:HA	1:G:780:ILE:HG23	1.88	0.53
1:G:714:LEU:HB3	1:G:717:TYR:HB3	1.89	0.53
1:I:466:ARG:HG3	1:I:467:ILE:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:416:ASP:OD1	1:I:416:ASP:N	2.36	0.53
1:C:826:ILE:HG22	1:C:827:GLU:HG3	1.90	0.53
1:A:455:LYS:NZ	1:E:457:GLN:HE21	2.07	0.53
1:G:861:LYS:HD2	1:G:875:ILE:HG22	1.90	0.53
1:K:321:VAL:HG22	1:K:343:ILE:HB	1.91	0.52
1:E:895:GLU:HG3	1:E:902:GLN:HG3	1.91	0.52
1:G:896:ASP:O	1:G:900:GLY:N	2.38	0.52
1:K:569:ASP:O	1:K:573:ASN:ND2	2.30	0.52
1:G:451:GLN:N	1:G:451:GLN:OE1	2.42	0.52
1:I:461:ARG:HG3	1:I:617:ILE:HD11	1.91	0.52
1:K:861:LYS:HD2	1:K:875:ILE:HG22	1.91	0.52
1:G:895:GLU:HB2	1:G:902:GLN:HG2	1.92	0.52
1:K:919:ASP:HB3	1:K:922:GLU:HG3	1.91	0.52
1:E:837:ALA:O	1:E:840:GLU:HB2	2.10	0.52
1:E:862:ILE:HG22	1:E:873:TRP:HB2	1.92	0.52
1:E:579:PHE:O	1:E:580:ASP:HB2	2.09	0.52
1:E:858:LYS:HA	1:E:877:VAL:HG12	1.91	0.52
1:G:888:LYS:HB3	5:H:101:GTP:H5'	1.90	0.52
1:E:293:VAL:HG22	1:E:368:LEU:HB3	1.92	0.52
1:I:353:ASN:O	1:I:357:LYS:HG2	2.09	0.51
1:I:411:SER:HB2	1:I:725:ILE:HD12	1.92	0.51
1:G:320:ARG:HD2	1:K:332:VAL:HG11	1.92	0.51
1:K:465:SER:HA	1:K:609:PRO:HG2	1.92	0.51
1:K:477:GLN:HA	1:K:480:ARG:HG2	1.90	0.51
1:K:350:ILE:O	1:K:354:ASN:ND2	2.40	0.51
1:C:298:ASN:HD21	1:C:381:HIS:CE1	2.28	0.51
1:I:528:LYS:O	1:I:531:GLU:N	2.44	0.51
1:G:469:ASP:HB3	1:G:472:LYS:HB3	1.93	0.51
1:A:746:GLY:O	1:A:750:LYS:HG2	2.11	0.51
1:E:708:GLN:HE22	1:E:732:ARG:CZ	2.24	0.50
1:E:806:LYS:HA	1:E:896:ASP:CG	2.30	0.50
1:I:745:ALA:O	1:I:749:GLU:HG3	2.11	0.50
1:I:599:SER:HA	1:I:602:ARG:H	1.77	0.50
1:A:815:ALA:HB2	1:A:866:ARG:HD2	1.93	0.50
1:C:814:LYS:NZ	1:C:902:GLN:OE1	2.41	0.50
1:A:485:LEU:HB3	1:A:541:TYR:CZ	2.46	0.49
1:C:487:LYS:HA	1:C:490:CYS:SG	2.51	0.49
1:G:719:GLY:O	1:G:754:ASN:ND2	2.43	0.49
1:I:476:ALA:O	1:I:480:ARG:HG3	2.11	0.49
1:C:619:GLN:HE22	1:C:652:LYS:HE2	1.77	0.49
1:G:580:ASP:OD2	1:G:581:GLU:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:809:LEU:HB2	1:G:893:VAL:HG13	1.94	0.49
1:I:243:PRO:HB3	1:I:272:PHE:CE2	2.48	0.49
1:C:555:SER:OG	1:C:560:MET:HG2	2.12	0.49
1:K:559:ARG:HD3	1:K:646:TRP:HD1	1.77	0.49
1:G:824:ARG:HG3	1:G:916:ILE:HD13	1.94	0.49
1:A:508:LYS:HE2	2:B:9:U:H4'	1.94	0.49
1:E:718:VAL:HG13	1:E:750:LYS:HG2	1.95	0.49
1:E:813:CYS:HB2	1:E:866:ARG:NH1	2.28	0.49
1:K:363:LEU:HB3	1:K:369:MET:HE3	1.95	0.49
1:G:919:ASP:HB3	1:G:922:GLU:HG3	1.95	0.48
1:E:524:GLN:HG2	1:E:902:GLN:NE2	2.28	0.48
1:G:750:LYS:O	1:G:753:ILE:HG12	2.14	0.48
2:B:9:U:H2'	2:B:10:A:C8	2.47	0.48
1:G:629:ILE:HD11	1:G:687:ALA:HA	1.95	0.48
1:I:584:GLN:HA	1:I:587:THR:HG22	1.96	0.48
1:A:637:ARG:HH22	1:A:664:ARG:HG2	1.78	0.48
2:F:7:A:H2'	2:F:8:A:C8	2.49	0.48
1:K:243:PRO:HB3	1:K:272:PHE:CE2	2.49	0.48
1:A:461:ARG:HG3	1:A:617:ILE:HD11	1.95	0.48
1:K:814:LYS:NZ	1:K:902:GLN:OE1	2.36	0.48
1:A:888:LYS:HE3	1:A:891:SER:HB2	1.96	0.47
1:E:519:ALA:HA	1:E:522:VAL:HG22	1.95	0.47
1:A:581:GLU:HB3	1:A:582:ILE:H	1.25	0.47
1:G:744:ASN:HB3	1:G:747:VAL:HG23	1.96	0.47
1:K:899:THR:HG23	1:K:901:VAL:H	1.78	0.47
1:G:698:SER:HG	2:H:20:U:HO2'	1.57	0.47
1:G:742:THR:HG21	1:G:747:VAL:HB	1.96	0.47
1:E:809:LEU:HB2	1:E:893:VAL:HG13	1.97	0.47
1:I:529:ASP:OD1	1:I:529:ASP:N	2.44	0.47
1:I:830:HIS:CE1	5:J:101:GTP:HN22	2.32	0.47
1:A:450:GLU:OE2	1:E:734:ARG:NH1	2.44	0.47
1:C:503:GLU:O	1:C:509:TYR:HB2	2.15	0.47
1:G:818:CYS:SG	1:G:819:TYR:N	2.88	0.47
1:G:839:LYS:HA	1:G:842:PHE:CE2	2.50	0.47
1:I:344:ILE:HG22	1:I:346:LEU:HD13	1.96	0.47
1:A:460:PHE:HE1	1:A:751:GLU:HG2	1.79	0.47
1:E:411:SER:HB2	1:E:725:ILE:HD12	1.97	0.47
1:E:826:ILE:HG22	1:E:827:GLU:HG3	1.95	0.47
1:E:854:SER:OG	1:E:855:SER:N	2.47	0.47
1:E:860:ALA:HB3	1:E:876:HIS:HB3	1.95	0.47
1:K:462:LYS:NZ	1:K:743:SER:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:520:CYS:SG	1:I:538:LEU:HD23	2.55	0.47
1:K:460:PHE:HB3	1:K:748:ILE:HD12	1.96	0.47
1:E:356:LYS:HD2	1:E:356:LYS:O	2.14	0.47
1:I:750:LYS:HE3	2:J:8:A:H5"	1.96	0.47
1:I:861:LYS:HD2	1:I:875:ILE:HG22	1.96	0.47
1:I:839:LYS:HA	1:I:842:PHE:CE2	2.51	0.46
1:K:860:ALA:HB3	1:K:876:HIS:HB3	1.97	0.46
1:G:467:ILE:HG22	1:G:468:SER:N	2.30	0.46
1:I:748:ILE:O	1:I:752:GLN:HG2	2.16	0.46
1:K:478:LEU:HD11	1:K:593:LYS:HE2	1.97	0.46
1:C:742:THR:HG21	1:C:747:VAL:HB	1.97	0.46
1:C:858:LYS:HA	1:C:877:VAL:HG12	1.98	0.46
1:G:706:ILE:HG12	1:G:707:ALA:H	1.79	0.46
1:A:598:GLU:OE1	1:A:602:ARG:NH2	2.48	0.46
1:I:749:GLU:O	1:I:753:ILE:HG23	2.16	0.46
1:K:480:ARG:HA	1:K:483:GLU:HB2	1.98	0.46
1:A:411:SER:HB2	1:A:725:ILE:HD12	1.98	0.46
1:C:524:GLN:HA	1:C:531:GLU:OE2	2.15	0.46
1:A:872:ASP:O	1:A:891:SER:OG	2.21	0.46
1:G:747:VAL:HA	1:G:750:LYS:HG2	1.97	0.46
1:I:503:GLU:CG	1:I:504:PHE:N	2.79	0.46
1:I:514:VAL:O	1:I:518:LYS:HG3	2.16	0.46
1:C:595:GLN:O	1:C:599:SER:OG	2.22	0.46
1:C:650:ASN:OD1	1:C:652:LYS:HG3	2.16	0.46
1:G:463:VAL:O	1:G:743:SER:HA	2.15	0.46
1:G:749:GLU:O	1:G:753:ILE:HG23	2.16	0.46
1:E:529:ASP:O	1:E:532:SER:HB3	2.16	0.46
1:E:922:GLU:HG2	1:E:922:GLU:H	1.53	0.46
2:F:18:U:H2'	2:F:19:A:C8	2.51	0.45
1:I:594:LEU:O	1:I:597:LEU:HB2	2.17	0.45
1:I:598:GLU:HG2	1:I:599:SER:N	2.31	0.45
1:K:298:ASN:HD21	1:K:381:HIS:CE1	2.35	0.45
1:A:502:ARG:HG2	1:A:503:GLU:HG3	1.97	0.45
1:E:243:PRO:HB3	1:E:272:PHE:CE2	2.50	0.45
1:E:603:ASP:HA	1:E:604:PRO:HD3	1.84	0.45
1:I:807:LYS:HD2	1:I:816:LEU:HD13	1.99	0.45
1:A:637:ARG:NH2	2:B:21:A:OP2	2.41	0.45
1:C:824:ARG:NH2	1:C:922:GLU:OE1	2.39	0.45
1:I:527:ASP:OD1	1:I:530:GLU:HB3	2.17	0.45
1:C:466:ARG:HB2	1:C:608:ASN:OD1	2.17	0.45
1:C:714:LEU:HD13	1:C:717:TYR:CD2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:MET:SD	1:E:530:GLU:HB3	2.57	0.45
1:E:594:LEU:HG	1:E:595:GLN:H	1.81	0.45
1:E:708:GLN:HE22	1:E:732:ARG:NH1	2.14	0.45
1:I:432:ALA:HA	1:I:780:ILE:HG23	1.98	0.45
1:A:779:LYS:O	1:A:783:ILE:HG13	2.16	0.45
1:E:603:ASP:OD2	1:E:605:SER:OG	2.30	0.45
1:A:350:ILE:O	1:A:354:ASN:ND2	2.43	0.45
1:I:510:GLU:HA	1:I:513:ILE:HG22	1.99	0.45
1:K:263:CYS:HA	1:K:409:THR:O	2.17	0.45
1:E:805:ASN:HD21	1:E:819:TYR:HD2	1.65	0.44
1:I:534:ILE:HG13	1:I:535:CYS:N	2.32	0.44
1:I:826:ILE:HG22	1:I:827:GLU:HG3	1.98	0.44
1:K:295:PHE:HB3	1:K:345:ILE:HG13	2.00	0.44
1:K:779:LYS:O	1:K:783:ILE:HG13	2.18	0.44
1:E:462:LYS:NZ	1:E:743:SER:O	2.51	0.44
1:C:888:LYS:HB3	5:D:101:GTP:H5'	1.99	0.44
1:A:734:ARG:NH1	1:E:450:GLU:OE2	2.31	0.44
1:E:470:LYS:O	1:E:474:ILE:HG13	2.18	0.44
1:E:585:ASP:O	1:E:589:ARG:HG3	2.16	0.44
1:G:569:ASP:OD1	1:G:573:ASN:ND2	2.51	0.44
1:G:863:PHE:HD2	1:G:872:ASP:HA	1.83	0.44
1:A:363:LEU:HB3	1:A:369:MET:HE3	2.00	0.44
1:E:432:ALA:HA	1:E:780:ILE:HG23	2.00	0.44
1:E:363:LEU:HB3	1:E:369:MET:HE3	2.00	0.44
1:I:503:GLU:HG3	1:I:504:PHE:CD1	2.52	0.44
1:I:814:LYS:NZ	1:I:902:GLN:OE1	2.37	0.44
1:E:263:CYS:HA	1:E:409:THR:O	2.17	0.44
1:G:366:PHE:O	1:G:403:PRO:HB3	2.18	0.44
1:K:750:LYS:HA	1:K:753:ILE:HG12	1.99	0.44
2:L:11:G:N2	2:L:14:A:OP2	2.44	0.44
1:A:299:GLN:NE2	1:A:700:ALA:HB3	2.33	0.43
1:G:411:SER:HB2	1:G:725:ILE:HD12	1.99	0.43
1:A:547:LYS:HG3	1:A:570:PHE:CE1	2.54	0.43
1:A:839:LYS:HA	1:A:842:PHE:CE2	2.53	0.43
1:E:512:TRP:O	1:E:516:VAL:HG23	2.19	0.43
1:E:839:LYS:HA	1:E:842:PHE:CE2	2.53	0.43
1:G:524:GLN:NE2	1:G:895:GLU:OE2	2.52	0.43
2:L:9:U:H2'	2:L:10:A:C8	2.53	0.43
1:A:263:CYS:HA	1:A:409:THR:O	2.18	0.43
1:A:366:PHE:O	1:A:403:PRO:HB3	2.19	0.43
1:G:357:LYS:HE2	1:G:357:LYS:HB3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:528:LYS:HA	1:I:531:GLU:HB3	2.00	0.43
1:E:524:GLN:NE2	1:E:531:GLU:OE1	2.51	0.43
1:I:595:GLN:HA	1:I:598:GLU:OE1	2.19	0.43
1:I:887:ILE:HB	1:I:892:PHE:HE2	1.83	0.43
1:E:524:GLN:HG2	1:E:902:GLN:HE22	1.83	0.43
2:F:18:U:H2'	2:F:19:A:H8	1.83	0.43
1:G:467:ILE:HG22	1:G:468:SER:H	1.83	0.43
1:G:839:LYS:HA	1:G:842:PHE:HE2	1.84	0.43
1:I:742:THR:HG21	1:I:747:VAL:HB	2.01	0.43
1:E:858:LYS:HG2	1:E:875:ILE:HD12	2.00	0.43
1:G:253:PRO:HG2	1:G:440:ALA:HB2	2.00	0.43
1:A:416:ASP:OD1	1:A:416:ASP:N	2.41	0.43
1:A:492:ASP:HB3	1:A:493:LEU:H	1.42	0.43
1:C:466:ARG:NH2	1:C:555:SER:O	2.52	0.43
1:G:608:ASN:HA	1:G:609:PRO:HD2	1.88	0.43
1:I:524:GLN:O	1:I:525:MET:HG3	2.19	0.43
1:E:779:LYS:O	1:E:783:ILE:HG13	2.19	0.42
1:G:598:GLU:O	1:G:602:ARG:HG3	2.19	0.42
1:I:466:ARG:HG2	1:I:467:ILE:HG12	2.01	0.42
1:G:490:CYS:SG	1:G:491:LYS:N	2.92	0.42
1:G:619:GLN:NE2	1:G:652:LYS:HB3	2.34	0.42
1:G:800:VAL:HA	1:G:801:PRO:HD3	1.91	0.42
1:I:608:ASN:HA	1:I:609:PRO:HD2	1.90	0.42
1:K:404:GLN:HE21	1:K:406:ILE:HD11	1.84	0.42
1:I:363:LEU:HB3	1:I:369:MET:HE3	2.01	0.42
1:I:878:LYS:HD3	1:I:883:GLU:HG2	2.02	0.42
1:K:564:LEU:HA	1:K:564:LEU:HD23	1.87	0.42
1:A:364:SER:HG	1:A:393:GLN:HE22	1.64	0.42
1:G:344:ILE:HG22	1:G:346:LEU:HD13	2.02	0.42
1:G:564:LEU:HA	1:G:564:LEU:HD23	1.85	0.42
1:I:540:LEU:O	1:I:544:HIS:ND1	2.47	0.42
1:K:298:ASN:HD21	1:K:381:HIS:HE2	1.67	0.42
1:K:634:VAL:HG12	1:K:715:TYR:HB3	2.00	0.42
1:K:826:ILE:HG22	1:K:827:GLU:HG3	2.01	0.42
1:E:591:GLU:HA	1:E:594:LEU:HB2	2.02	0.42
1:G:858:LYS:HA	1:G:877:VAL:HG12	2.01	0.42
2:B:7:A:H2'	2:B:8:A:C8	2.54	0.42
1:E:533:ARG:HA	1:E:536:LYS:HB3	2.02	0.42
1:E:453:VAL:HG22	1:E:732:ARG:HD2	2.01	0.42
1:E:773:GLU:OE2	1:E:777:ARG:NH2	2.44	0.42
1:I:714:LEU:HD13	1:I:717:TYR:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:887:ILE:HB	1:K:892:PHE:HE2	1.84	0.42
1:G:350:ILE:O	1:G:354:ASN:ND2	2.43	0.42
1:I:619:GLN:NE2	1:I:652:LYS:HB3	2.35	0.42
1:A:249:GLU:OE1	1:A:445:ASN:ND2	2.33	0.42
1:A:587:THR:O	1:A:591:GLU:HG3	2.19	0.42
1:A:729:GLY:O	1:A:732:ARG:HG3	2.20	0.42
1:G:381:HIS:HD1	1:G:383:TYR:H	1.67	0.42
2:L:13:G:H2'	2:L:14:A:C8	2.55	0.42
2:D:13:G:H2'	2:D:14:A:C8	2.55	0.42
1:E:714:LEU:HD13	1:E:717:TYR:CD2	2.55	0.42
2:H:11:G:N2	2:H:14:A:OP2	2.40	0.42
1:E:344:ILE:HG22	1:E:346:LEU:HD13	2.02	0.41
1:G:662:THR:HG22	1:G:697:THR:HG23	2.02	0.41
1:I:863:PHE:HD2	1:I:872:ASP:HA	1.84	0.41
1:G:916:ILE:HA	1:G:917:PRO:HD3	1.96	0.41
1:C:629:ILE:H	1:C:710:ASN:HD21	1.67	0.41
1:E:466:ARG:NH2	1:E:606:ASN:O	2.39	0.41
1:G:394:LYS:NZ	1:G:435:ASP:OD1	2.52	0.41
1:G:625:ASN:HA	1:G:626:PRO:HD2	1.90	0.41
1:I:334:VAL:HG11	1:I:354:ASN:OD1	2.20	0.41
1:I:503:GLU:O	1:I:509:TYR:HB2	2.20	0.41
1:K:480:ARG:HG2	1:K:480:ARG:H	1.65	0.41
1:A:624:LEU:HD11	1:E:420:THR:HG21	2.01	0.41
1:C:608:ASN:HA	1:C:609:PRO:HD2	1.76	0.41
1:C:625:ASN:HA	1:C:626:PRO:HD2	1.96	0.41
1:C:658:PRO:HA	1:C:693:ILE:HG23	2.01	0.41
1:E:346:LEU:HD23	1:E:351:LEU:HB2	2.03	0.41
1:E:807:LYS:HE3	1:E:819:TYR:CE2	2.54	0.41
1:G:798:LYS:HA	1:G:799:PRO:HD3	1.94	0.41
1:C:629:ILE:HD11	1:C:687:ALA:HA	2.01	0.41
1:C:807:LYS:HZ1	1:C:897:ILE:HG23	1.85	0.41
1:G:897:ILE:HG12	1:G:897:ILE:O	2.21	0.41
1:I:546:ARG:O	1:I:549:ASN:HB3	2.20	0.41
1:C:610:LYS:HE2	1:C:715:TYR:HE1	1.85	0.41
1:E:334:VAL:HG21	1:E:354:ASN:ND2	2.35	0.41
1:E:547:LYS:HG3	1:E:570:PHE:CE1	2.56	0.41
1:G:456:PRO:HB3	1:G:736:SER:HB2	2.03	0.41
1:I:528:LYS:O	1:I:532:SER:N	2.46	0.41
2:L:18:U:H2'	2:L:19:A:C8	2.56	0.41
1:E:324:ILE:HG22	1:E:350:ILE:HG12	2.03	0.41
2:L:18:U:H2'	2:L:19:A:H8	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:PRO:HA	1:A:693:ILE:HG23	2.02	0.41
1:A:888:LYS:HA	1:A:908:TRP:HE1	1.86	0.41
1:C:661:LEU:HB3	1:C:696:ALA:HB2	2.02	0.41
1:C:818:CYS:SG	1:C:819:TYR:N	2.94	0.41
1:E:706:ILE:HD12	1:E:707:ALA:O	2.20	0.41
1:I:381:HIS:CG	1:I:382:PRO:HD2	2.56	0.41
1:I:507:GLN:HE22	2:J:9:U:H1'	1.85	0.41
1:E:508:LYS:HE2	1:E:508:LYS:HB3	1.71	0.41
1:G:547:LYS:HG3	1:G:570:PHE:CE1	2.56	0.41
1:I:482:THR:HA	1:I:485:LEU:HD22	2.03	0.41
1:I:862:ILE:HG22	1:I:873:TRP:HB2	2.03	0.41
1:A:299:GLN:HE21	1:A:700:ALA:HB3	1.86	0.41
1:G:825:VAL:HG12	1:G:916:ILE:O	2.20	0.41
1:I:545:LEU:HA	1:I:545:LEU:HD12	1.86	0.41
1:K:714:LEU:HD13	1:K:717:TYR:CD2	2.56	0.41
1:A:887:ILE:HB	1:A:892:PHE:HE2	1.86	0.40
1:A:809:LEU:HD11	1:A:895:GLU:HG3	2.03	0.40
1:A:803:LYS:HD2	1:A:914:GLU:HG3	2.03	0.40
1:C:843:VAL:HG12	1:G:845:ARG:HE	1.86	0.40
1:E:374:CYS:HB2	1:E:434:LEU:HD11	2.02	0.40
1:G:334:VAL:HG11	1:G:354:ASN:OD1	2.22	0.40
1:I:547:LYS:NZ	1:I:570:PHE:CE1	2.87	0.40
1:I:861:LYS:HB3	1:I:861:LYS:HE3	1.87	0.40
1:C:263:CYS:HA	1:C:409:THR:O	2.21	0.40
1:E:281:HIS:O	1:E:284:LYS:HG2	2.20	0.40
1:G:545:LEU:HA	1:G:545:LEU:HD12	1.85	0.40
2:H:9:U:H2'	2:H:10:A:C8	2.56	0.40
1:I:350:ILE:O	1:I:354:ASN:ND2	2.54	0.40
1:I:858:LYS:NZ	5:J:101:GTP:O2B	2.39	0.40
1:K:334:VAL:HG11	1:K:354:ASN:OD1	2.21	0.40
1:K:366:PHE:O	1:K:403:PRO:HB3	2.21	0.40
1:G:346:LEU:HD23	1:G:351:LEU:HB2	2.03	0.40
1:K:570:PHE:O	1:K:574:VAL:HG13	2.21	0.40
1:E:263:CYS:HB3	1:E:441:THR:HG22	2.03	0.40
1:I:603:ASP:OD1	1:I:605:SER:N	2.49	0.40
1:K:888:LYS:HB3	5:L:101:GTP:H5'	2.04	0.40
1:A:381:HIS:HD1	1:A:383:TYR:H	1.68	0.40
1:A:888:LYS:HB3	5:B:101:GTP:H5'	2.04	0.40
1:E:351:LEU:HD23	1:E:386:ILE:HD13	2.03	0.40
1:E:887:ILE:HB	1:E:892:PHE:HE2	1.87	0.40
1:K:608:ASN:HA	1:K:609:PRO:HD2	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:888:LYS:HA	1:K:908:TRP:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/695 (92%)	618 (97%)	18 (3%)	0	100	100
1	C	639/695 (92%)	621 (97%)	18 (3%)	0	100	100
1	E	624/695 (90%)	602 (96%)	19 (3%)	3 (0%)	34	72
1	G	645/695 (93%)	628 (97%)	16 (2%)	1 (0%)	52	84
1	I	630/695 (91%)	611 (97%)	19 (3%)	0	100	100
1	K	625/695 (90%)	607 (97%)	18 (3%)	0	100	100
All	All	3799/4170 (91%)	3687 (97%)	108 (3%)	4 (0%)	56	88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	580	ASP
1	G	467	ILE
1	E	581	GLU
1	E	594	LEU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	559/623 (90%)	555 (99%)	4 (1%)	88 95
1	C	551/623 (88%)	548 (100%)	3 (0%)	92 96
1	E	549/623 (88%)	545 (99%)	4 (1%)	88 95
1	G	562/623 (90%)	557 (99%)	5 (1%)	84 94
1	I	542/623 (87%)	540 (100%)	2 (0%)	93 97
1	K	545/623 (88%)	543 (100%)	2 (0%)	93 97
All	All	3308/3738 (88%)	3288 (99%)	20 (1%)	90 95

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	LYS
1	A	529	ASP
1	A	580	ASP
1	A	895	GLU
1	C	474	ILE
1	C	490	CYS
1	C	907	LYS
1	E	529	ASP
1	E	531	GLU
1	E	582	ILE
1	E	866	ARG
1	G	681	ILE
1	G	803	LYS
1	G	816	LEU
1	G	843	VAL
1	G	916	ILE
1	I	485	LEU
1	I	547	LYS
1	K	583	GLU
1	K	654	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	A	524	GLN
1	C	298	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	619	GLN
1	C	692	ASN
1	C	710	ASN
1	C	852	GLN
1	E	298	ASN
1	E	299	GLN
1	E	457	GLN
1	E	692	ASN
1	E	708	GLN
1	E	902	GLN
1	G	524	GLN
1	G	619	GLN
1	I	619	GLN
1	K	298	ASN
1	K	619	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	22/23 (95%)	1 (4%)	0
2	D	22/23 (95%)	0	0
2	F	22/23 (95%)	0	0
2	H	22/23 (95%)	0	0
2	J	22/23 (95%)	0	0
2	L	22/23 (95%)	0	0
All	All	132/138 (95%)	1 (0%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	13	G

There are no RNA pucker outliers to report.

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

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	GTP	B	101	2	26,34,34	0.93	1 (3%)	29,54,54	1.55	3 (10%)
5	GTP	D	101	2	26,34,34	0.92	1 (3%)	29,54,54	1.53	3 (10%)
5	GTP	F	101	2	26,34,34	0.92	1 (3%)	29,54,54	1.55	4 (13%)
5	GTP	H	101	2	26,34,34	0.94	1 (3%)	29,54,54	1.50	3 (10%)
5	GTP	J	101	2	26,34,34	0.91	1 (3%)	29,54,54	1.52	3 (10%)
5	GTP	L	101	2	26,34,34	0.92	1 (3%)	29,54,54	1.48	3 (10%)

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	GTP	B	101	2	-	0/18/38/38	0/3/3/3
5	GTP	D	101	2	-	0/18/38/38	0/3/3/3
5	GTP	F	101	2	-	0/18/38/38	0/3/3/3
5	GTP	H	101	2	-	0/18/38/38	0/3/3/3
5	GTP	J	101	2	-	0/18/38/38	0/3/3/3
5	GTP	L	101	2	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	GTP	C6-N1	2.77	1.38	1.33
5	J	101	GTP	C6-N1	2.77	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	101	GTP	C6-N1	2.83	1.38	1.33
5	L	101	GTP	C6-N1	2.84	1.38	1.33
5	H	101	GTP	C6-N1	2.88	1.38	1.33
5	B	101	GTP	C6-N1	2.90	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	101	GTP	N3-C2-N1	-5.42	120.19	127.56
5	D	101	GTP	N3-C2-N1	-5.40	120.21	127.56
5	J	101	GTP	N3-C2-N1	-5.39	120.22	127.56
5	H	101	GTP	N3-C2-N1	-5.35	120.28	127.56
5	F	101	GTP	N3-C2-N1	-5.32	120.32	127.56
5	L	101	GTP	N3-C2-N1	-5.32	120.33	127.56
5	F	101	GTP	C5-C6-N1	-2.96	119.65	123.52
5	L	101	GTP	C5-C6-N1	-2.96	119.65	123.52
5	H	101	GTP	C5-C6-N1	-2.96	119.65	123.52
5	D	101	GTP	C5-C6-N1	-2.92	119.70	123.52
5	B	101	GTP	C5-C6-N1	-2.91	119.72	123.52
5	J	101	GTP	C5-C6-N1	-2.86	119.78	123.52
5	F	101	GTP	C1'-N9-C4	2.11	129.16	126.81
5	F	101	GTP	C6-N1-C2	3.17	119.60	115.88
5	J	101	GTP	C6-N1-C2	3.21	119.64	115.88
5	H	101	GTP	C6-N1-C2	3.22	119.66	115.88
5	L	101	GTP	C6-N1-C2	3.23	119.67	115.88
5	B	101	GTP	C6-N1-C2	3.23	119.67	115.88
5	D	101	GTP	C6-N1-C2	3.28	119.72	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	101	GTP	1	0
5	D	101	GTP	2	0
5	H	101	GTP	2	0
5	J	101	GTP	4	0
5	L	101	GTP	1	0

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	646/695 (92%)	-0.25	4 (0%) 90 80	23, 53, 121, 244	0
1	C	647/695 (93%)	-0.15	14 (2%) 65 42	25, 56, 126, 229	0
1	E	638/695 (91%)	-0.15	3 (0%) 91 83	33, 59, 133, 252	0
1	G	653/695 (93%)	-0.11	3 (0%) 91 83	34, 61, 108, 186	0
1	I	644/695 (92%)	-0.05	5 (0%) 87 75	34, 63, 151, 267	0
1	K	637/695 (91%)	-0.17	3 (0%) 91 83	30, 58, 115, 220	0
2	B	23/23 (100%)	-0.03	0 100 100	33, 47, 158, 204	0
2	D	23/23 (100%)	-0.08	0 100 100	32, 48, 135, 159	0
2	F	23/23 (100%)	-0.28	0 100 100	40, 47, 117, 132	0
2	H	23/23 (100%)	0.02	0 100 100	36, 58, 138, 154	0
2	J	23/23 (100%)	-0.17	0 100 100	35, 55, 133, 159	0
2	L	23/23 (100%)	-0.38	0 100 100	37, 49, 133, 169	0
All	All	4003/4308 (92%)	-0.15	32 (0%) 87 75	23, 59, 130, 267	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	482	THR	3.1
1	C	688	SER	3.1
1	C	545	LEU	3.0
1	I	475	ILE	3.0
1	C	509	TYR	2.9
1	G	688	SER	2.8
1	C	548	TYR	2.8
1	C	471	PHE	2.7
1	C	482	THR	2.7
1	C	479	MET	2.6
1	I	516	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	548	TYR	2.6
1	E	564	LEU	2.5
1	C	603	ASP	2.5
1	I	579	PHE	2.4
1	E	601	SER	2.4
1	A	479	MET	2.3
1	A	509	TYR	2.3
1	K	604	PRO	2.3
1	E	606	ASN	2.3
1	A	816	LEU	2.3
1	C	469	ASP	2.2
1	K	526	PRO	2.2
1	C	481	ASP	2.1
1	G	551	ALA	2.1
1	C	604	PRO	2.1
1	C	906	SER	2.1
1	C	477	GLN	2.1
1	C	914	GLU	2.1
1	G	687	ALA	2.0
1	I	545	LEU	2.0
1	K	857	GLU	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
4	MG	G	1003	1/1	0.97	0.16	-0.31	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GTP	B	101	32/32	0.94	0.17	-0.80	33,47,88,95	0
5	GTP	D	101	32/32	0.96	0.16	-0.82	4,45,89,97	0
5	GTP	L	101	32/32	0.94	0.17	-0.86	27,56,96,105	0
4	MG	I	1002	1/1	0.97	0.13	-0.90	13,13,13,13	0
5	GTP	H	101	32/32	0.95	0.16	-1.09	22,44,88,90	0
5	GTP	J	101	32/32	0.95	0.17	-1.11	11,44,98,125	0
5	GTP	F	101	32/32	0.93	0.16	-1.11	36,60,84,88	0
3	ZN	G	1001	1/1	0.95	0.13	-1.61	77,77,77,77	0
3	ZN	E	1001	1/1	0.90	0.12	-1.65	82,82,82,82	0
3	ZN	C	1001	1/1	0.94	0.12	-1.76	74,74,74,74	0
4	MG	G	1002	1/1	0.90	0.15	-1.90	24,24,24,24	0
3	ZN	K	1001	1/1	0.98	0.10	-1.99	75,75,75,75	0
3	ZN	I	1001	1/1	0.89	0.14	-3.03	74,74,74,74	0
4	MG	E	1002	1/1	0.98	0.13	-3.83	46,46,46,46	0
3	ZN	A	1001	1/1	0.93	0.12	-3.92	75,75,75,75	0
4	MG	A	1004	1/1	0.94	0.16	-	50,50,50,50	0
4	MG	A	1002	1/1	0.98	0.08	-	28,28,28,28	0
4	MG	K	1002	1/1	0.92	0.09	-	39,39,39,39	0
4	MG	A	1003	1/1	0.85	0.31	-	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.