Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:55 AM GMT

PDB ID	:	3CJT
Title	:	Ribosomal protein L11 methyltransferase (PrmA) in complex with dimethylated ribosomal protein L11
Authors	:	Demirci, H.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2008-03-13
Resolution	:	2.30 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:

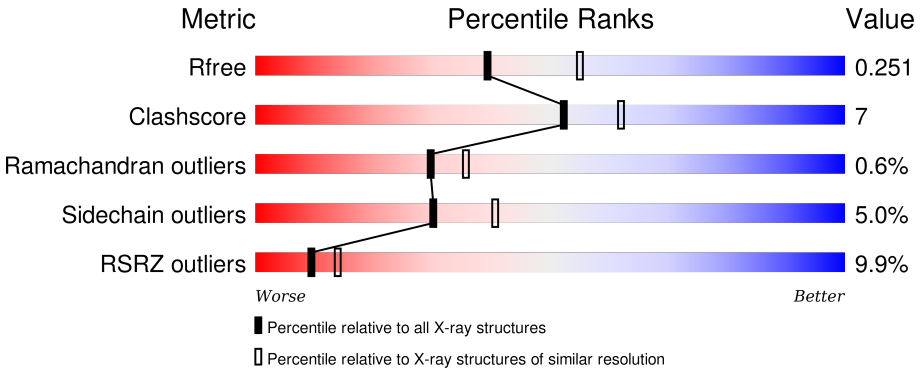
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	254	87% 11% •
1	C	254	6% 79% 17% • •
1	E	254	2% 85% 13% •
1	G	254	4% 83% 14% • •
1	I	254	88% 11% •

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Mol	Chain	Length	Quality of chain
1	K	254	13% 83% 14%
1	M	254	84% 15%
1	O	254	14% 84% 13%
2	B	147	11% 71% 13% 14%
2	D	147	18% 39% 8% 51%
2	F	147	12% 69% 17% 12%
2	H	147	5% 41% 5% 52%
2	J	147	10% 71% 14% 14%
2	L	147	27% 37% 9% 51%
2	N	147	14% 74% 14% 12%
2	P	147	24% 41% 5% 51%

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	NO3	A	255	-	X	-	-
3	NO3	B	148	-	X	-	-
3	NO3	E	255	-	X	-	-
3	NO3	F	148	-	X	-	-
3	NO3	I	255	-	X	-	-
3	NO3	I	256	-	X	-	-
3	NO3	M	255	-	X	-	X
3	NO3	N	148	-	X	-	X
4	CL	I	258	-	-	X	-
7	EDO	B	150	-	-	-	X
8	2MM	M	257	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23555 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 Ribosomal protein L11 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	2	0
			1966	1278	338	346	4			
1	C	250	Total	C	N	O	S	5	0	0
			1922	1245	333	341	3			
1	E	254	Total	C	N	O	S	0	0	0
			1953	1267	337	345	4			
1	G	251	Total	C	N	O	S	5	0	0
			1926	1247	334	342	3			
1	I	254	Total	C	N	O	S	0	1	0
			1961	1273	338	346	4			
1	K	250	Total	C	N	O	S	5	0	0
			1922	1245	333	341	3			
1	M	254	Total	C	N	O	S	0	1	0
			1961	1273	338	346	4			
1	O	250	Total	C	N	O	S	5	0	0
			1922	1245	333	341	3			

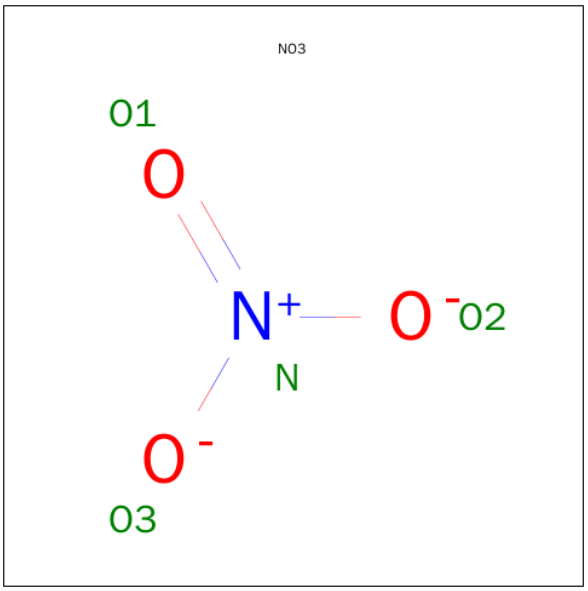
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ALA	HIS	ENGINEERED	UNP Q84BQ9
C	104	ALA	HIS	ENGINEERED	UNP Q84BQ9
E	104	ALA	HIS	ENGINEERED	UNP Q84BQ9
G	104	ALA	HIS	ENGINEERED	UNP Q84BQ9
I	104	ALA	HIS	ENGINEERED	UNP Q84BQ9
K	104	ALA	HIS	ENGINEERED	UNP Q84BQ9
M	104	ALA	HIS	ENGINEERED	UNP Q84BQ9
O	104	ALA	HIS	ENGINEERED	UNP Q84BQ9

- Molecule 2 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	126	Total C N O S 921 588 166 162 5	0	0	0
2	D	72	Total C N O S 525 341 88 93 3	4	0	0
2	F	130	Total C N O S 950 607 170 168 5	0	0	0
2	H	71	Total C N O S 520 338 87 92 3	4	0	0
2	J	127	Total C N O S 922 588 166 163 5	0	0	0
2	L	72	Total C N O S 525 341 88 93 3	4	0	0
2	N	130	Total C N O S 946 604 169 168 5	0	0	0
2	P	72	Total C N O S 525 341 88 93 3	4	0	0

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	E	1	Total N O 4 1 3	0	0
3	F	1	Total N O 4 1 3	0	0

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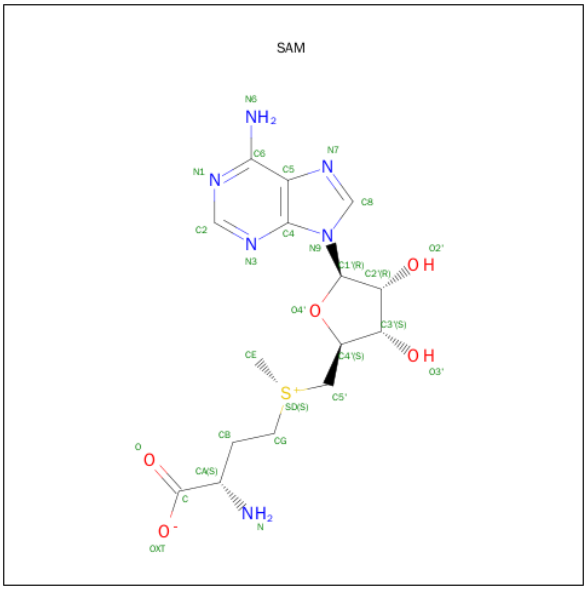
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total N O 4 1 3	0	0
3	I	1	Total N O 4 1 3	0	0
3	M	1	Total N O 4 1 3	0	0
3	N	1	Total N O 4 1 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	2	Total Cl 2 2	0	0
4	A	2	Total Cl 2 2	0	0

- Molecule 5 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O S 27 15 6 5 1	0	0
5	G	1	Total C N O S 27 15 6 5 1	0	0
5	K	1	Total C N O S 27 15 6 5 1	0	0

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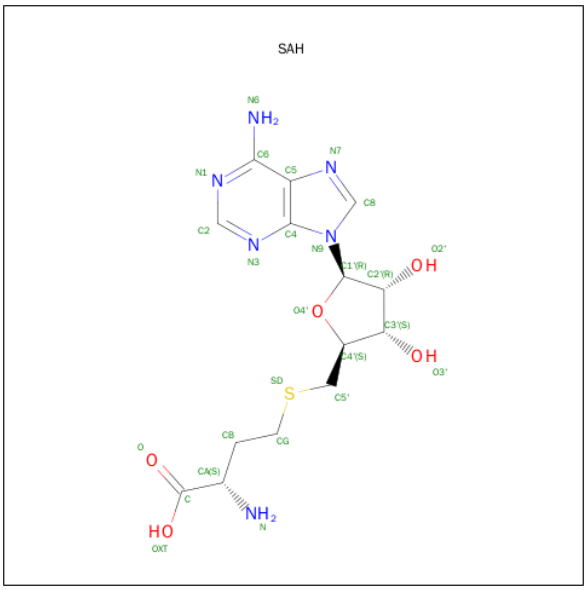
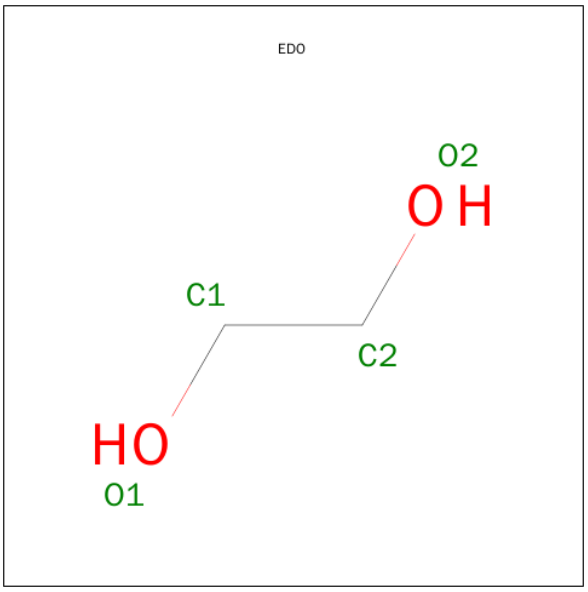
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	O	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 6 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



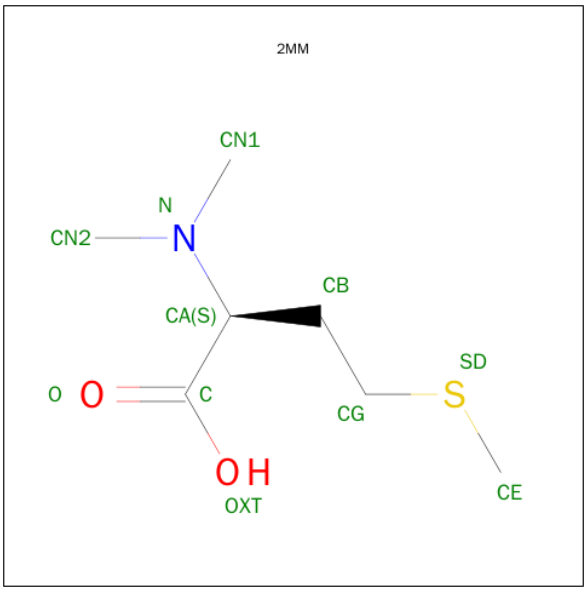
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
6	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is N,N-DIMETHYL-L-METHIONINE (three-letter code: 2MM) (formula: $C_7H_{15}NO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O S 10 7 1 1 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	F	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
8	J	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
8	M	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

- Molecule 9 is water.

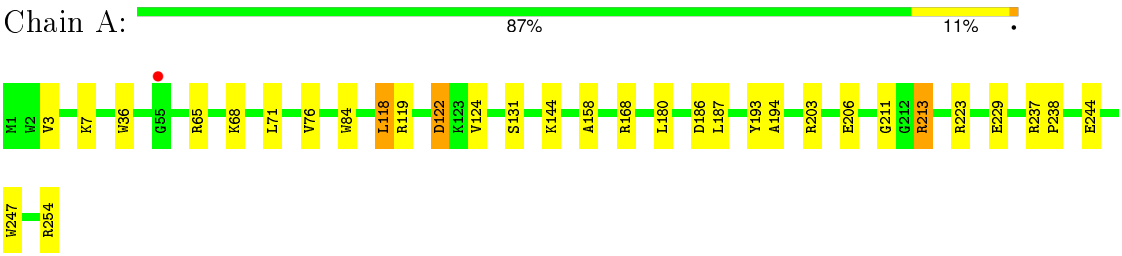
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	263	Total	O	0	5
			268	268		
9	B	87	Total	O	0	2
			89	89		
9	C	173	Total	O	0	0
			173	173		
9	D	25	Total	O	0	0
			25	25		
9	E	248	Total	O	0	0
			248	248		
9	F	61	Total	O	0	0
			61	61		
9	G	198	Total	O	0	0
			198	198		
9	H	22	Total	O	0	0
			22	22		
9	I	200	Total	O	0	0
			200	200		
9	J	67	Total	O	0	0
			67	67		
9	K	142	Total	O	0	0
			142	142		
9	L	10	Total	O	0	0
			10	10		
9	M	193	Total	O	0	0
			193	193		
9	N	46	Total	O	0	0
			46	46		
9	O	145	Total	O	0	0
			145	145		
9	P	5	Total	O	0	0
			5	5		

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.

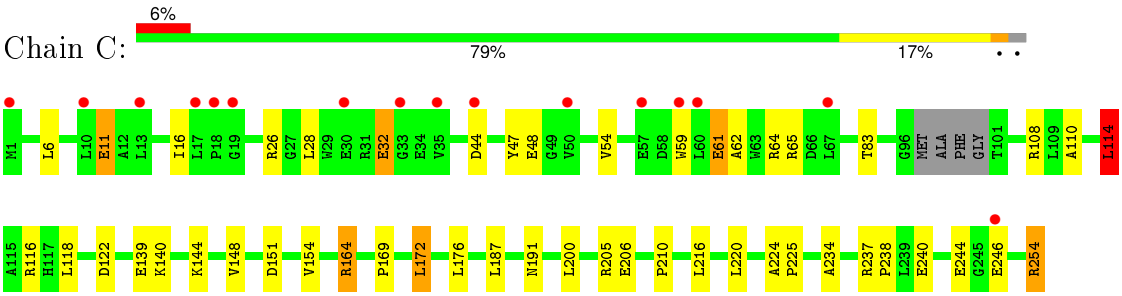
- Molecule 1: Ribosomal protein L11 methyltransferase

Chain A:



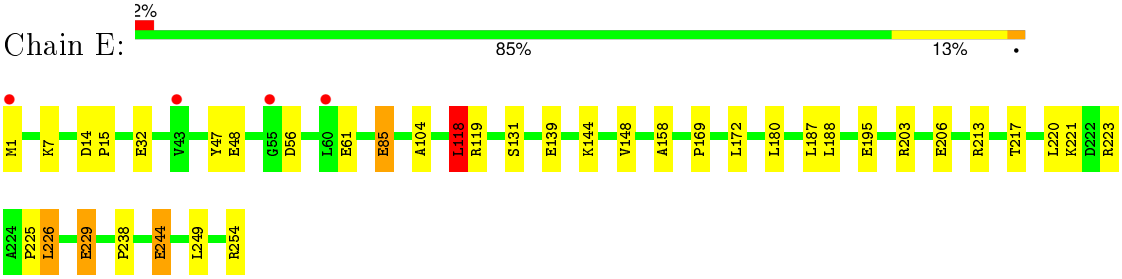
- Molecule 1: Ribosomal protein L11 methyltransferase

Chain C:



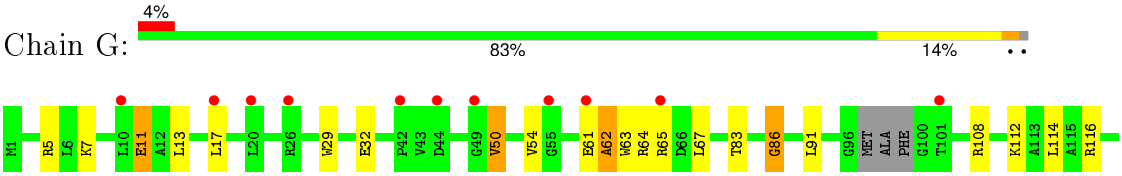
- Molecule 1: Ribosomal protein L11 methyltransferase

Chain E:



- Molecule 1: Ribosomal protein L11 methyltransferase

Chain G:

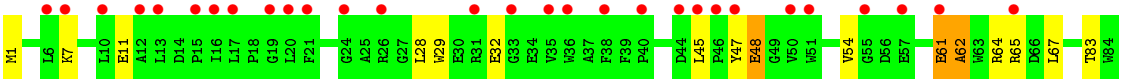


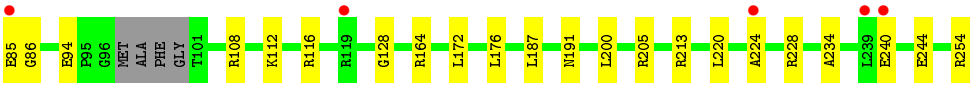
• Molecule 1: Ribosomal protein L11 methyltransferase

Chain I:

• Molecule 1: Ribosomal protein L11 methyltransferase

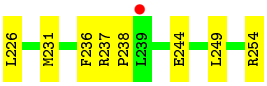
Chain K:





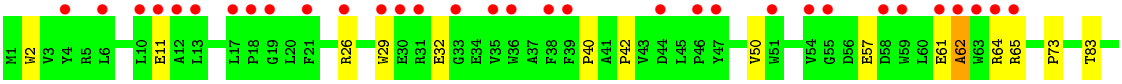
• Molecule 1: Ribosomal protein L11 methyltransferase

Chain M:



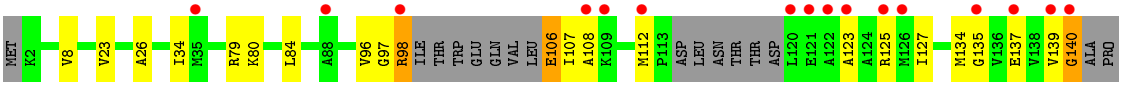
• Molecule 1: Ribosomal protein L11 methyltransferase

Chain O:



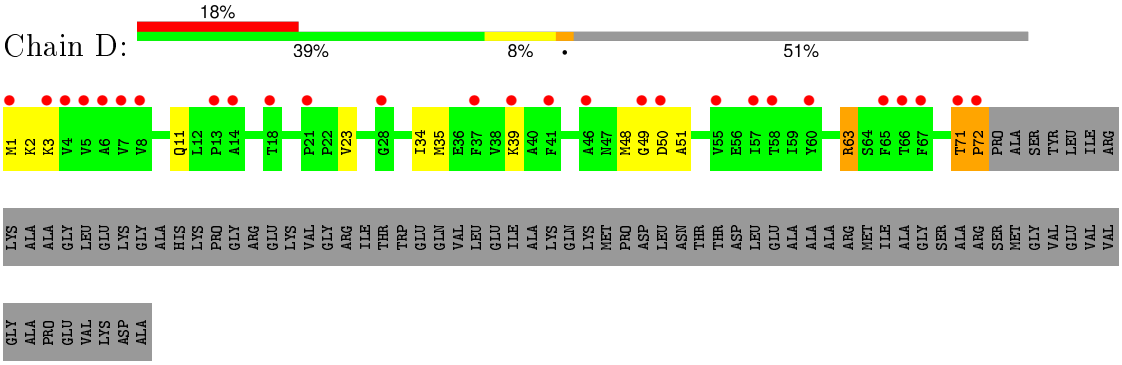
• Molecule 2: 50S ribosomal protein L11

Chain B:



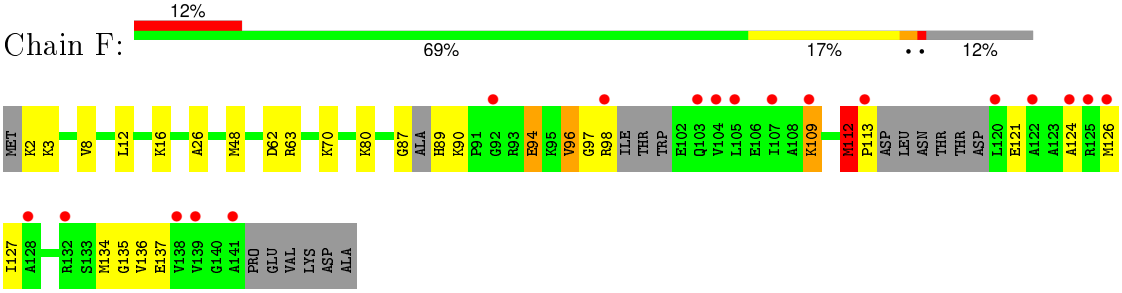
- Molecule 2: 50S ribosomal protein L11

Chain D:



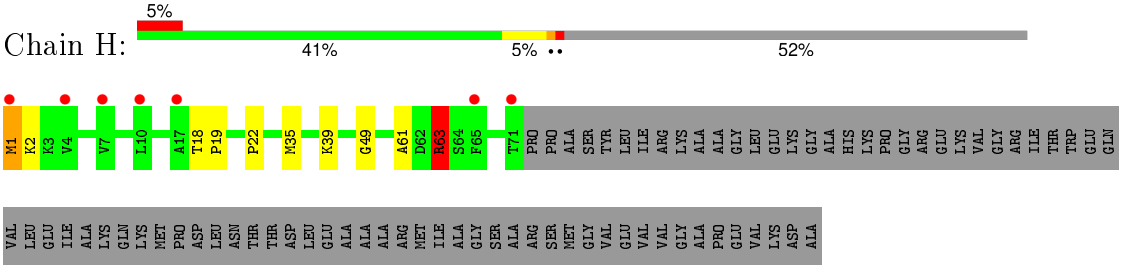
- Molecule 2: 50S ribosomal protein L11

Chain F:



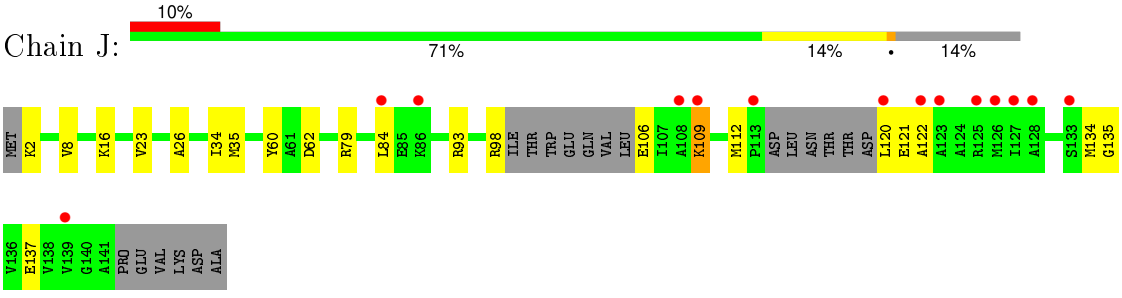
- Molecule 2: 50S ribosomal protein L11

Chain H:



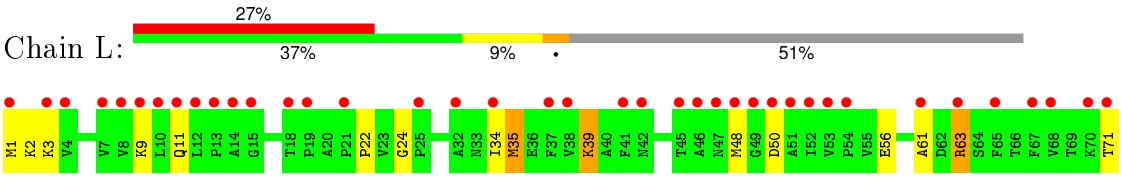
- Molecule 2: 50S ribosomal protein L11

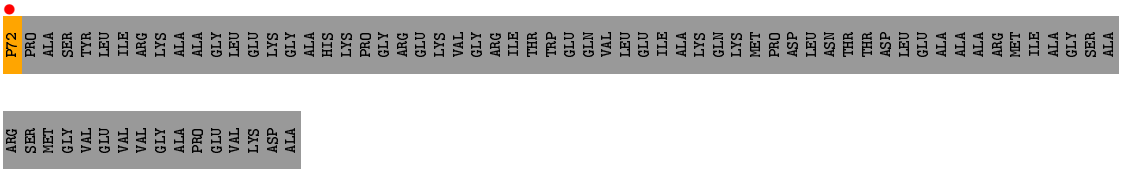
Chain J:



- Molecule 2: 50S ribosomal protein L11

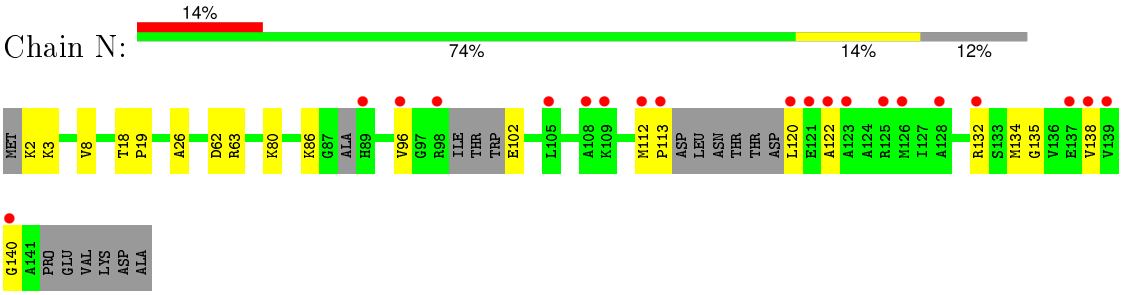
Chain L:





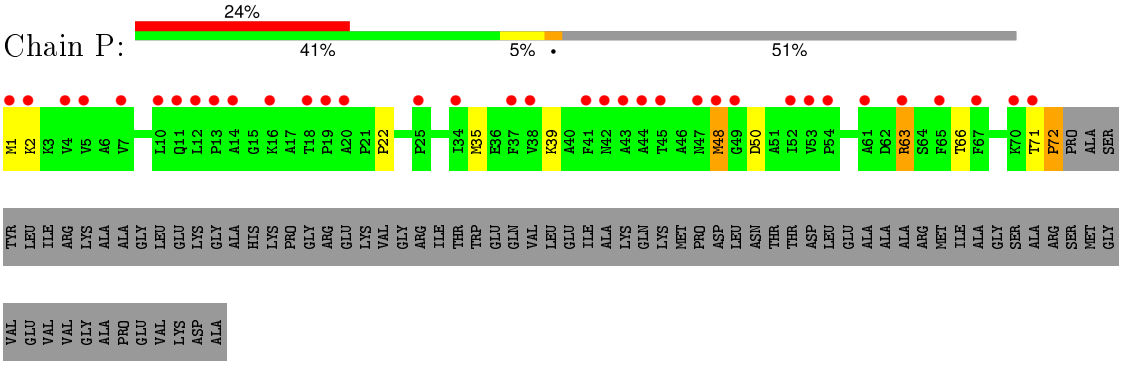
• Molecule 2: 50S ribosomal protein L11

Chain N:



• Molecule 2: 50S ribosomal protein L11

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.82Å 69.94Å 379.01Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	29.74 – 2.30 29.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.74-2.30) 94.1 (29.73-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.259 0.190 , 0.251	Depositor DCC
R_{free} test set	7898 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 31.4	EDS
Estimated twinning fraction	0.407 for -k,-h,-l 0.410 for k,h,-l 0.387 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 157884 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23555	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: SAH, SAM, CL, EDO, 2MM, NO3

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	0.67	1/2025 (0.0%)	0.73	4/2761 (0.1%)
1	C	2.15	4/1976 (0.2%)	0.84	5/2694 (0.2%)
1	E	0.67	2/2009 (0.1%)	0.74	1/2739 (0.0%)
1	G	2.25	3/1980 (0.2%)	0.86	4/2699 (0.1%)
1	I	0.59	0/2017	0.70	1/2750 (0.0%)
1	K	2.08	4/1976 (0.2%)	0.77	3/2694 (0.1%)
1	M	0.60	0/2017	0.70	2/2750 (0.1%)
1	O	1.67	4/1976 (0.2%)	0.77	5/2694 (0.2%)
2	B	2.00	2/936 (0.2%)	0.84	1/1261 (0.1%)
2	D	1.56	2/536 (0.4%)	1.31	5/730 (0.7%)
2	F	0.62	2/964 (0.2%)	0.70	0/1298
2	H	0.86	2/531 (0.4%)	2.78	4/723 (0.6%)
2	J	0.54	0/937	0.67	0/1264
2	L	1.52	3/536 (0.6%)	1.14	4/730 (0.5%)
2	N	0.53	1/960 (0.1%)	0.62	0/1294
2	P	0.96	2/536 (0.4%)	1.17	5/730 (0.7%)
All	All	1.43	32/21912 (0.1%)	0.90	44/29811 (0.1%)

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	C	0	1
1	G	0	1
2	D	0	1
2	H	0	1
2	L	0	1
2	P	0	1
All	All	0	6

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	11	GLU	CD-OE1	77.43	2.10	1.25
1	C	11	GLU	CD-OE1	71.32	2.04	1.25
1	K	11	GLU	CG-CD	62.97	2.46	1.51
2	B	140	GLY	C-O	58.07	2.16	1.23
1	G	11	GLU	CD-OE2	56.12	1.87	1.25
1	C	11	GLU	CD-OE2	54.90	1.86	1.25
1	K	11	GLU	CD-OE2	52.45	1.83	1.25
1	O	11	GLU	CD-OE1	50.35	1.81	1.25
1	O	11	GLU	CD-OE2	41.38	1.71	1.25
2	D	63	ARG	CZ-NH2	33.51	1.76	1.33
1	K	32	GLU	CB-CG	25.67	2.00	1.52
2	L	35	MET	SD-CE	25.11	3.18	1.77
1	K	11	GLU	CD-OE1	23.07	1.51	1.25
1	O	11	GLU	CG-CD	22.25	1.85	1.51
2	L	63	ARG	CZ-NH2	16.27	1.54	1.33
2	P	39	LYS	CD-CE	15.82	1.90	1.51
2	L	39	LYS	CD-CE	-14.69	1.14	1.51
2	H	39	LYS	CD-CE	-14.08	1.16	1.51
1	C	11	GLU	CG-CD	12.67	1.71	1.51
2	P	63	ARG	CZ-NH2	11.34	1.47	1.33
1	C	32	GLU	CB-CG	9.89	1.71	1.52
1	G	11	GLU	CG-CD	-8.72	1.38	1.51
2	H	63	ARG	CZ-NH2	7.97	1.43	1.33
1	O	32	GLU	CB-CG	-7.42	1.38	1.52
2	F	121	GLU	CD-OE2	6.91	1.33	1.25
2	F	121	GLU	CD-OE1	6.70	1.33	1.25
1	A	229	GLU	CG-CD	6.34	1.61	1.51
2	B	140	GLY	CA-C	6.24	1.61	1.51
2	N	80	LYS	CD-CE	6.07	1.66	1.51
1	E	229	GLU	CG-CD	5.72	1.60	1.51
2	D	35	MET	SD-CE	-5.56	1.46	1.77
1	E	244	GLU	CG-CD	5.38	1.60	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	63	ARG	NE-CZ-NH2	-68.41	86.10	120.30
2	D	63	ARG	NE-CZ-NH2	-26.56	107.02	120.30
2	P	63	ARG	NE-CZ-NH2	-22.95	108.82	120.30
2	H	63	ARG	NH1-CZ-NH2	22.45	144.10	119.40
2	L	63	ARG	NH1-CZ-NH2	-22.45	94.70	119.40
1	C	11	GLU	OE1-CD-OE2	-18.11	101.57	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	11	GLU	OE1-CD-OE2	-18.06	101.62	123.30
1	K	11	GLU	CB-CG-CD	-16.57	69.45	114.20
2	B	140	GLY	CA-C-O	-15.92	91.95	120.60
2	L	35	MET	CG-SD-CE	11.94	119.30	100.20
2	D	39	LYS	CD-CE-NZ	11.77	138.76	111.70
2	P	63	ARG	NH1-CZ-NH2	-10.73	107.60	119.40
2	H	39	LYS	CG-CD-CE	10.36	142.97	111.90
1	G	11	GLU	CG-CD-OE2	9.98	138.26	118.30
1	O	32	GLU	CB-CG-CD	-9.79	87.76	114.20
2	D	39	LYS	CG-CD-CE	8.98	138.85	111.90
1	E	118	LEU	CA-CB-CG	8.54	134.95	115.30
2	D	63	ARG	NH1-CZ-NH2	8.49	128.74	119.40
1	C	32	GLU	CA-CB-CG	-8.47	94.77	113.40
2	P	35	MET	CG-SD-CE	8.17	113.27	100.20
1	M	118	LEU	CA-CB-CG	7.82	133.28	115.30
2	H	39	LYS	CD-CE-NZ	-7.51	94.44	111.70
2	P	39	LYS	CG-CD-CE	-6.94	91.08	111.90
1	G	86	GLY	N-CA-C	6.50	129.36	113.10
1	C	11	GLU	CG-CD-OE2	6.48	131.26	118.30
2	P	72	PRO	N-CA-CB	6.36	110.93	103.30
1	G	220	LEU	CA-CB-CG	6.25	129.68	115.30
2	D	72	PRO	N-CA-CB	6.15	110.67	103.30
1	O	11	GLU	OE1-CD-OE2	-6.08	116.01	123.30
2	L	72	PRO	N-CA-CB	6.07	110.58	103.30
2	L	39	LYS	CG-CD-CE	5.88	129.55	111.90
1	O	11	GLU	CB-CG-CD	-5.87	98.36	114.20
1	C	114	LEU	CA-CB-CG	5.85	128.76	115.30
1	O	86	GLY	N-CA-C	5.55	126.99	113.10
1	K	11	GLU	OE1-CD-OE2	5.41	129.79	123.30
1	C	62	ALA	N-CA-C	5.29	125.28	111.00
1	M	67	LEU	CA-CB-CG	5.18	127.20	115.30
1	I	223	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	122	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	K	62	ALA	N-CA-C	5.09	124.76	111.00
1	A	122	ASP	CB-CA-C	5.08	120.56	110.40
1	O	168	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	118[A]	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	118[B]	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11	GLU	Sidechain
2	D	63	ARG	Sidechain
1	G	11	GLU	Sidechain
2	H	63	ARG	Sidechain
2	L	63	ARG	Sidechain
2	P	63	ARG	Sidechain

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	1966	0	1974	27	0
1	C	1922	0	1917	34	0
1	E	1953	0	1953	27	0
1	G	1926	0	1920	24	0
1	I	1961	0	1963	22	0
1	K	1922	0	1917	30	0
1	M	1961	0	1963	22	0
1	O	1922	0	1917	22	0
2	B	921	0	974	13	1
2	D	525	0	549	8	0
2	F	950	0	1001	22	0
2	H	520	0	548	7	0
2	J	922	0	968	14	0
2	L	525	0	549	9	0
2	N	946	0	990	16	0
2	P	525	0	549	5	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	1	0
3	I	8	0	0	0	0
3	M	4	0	0	0	0
3	N	4	0	0	0	0
4	A	2	0	0	0	0
4	I	2	0	0	2	0
5	C	27	0	22	3	0
5	G	27	0	22	2	0
5	K	27	0	22	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	27	0	22	5	0
6	A	26	0	19	0	0
6	E	26	0	19	0	0
6	I	26	0	19	0	0
6	M	26	0	19	0	0
7	A	4	0	6	1	0
7	B	4	0	6	0	0
8	B	10	0	14	2	0
8	F	10	0	14	4	0
8	J	10	0	14	1	0
8	M	10	0	14	9	0
9	A	268	0	0	7	0
9	B	89	0	0	0	0
9	C	173	0	0	7	0
9	D	25	0	0	1	0
9	E	248	0	0	5	0
9	F	61	0	0	3	0
9	G	198	0	0	6	1
9	H	22	0	0	1	0
9	I	200	0	0	7	0
9	J	67	0	0	1	0
9	K	142	0	0	8	0
9	L	10	0	0	1	0
9	M	193	0	0	5	0
9	N	46	0	0	0	0
9	O	145	0	0	2	0
9	P	5	0	0	0	0
All	All	23555	0	21884	290	1

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 7.

All (290) 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:244:GLU:HG3	9:E:297:HOH:O	1.33	1.26
8:M:257:2MM:O	2:N:2:LYS:N	1.78	1.17
1:O:61:GLU:HG3	1:O:65:ARG:HB3	1.38	1.04
1:C:164:ARG:HG2	1:C:164:ARG:HH11	1.25	1.01
2:L:1:MET:H3	2:L:2:LYS:HA	1.31	0.95
1:O:73:PRO:O	1:O:112:LYS:HG2	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:302:SAM:HA	9:C:330:HOH:O	1.71	0.91
2:L:1:MET:N	2:L:2:LYS:HA	1.82	0.90
2:P:1:MET:N	2:P:2:LYS:HA	1.88	0.88
8:M:257:2MM:O	2:N:2:LYS:CA	2.21	0.88
1:C:206:GLU:HG3	9:C:456:HOH:O	1.73	0.87
1:E:187:LEU:HD12	1:E:213:ARG:HB2	1.58	0.86
1:I:244:GLU:HG3	9:I:327:HOH:O	1.75	0.86
1:A:203:ARG:NH1	1:A:206:GLU:OE2	2.09	0.85
1:G:61:GLU:HB2	1:G:64:ARG:HB2	1.55	0.85
2:B:140:GLY:O	2:B:140:GLY:C	2.16	0.84
1:K:61:GLU:HB2	1:K:64:ARG:HB2	1.58	0.84
1:M:187:LEU:HD13	1:M:213:ARG:HB2	1.61	0.82
1:C:61:GLU:HB2	1:C:64:ARG:HB2	1.62	0.81
1:E:238:PRO:HD3	9:E:431:HOH:O	1.79	0.81
2:J:16:LYS:CB	9:J:149:HOH:O	2.29	0.80
1:K:164:ARG:HG2	1:K:164:ARG:HH11	1.47	0.80
1:C:108:ARG:NH1	1:C:244:GLU:OE2	2.15	0.80
1:G:62:ALA:O	1:G:65:ARG:HG2	1.81	0.80
1:K:108:ARG:NH1	1:K:244:GLU:OE2	2.18	0.76
1:A:144:LYS:CD	9:A:517:HOH:O	2.33	0.76
1:A:168:ARG:HG2	9:A:518:HOH:O	1.86	0.76
1:C:61:GLU:H	1:C:64:ARG:H	1.34	0.75
1:M:187:LEU:CD1	1:M:213:ARG:HB2	2.17	0.75
1:E:187:LEU:CD1	1:E:213:ARG:HB2	2.17	0.74
1:C:191:ASN:HB3	5:C:302:SAM:HB2	1.68	0.74
1:G:237:ARG:NH2	9:G:355:HOH:O	1.90	0.73
1:E:47:TYR:O	1:E:48:GLU:HG2	1.87	0.73
1:A:144:LYS:HD2	9:A:517:HOH:O	1.87	0.73
8:M:257:2MM:HA	2:N:2:LYS:N	2.03	0.73
1:I:244:GLU:CG	9:I:327:HOH:O	2.33	0.73
2:F:112:MET:CB	2:F:113:PRO:HD3	2.20	0.72
2:D:1:MET:H3	2:D:2:LYS:HA	1.53	0.71
1:O:73:PRO:O	1:O:112:LYS:CG	2.40	0.70
2:B:106:GLU:HG3	2:B:107:ILE:N	2.06	0.70
1:A:238:PRO:HD3	9:A:400:HOH:O	1.92	0.70
1:A:71:LEU:HD22	1:A:76:VAL:HG23	1.73	0.69
2:N:134:MET:H	2:N:135:GLY:HA2	1.56	0.68
1:O:191:ASN:O	5:O:302:SAM:CE	2.41	0.68
1:I:203:ARG:CZ	1:I:206:GLU:OE2	2.41	0.68
1:O:96:GLY:C	9:O:384:HOH:O	2.31	0.68
8:M:257:2MM:C	2:N:2:LYS:N	2.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187[A]:LEU:HD12	1:A:213:ARG:HB2	1.75	0.67
2:P:1:MET:H3	2:P:2:LYS:HA	1.59	0.67
1:E:203:ARG:CZ	1:E:206:GLU:OE2	2.42	0.66
1:K:94:GLU:OE1	9:K:402:HOH:O	2.12	0.66
1:A:244:GLU:HG2	9:A:464:HOH:O	1.95	0.65
2:J:79:ARG:HG2	2:J:84:LEU:HD12	1.77	0.65
1:K:86:GLY:N	9:K:368:HOH:O	2.30	0.65
2:D:49:GLY:C	2:D:51:ALA:H	1.99	0.65
1:C:61:GLU:HG3	1:C:65:ARG:HB3	1.79	0.64
1:A:119:ARG:HD2	1:C:144:LYS:HD2	1.79	0.64
2:H:1:MET:N	2:H:2:LYS:HA	2.12	0.64
8:M:257:2MM:CA	2:N:2:LYS:N	2.61	0.64
5:K:302:SAM:N	9:K:325:HOH:O	2.30	0.64
1:E:119:ARG:HD2	1:G:144:LYS:HD2	1.78	0.64
1:C:164:ARG:CG	1:C:164:ARG:HH11	2.06	0.64
2:B:106:GLU:HG3	2:B:107:ILE:H	1.61	0.64
1:C:59:TRP:HA	9:D:1842:HOH:O	1.98	0.64
2:N:134:MET:N	2:N:135:GLY:HA2	2.14	0.63
1:K:112:LYS:HG2	1:K:116:ARG:HH21	1.64	0.63
2:F:134:MET:H	2:F:135:GLY:HA2	1.63	0.63
3:F:148:NO3:O1	9:F:756:HOH:O	2.15	0.62
2:H:1:MET:H2	2:H:2:LYS:HA	1.64	0.61
1:C:237:ARG:NH2	9:C:336:HOH:O	1.99	0.61
1:G:116:ARG:NH1	1:G:240:GLU:OE2	2.34	0.61
2:J:121:GLU:HG3	2:J:122:ALA:H	1.66	0.61
1:O:191:ASN:O	5:O:302:SAM:HE1	1.99	0.61
1:O:62:ALA:O	1:O:65:ARG:HG2	2.01	0.61
1:O:61:GLU:HA	1:O:62:ALA:C	2.21	0.61
1:C:246:GLU:OE1	9:C:360:HOH:O	2.17	0.60
1:G:61:GLU:HA	1:G:62:ALA:C	2.21	0.60
1:A:144:LYS:HD3	9:A:517:HOH:O	2.00	0.60
2:P:1:MET:H2	2:P:2:LYS:HA	1.65	0.60
1:A:71:LEU:HD21	1:A:84:TRP:CH2	2.37	0.59
5:O:302:SAM:HE3	9:O:438:HOH:O	2.03	0.58
1:E:148:VAL:HG12	1:E:172:LEU:HB3	1.85	0.58
1:G:61:GLU:HG3	1:G:65:ARG:HB3	1.85	0.58
1:K:191:ASN:O	5:K:302:SAM:HG1	2.04	0.58
2:F:134:MET:N	2:F:135:GLY:HA2	2.17	0.57
1:G:128:GLY:O	5:G:302:SAM:HG2	2.04	0.57
1:I:81:TRP:NE1	9:I:291:HOH:O	2.27	0.56
1:K:85:GLU:C	9:K:368:HOH:O	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:302:SAM:H5'2	9:K:414:HOH:O	2.06	0.56
1:K:47:TYR:O	1:K:48:GLU:HB2	2.04	0.56
1:A:193:TYR:HB3	8:B:149:2MM:HB	1.88	0.56
1:K:224:ALA:O	1:K:228:ARG:HG3	2.04	0.56
2:J:134:MET:N	2:J:135:GLY:HA2	2.19	0.56
1:O:191:ASN:O	5:O:302:SAM:HE2	2.05	0.56
1:E:1:MET:N	1:E:56:ASP:OD1	2.37	0.55
1:O:164:ARG:HH11	1:O:164:ARG:HG2	1.71	0.55
1:K:116:ARG:NH1	1:K:240:GLU:OE2	2.40	0.55
2:F:112:MET:HB3	2:F:113:PRO:HD3	1.87	0.55
2:F:2:LYS:CA	8:F:149:2MM:C	2.78	0.55
1:C:164:ARG:HG2	1:C:164:ARG:NH1	2.04	0.55
1:K:128:GLY:O	5:K:302:SAM:HA	2.06	0.55
1:E:61:GLU:OE1	9:E:362:HOH:O	2.18	0.55
1:G:237:ARG:NE	9:G:355:HOH:O	2.31	0.55
1:A:124:VAL:HG22	1:A:187[A]:LEU:HB3	1.88	0.54
1:C:191:ASN:HD22	5:C:302:SAM:C	2.19	0.54
2:F:98:ARG:HA	2:F:137:GLU:O	2.06	0.54
1:O:61:GLU:HB2	1:O:64:ARG:HB2	1.88	0.54
1:K:1:MET:O	1:K:54:VAL:HG13	2.07	0.54
2:B:134:MET:H	2:B:135:GLY:HA2	1.72	0.54
1:A:144:LYS:HE2	1:E:144:LYS:HG2	1.89	0.54
2:N:62:ASP:O	2:N:63:ARG:HB2	2.08	0.53
1:M:237:ARG:NH1	9:M:367:HOH:O	2.40	0.53
1:I:170:ARG:NH1	4:I:258:CL:CL	2.77	0.53
1:E:220:LEU:HG	8:F:149:2MM:CE	2.39	0.53
1:I:60:LEU:HD11	2:J:35:MET:HG2	1.92	0.52
1:G:238:PRO:HD3	9:G:381:HOH:O	2.10	0.52
1:A:211:GLY:HA3	7:A:259:EDO:H12	1.91	0.52
1:K:61:GLU:H	1:K:64:ARG:H	1.57	0.52
2:N:8:VAL:HG11	2:N:26:ALA:HB1	1.90	0.52
1:G:83:THR:O	1:G:83:THR:HG22	2.09	0.52
2:F:94:GLU:HG3	1:O:89:ILE:HG23	1.92	0.52
1:C:238:PRO:HG2	9:C:475:HOH:O	2.11	0.51
2:J:134:MET:H	2:J:135:GLY:HA2	1.74	0.51
1:I:60:LEU:HD21	2:J:35:MET:HG2	1.92	0.51
1:G:238:PRO:CD	9:G:381:HOH:O	2.59	0.51
2:F:112:MET:HB2	2:F:113:PRO:HD3	1.91	0.51
1:G:191:ASN:O	5:G:302:SAM:HG1	2.10	0.51
1:I:148:VAL:HG12	1:I:172:LEU:HB3	1.92	0.51
1:K:164:ARG:HD2	9:K:394:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:GLY:O	2:D:51:ALA:N	2.43	0.51
1:K:45:LEU:HB3	1:K:47:TYR:CD1	2.46	0.51
1:G:61:GLU:H	1:G:63:TRP:N	2.09	0.50
1:K:85:GLU:HA	9:K:408:HOH:O	2.10	0.50
1:K:164:ARG:NH1	1:K:164:ARG:HG2	2.21	0.50
1:I:103:HIS:HE1	9:I:272:HOH:O	1.93	0.50
1:M:144:LYS:HB2	9:M:375:HOH:O	2.12	0.50
1:C:164:ARG:CG	1:C:164:ARG:NH1	2.71	0.50
2:B:108:ALA:HA	2:B:127:ILE:HD13	1.93	0.50
1:I:5:ARG:NH2	9:I:314:HOH:O	2.45	0.50
2:B:134:MET:N	2:B:135:GLY:HA2	2.26	0.50
1:M:14:ASP:HB3	1:M:15:PRO:HD3	1.94	0.50
1:M:192:LEU:O	8:M:257:2MM:HBA	2.13	0.49
1:M:104:ALA:HB2	2:N:62:ASP:HB3	1.94	0.49
1:A:3:VAL:HG21	1:A:36:TRP:CE3	2.47	0.49
2:B:79:ARG:HG2	2:B:84:LEU:HD12	1.94	0.49
1:E:104:ALA:HB2	2:F:62:ASP:HB3	1.94	0.49
1:C:116:ARG:NH1	1:C:240:GLU:OE2	2.46	0.49
1:K:62:ALA:HB1	9:L:957:HOH:O	2.12	0.49
1:A:187[A]:LEU:CD1	1:A:213:ARG:HB2	2.41	0.49
2:F:112:MET:CB	2:F:113:PRO:CD	2.90	0.49
1:K:83:THR:O	1:K:83:THR:HG22	2.13	0.49
1:C:47:TYR:O	1:C:48:GLU:HB2	2.13	0.49
1:C:140:LYS:HE3	9:C:335:HOH:O	2.12	0.48
1:M:244:GLU:HG2	9:M:299:HOH:O	2.13	0.48
1:M:220:LEU:HD11	8:M:257:2MM:CE	2.43	0.48
1:M:238:PRO:HD3	9:M:355:HOH:O	2.12	0.48
2:D:49:GLY:C	2:D:51:ALA:N	2.66	0.48
1:M:217:THR:HB	1:M:249:LEU:HD12	1.96	0.48
2:J:8:VAL:HG11	2:J:26:ALA:HB1	1.94	0.48
1:K:28:LEU:HB2	2:L:11:GLN:HB2	1.96	0.48
1:C:210:PRO:HA	1:C:254:ARG:HD2	1.95	0.48
2:D:1:MET:N	2:D:2:LYS:HA	2.25	0.48
2:F:96:VAL:CG1	2:F:97:GLY:N	2.77	0.48
1:E:220:LEU:HG	8:F:149:2MM:HEB	1.96	0.48
1:A:194:ALA:CB	1:A:223:ARG:HB3	2.44	0.48
1:A:118[A]:LEU:CD1	1:A:122:ASP:OD1	2.62	0.47
1:A:65:ARG:O	1:A:68:LYS:NZ	2.48	0.47
2:B:23:VAL:HG12	2:B:34:ILE:HG23	1.96	0.47
1:M:17:LEU:HD22	1:M:28:LEU:HD13	1.96	0.47
1:K:29:TRP:HB2	2:L:22:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LEU:HB2	1:E:187:LEU:HD22	1.96	0.47
1:G:205:ARG:HD2	1:G:234:ALA:O	2.15	0.47
1:K:45:LEU:HB3	1:K:47:TYR:HD1	1.80	0.47
1:G:5:ARG:HB2	1:G:50:VAL:HG12	1.97	0.47
1:K:187:LEU:HD12	1:K:213:ARG:HB2	1.96	0.47
2:H:61:ALA:HB3	9:H:161:HOH:O	2.14	0.46
1:I:104:ALA:HB2	2:J:62:ASP:HB3	1.97	0.46
2:J:2:LYS:HB3	2:J:60:TYR:CE1	2.50	0.46
8:M:257:2MM:O	2:N:2:LYS:HA	2.13	0.46
1:A:119:ARG:CD	1:C:144:LYS:HD2	2.44	0.46
1:E:195:GLU:OE2	1:E:223:ARG:HD2	2.15	0.46
2:F:89:HIS:O	2:F:90:LYS:HD2	2.15	0.46
2:F:112:MET:HB3	2:F:113:PRO:CD	2.46	0.46
1:A:122:ASP:HB2	1:A:186:ASP:CB	2.46	0.46
1:O:116:ARG:NH1	1:O:240:GLU:OE2	2.47	0.46
1:C:205:ARG:HD2	1:C:234:ALA:O	2.16	0.46
1:C:83:THR:HG22	1:C:83:THR:O	2.16	0.46
1:A:131:SER:O	1:A:158:ALA:HA	2.16	0.46
1:C:108:ARG:HD2	1:C:244:GLU:OE1	2.15	0.46
2:L:3:LYS:HB2	2:L:61:ALA:HB2	1.98	0.46
2:J:98:ARG:HB3	2:J:137:GLU:HB2	1.98	0.46
1:O:164:ARG:NH1	1:O:164:ARG:HG2	2.30	0.45
1:C:6:LEU:HD13	1:C:16:ILE:HD11	1.98	0.45
1:O:108:ARG:O	1:O:112:LYS:HD3	2.16	0.45
1:C:118:LEU:CD1	1:C:122:ASP:HB2	2.46	0.45
1:C:61:GLU:N	1:C:64:ARG:H	2.08	0.45
2:N:112:MET:HB3	2:N:113:PRO:HD3	1.98	0.45
2:F:8:VAL:HG11	2:F:26:ALA:HB1	1.99	0.45
1:E:118:LEU:HB2	1:E:187:LEU:CD2	2.46	0.45
2:N:102:GLU:HB2	2:N:140:GLY:H	1.82	0.45
2:P:71:THR:HA	2:P:72:PRO:HA	1.72	0.45
2:F:96:VAL:HG13	2:F:97:GLY:H	1.81	0.45
1:C:110:ALA:O	1:C:114:LEU:HB2	2.17	0.45
2:J:109:LYS:HA	2:J:112:MET:HB2	1.98	0.45
1:M:194:ALA:CB	1:M:223:ARG:HB3	2.46	0.45
2:D:71:THR:HA	2:D:72:PRO:HA	1.72	0.45
1:M:105:GLU:HG2	1:M:244:GLU:HG3	1.99	0.45
1:M:59:TRP:HD1	9:M:408:HOH:O	2.00	0.45
1:G:254:ARG:O	1:G:254:ARG:HD3	2.17	0.44
2:B:98:ARG:HA	2:B:137:GLU:O	2.17	0.44
1:E:223:ARG:O	1:E:226:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:108:ARG:HH11	1:O:244:GLU:CD	2.19	0.44
1:I:210:PRO:HA	1:I:254:ARG:HD2	1.98	0.44
1:I:193:TYR:HB3	8:J:148:2MM:HB	1.99	0.44
1:I:223:ARG:NE	9:I:311:HOH:O	2.43	0.44
2:F:62:ASP:O	2:F:63:ARG:HB2	2.17	0.44
1:O:57:GLU:H	1:O:57:GLU:CD	2.20	0.44
1:C:224:ALA:N	1:C:225:PRO:CD	2.80	0.44
1:C:148:VAL:HA	1:C:172:LEU:O	2.18	0.44
1:I:118[A]:LEU:CD1	1:I:122:ASP:HB2	2.48	0.44
1:C:139:GLU:HG3	1:C:169:PRO:HG3	1.99	0.43
2:H:1:MET:N	2:H:2:LYS:CA	2.80	0.43
1:C:237:ARG:NE	9:C:336:HOH:O	2.41	0.43
1:I:127:LEU:HD12	1:I:148:VAL:HG23	1.99	0.43
1:C:151:ASP:O	1:C:154:VAL:HG22	2.18	0.43
2:J:23:VAL:HG12	2:J:34:ILE:HG23	1.99	0.43
1:K:61:GLU:HG3	1:K:65:ARG:HB3	2.01	0.43
1:E:14:ASP:HB3	1:E:15:PRO:HD3	2.00	0.43
1:E:7:LYS:HB2	9:E:278:HOH:O	2.18	0.43
1:K:164:ARG:CG	1:K:164:ARG:HH11	2.25	0.43
1:I:195:GLU:OE2	1:I:223:ARG:HD2	2.18	0.43
1:I:244:GLU:HG2	9:I:327:HOH:O	2.12	0.43
1:M:231:MET:O	1:M:236:PHE:HB2	2.18	0.43
1:I:109:LEU:HD21	1:I:244:GLU:HB2	2.01	0.43
1:G:61:GLU:CA	1:G:62:ALA:C	2.87	0.43
1:C:28:LEU:HB2	2:D:11:GLN:HB2	2.01	0.42
1:O:2:TRP:CG	1:O:42:PRO:HD3	2.54	0.42
1:G:29:TRP:HB2	2:H:22:PRO:HB3	2.01	0.42
2:L:71:THR:HA	2:L:72:PRO:HA	1.70	0.42
1:K:1:MET:HB2	9:K:345:HOH:O	2.19	0.42
2:D:23:VAL:HG12	2:D:34:ILE:HG23	2.01	0.42
1:K:205:ARG:HD2	1:K:234:ALA:O	2.20	0.42
1:O:61:GLU:H	1:O:64:ARG:H	1.66	0.42
1:I:127:LEU:HD12	1:I:148:VAL:CG2	2.50	0.42
1:M:63:TRP:CH2	1:M:81:TRP:CH2	3.07	0.42
1:A:144:LYS:HG2	1:E:144:LYS:HE2	2.01	0.42
2:H:18:THR:HB	2:H:19:PRO:HD2	2.01	0.42
2:L:9:LYS:HG3	2:L:56:GLU:HG2	2.01	0.42
1:G:237:ARG:CZ	9:G:355:HOH:O	2.43	0.42
1:M:3:VAL:HG21	1:M:36:TRP:CE3	2.55	0.42
2:L:24:GLY:HA2	2:L:34:ILE:HD13	2.00	0.42
1:O:254:ARG:O	1:O:254:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:GLU:HG3	1:E:169:PRO:HG3	2.02	0.42
1:M:106:THR:HG21	1:M:218:GLY:HA2	2.02	0.42
1:M:177:GLU:HA	1:M:180:LEU:HD13	2.00	0.41
1:O:29:TRP:HB2	2:P:22:PRO:HB3	2.02	0.41
1:G:224:ALA:N	1:G:225:PRO:CD	2.83	0.41
1:E:119:ARG:HD3	9:G:332:HOH:O	2.20	0.41
2:B:8:VAL:HG11	2:B:26:ALA:HB1	2.03	0.41
2:F:126:MET:O	2:F:127:ILE:HG13	2.20	0.41
2:N:18:THR:HB	2:N:19:PRO:HD2	2.03	0.41
1:A:237:ARG:HD3	9:A:369:HOH:O	2.20	0.41
1:K:67:LEU:HD21	2:L:35:MET:HG3	2.02	0.41
1:K:61:GLU:N	1:K:64:ARG:H	2.18	0.41
2:N:132:ARG:NH2	2:N:138:VAL:HB	2.36	0.41
2:B:96:VAL:CG1	2:B:97:GLY:N	2.83	0.41
2:F:109:LYS:NZ	9:F:689:HOH:O	2.52	0.41
1:G:67:LEU:HD21	2:H:35:MET:HG3	2.03	0.41
2:F:134:MET:HB3	2:F:136:VAL:HG23	2.01	0.41
1:I:176:LEU:O	1:I:180:LEU:HD13	2.20	0.41
2:B:123:ALA:C	2:B:125:ARG:H	2.24	0.41
1:I:217:THR:HB	1:I:249:LEU:HD12	2.02	0.41
2:B:108:ALA:O	2:B:112:MET:HB2	2.21	0.41
1:G:13:LEU:O	1:G:17:LEU:HG	2.21	0.41
8:M:257:2MM:HEB	2:N:3:LYS:HE2	2.03	0.41
2:F:87:GLY:O	2:F:89:HIS:N	2.53	0.41
1:A:247:TRP:CH2	8:B:149:2MM:HG	2.56	0.41
4:I:258:CL:CL	1:M:170:ARG:NH2	2.90	0.40
1:G:180:LEU:HB3	1:G:181:PRO:HD3	2.03	0.40
1:O:26:ARG:HE	1:O:40:PRO:HG3	1.86	0.40
2:J:112:MET:SD	2:J:120:LEU:HA	2.61	0.40
1:E:217:THR:HB	1:E:249:LEU:HD12	2.03	0.40
2:F:2:LYS:N	8:F:149:2MM:O	2.35	0.40
5:O:302:SAM:H4'	5:O:302:SAM:HG2	2.01	0.40
1:A:124:VAL:HG22	1:A:187[B]:LEU:HB3	2.02	0.40
1:M:1:MET:HG2	1:M:39:PHE:O	2.21	0.40
1:E:225:PRO:O	1:E:229:GLU:HG3	2.21	0.40
1:E:131:SER:O	1:E:158:ALA:HA	2.21	0.40
2:F:12:LEU:HD22	9:F:380:HOH:O	2.22	0.40
1:E:85:GLU:HG3	9:E:272:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:MET:O	9:G:459:HOH:O[2_555]	2.15	0.05

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	254/254 (100%)	243 (96%)	11 (4%)	0	100	100
1	C	246/254 (97%)	237 (96%)	8 (3%)	1 (0%)	39	48
1	E	252/254 (99%)	247 (98%)	4 (2%)	1 (0%)	39	48
1	G	247/254 (97%)	238 (96%)	6 (2%)	3 (1%)	16	16
1	I	253/254 (100%)	242 (96%)	11 (4%)	0	100	100
1	K	246/254 (97%)	236 (96%)	8 (3%)	2 (1%)	24	27
1	M	253/254 (100%)	246 (97%)	7 (3%)	0	100	100
1	O	246/254 (97%)	236 (96%)	8 (3%)	2 (1%)	24	27
2	B	120/147 (82%)	112 (93%)	7 (6%)	1 (1%)	24	27
2	D	70/147 (48%)	64 (91%)	4 (6%)	2 (3%)	6	3
2	F	122/147 (83%)	113 (93%)	7 (6%)	2 (2%)	12	11
2	H	69/147 (47%)	65 (94%)	3 (4%)	1 (1%)	14	13
2	J	121/147 (82%)	115 (95%)	6 (5%)	0	100	100
2	L	70/147 (48%)	66 (94%)	4 (6%)	0	100	100
2	N	122/147 (83%)	120 (98%)	1 (1%)	1 (1%)	24	27
2	P	70/147 (48%)	66 (94%)	3 (4%)	1 (1%)	14	13
All	All	2761/3208 (86%)	2646 (96%)	98 (4%)	17 (1%)	30	36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	50	ASP

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Mol	Chain	Res	Type
1	E	32	GLU
2	F	124	ALA
1	G	62	ALA
1	G	86	GLY
2	H	49	GLY
1	O	62	ALA
1	O	86	GLY
1	C	61	GLU
2	D	48	MET
2	F	112	MET
1	G	32	GLU
1	K	61	GLU
2	N	122	ALA
1	K	48	GLU
2	P	48	MET
2	B	139	VAL

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	190/188 (101%)	186 (98%)	4 (2%)	61	78
1	C	185/188 (98%)	172 (93%)	13 (7%)	19	23
1	E	188/188 (100%)	181 (96%)	7 (4%)	41	55
1	G	185/188 (98%)	171 (92%)	14 (8%)	16	20
1	I	189/188 (100%)	181 (96%)	8 (4%)	36	49
1	K	185/188 (98%)	179 (97%)	6 (3%)	46	62
1	M	189/188 (100%)	178 (94%)	11 (6%)	25	33
1	O	185/188 (98%)	172 (93%)	13 (7%)	19	23
2	B	92/111 (83%)	89 (97%)	3 (3%)	45	61
2	D	54/111 (49%)	52 (96%)	2 (4%)	41	55
2	F	95/111 (86%)	86 (90%)	9 (10%)	11	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	54/111 (49%)	52 (96%)	2 (4%)	41 55
2	J	91/111 (82%)	88 (97%)	3 (3%)	45 61
2	L	54/111 (49%)	51 (94%)	3 (6%)	26 35
2	N	94/111 (85%)	91 (97%)	3 (3%)	46 62
2	P	54/111 (49%)	51 (94%)	3 (6%)	26 35
All	All	2084/2392 (87%)	1980 (95%)	104 (5%)	30 41

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	180	LEU
1	A	213	ARG
1	A	254	ARG
2	B	80	LYS
2	B	98	ARG
2	B	106	GLU
1	C	26	ARG
1	C	32	GLU
1	C	44	ASP
1	C	54	VAL
1	C	114	LEU
1	C	164	ARG
1	C	172	LEU
1	C	176	LEU
1	C	187	LEU
1	C	200	LEU
1	C	216	LEU
1	C	220	LEU
1	C	254	ARG
2	D	3	LYS
2	D	71	THR
1	E	85	GLU
1	E	118	LEU
1	E	180	LEU
1	E	188	LEU
1	E	221	LYS
1	E	226	LEU
1	E	254	ARG
2	F	3	LYS

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Mol	Chain	Res	Type
2	F	16	LYS
2	F	48	MET
2	F	70	LYS
2	F	80	LYS
2	F	94	GLU
2	F	96	VAL
2	F	109	LYS
2	F	112	MET
1	G	7	LYS
1	G	50	VAL
1	G	54	VAL
1	G	91	LEU
1	G	108	ARG
1	G	112	LYS
1	G	114	LEU
1	G	140	LYS
1	G	172	LEU
1	G	176	LEU
1	G	200	LEU
1	G	220	LEU
1	G	244	GLU
1	G	254	ARG
2	H	1	MET
2	H	63	ARG
1	I	7	LYS
1	I	56	ASP
1	I	57	GLU
1	I	180	LEU
1	I	213	ARG
1	I	221	LYS
1	I	226	LEU
1	I	254	ARG
2	J	93	ARG
2	J	106	GLU
2	J	109	LYS
1	K	7	LYS
1	K	172	LEU
1	K	176	LEU
1	K	200	LEU
1	K	220	LEU
1	K	254	ARG
2	L	39	LYS

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Mol	Chain	Res	Type
2	L	48	MET
2	L	50	ASP
1	M	56	ASP
1	M	67	LEU
1	M	71	LEU
1	M	83	THR
1	M	118	LEU
1	M	188	LEU
1	M	221	LYS
1	M	223	ARG
1	M	226[A]	LEU
1	M	226[B]	LEU
1	M	254	ARG
2	N	86	LYS
2	N	96	VAL
2	N	120	LEU
1	O	50	VAL
1	O	83	THR
1	O	91	LEU
1	O	101	THR
1	O	114	LEU
1	O	172	LEU
1	O	176	LEU
1	O	177	GLU
1	O	180	LEU
1	O	200	LEU
1	O	216	LEU
1	O	220	LEU
1	O	254	ARG
2	P	48	MET
2	P	50	ASP
2	P	66	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	89	HIS
1	I	103	HIS
1	M	103	HIS
2	N	89	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	$\#\|Z\|>2$
3	NO3	A	255	-	3,3,3	2.72	3 (100%)	3,3,3	0.25	0
6	SAH	A	258	-	20,28,28	0.95	2 (10%)	19,40,40	3.17	2 (10%)
7	EDO	A	259	-	3,3,3	0.56	0	2,2,2	0.17	0
3	NO3	B	148	-	3,3,3	2.88	3 (100%)	3,3,3	0.20	0
8	2MM	B	149	2	7,9,10	0.67	0	6,10,12	1.65	2 (33%)
7	EDO	B	150	-	3,3,3	0.50	0	2,2,2	0.41	0
5	SAM	C	302	-	21,29,29	1.36	2 (9%)	17,42,42	3.19	2 (11%)
3	NO3	E	255	-	3,3,3	2.73	3 (100%)	3,3,3	0.23	0
6	SAH	E	256	-	20,28,28	1.03	2 (10%)	19,40,40	3.69	3 (15%)
3	NO3	F	148	-	3,3,3	2.99	3 (100%)	3,3,3	0.12	0
8	2MM	F	149	2	7,9,10	0.68	0	6,10,12	2.59	4 (66%)
5	SAM	G	302	-	21,29,29	1.21	2 (9%)	17,42,42	3.00	1 (5%)
3	NO3	I	255	-	3,3,3	2.98	3 (100%)	3,3,3	0.27	0
3	NO3	I	256	-	3,3,3	2.66	3 (100%)	3,3,3	0.09	0
6	SAH	I	259	-	20,28,28	0.99	2 (10%)	19,40,40	3.21	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	2MM	J	148	2	7,9,10	0.73	0	6,10,12	1.57	1 (16%)
5	SAM	K	302	-	21,29,29	1.14	2 (9%)	17,42,42	3.36	2 (11%)
3	NO3	M	255	-	3,3,3	2.96	3 (100%)	3,3,3	0.18	0
6	SAH	M	256	-	20,28,28	1.00	2 (10%)	19,40,40	3.57	2 (10%)
8	2MM	M	257	-	7,9,10	0.61	0	6,10,12	2.11	2 (33%)
3	NO3	N	148	-	3,3,3	3.02	3 (100%)	3,3,3	0.47	0
5	SAM	O	302	-	21,29,29	1.22	2 (9%)	17,42,42	3.34	2 (11%)

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	NO3	A	255	-	-	0/0/0/0	0/0/0/0
6	SAH	A	258	-	-	0/7/31/31	0/3/3/3
7	EDO	A	259	-	-	0/1/1/1	0/0/0/0
3	NO3	B	148	-	-	0/0/0/0	0/0/0/0
8	2MM	B	149	2	-	0/6/10/12	0/0/0/0
7	EDO	B	150	-	-	0/1/1/1	0/0/0/0
5	SAM	C	302	-	-	0/8/33/33	0/3/3/3
3	NO3	E	255	-	-	0/0/0/0	0/0/0/0
6	SAH	E	256	-	-	0/7/31/31	0/3/3/3
3	NO3	F	148	-	-	0/0/0/0	0/0/0/0
8	2MM	F	149	2	-	0/6/10/12	0/0/0/0
5	SAM	G	302	-	-	0/8/33/33	0/3/3/3
3	NO3	I	255	-	-	0/0/0/0	0/0/0/0
3	NO3	I	256	-	-	0/0/0/0	0/0/0/0
6	SAH	I	259	-	-	0/7/31/31	0/3/3/3
8	2MM	J	148	2	-	0/6/10/12	0/0/0/0
5	SAM	K	302	-	-	0/8/33/33	0/3/3/3
3	NO3	M	255	-	-	0/0/0/0	0/0/0/0
6	SAH	M	256	-	-	0/7/31/31	0/3/3/3
8	2MM	M	257	-	-	0/6/10/12	0/0/0/0
3	NO3	N	148	-	-	0/0/0/0	0/0/0/0
5	SAM	O	302	-	-	0/8/33/33	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	256	NO3	O3-N	2.05	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	256	NO3	O2-N	2.22	1.36	1.25
3	A	255	NO3	O3-N	2.30	1.37	1.25
6	A	258	SAH	C2-N1	2.35	1.38	1.33
3	E	255	NO3	O3-N	2.42	1.37	1.25
6	E	256	SAH	C2-N1	2.48	1.38	1.33
3	F	148	NO3	O2-N	2.48	1.38	1.25
3	B	148	NO3	O3-N	2.50	1.38	1.25
3	E	255	NO3	O2-N	2.50	1.38	1.25
6	I	259	SAH	C2-N1	2.51	1.38	1.33
6	M	256	SAH	C2-N1	2.53	1.38	1.33
3	M	255	NO3	O2-N	2.53	1.38	1.25
3	B	148	NO3	O2-N	2.57	1.38	1.25
6	I	259	SAH	C2-N3	2.59	1.36	1.32
3	M	255	NO3	O3-N	2.60	1.38	1.25
5	K	302	SAM	C2-N1	2.62	1.38	1.33
3	A	255	NO3	O2-N	2.65	1.39	1.25
3	F	148	NO3	O3-N	2.65	1.39	1.25
3	I	255	NO3	O2-N	2.65	1.39	1.25
6	A	258	SAH	C2-N3	2.66	1.36	1.32
3	N	148	NO3	O2-N	2.72	1.39	1.25
3	I	255	NO3	O3-N	2.86	1.40	1.25
3	N	148	NO3	O3-N	2.87	1.40	1.25
5	O	302	SAM	C2-N1	2.97	1.39	1.33
5	G	302	SAM	C2-N1	3.11	1.39	1.33
5	C	302	SAM	C2-N1	3.12	1.39	1.33
3	A	255	NO3	O1-N	3.16	1.37	1.24
3	E	255	NO3	O1-N	3.19	1.37	1.24
6	M	256	SAH	C2-N3	3.20	1.37	1.32
6	E	256	SAH	C2-N3	3.30	1.38	1.32
3	I	255	NO3	O1-N	3.37	1.38	1.24
3	N	148	NO3	O1-N	3.43	1.38	1.24
3	B	148	NO3	O1-N	3.47	1.38	1.24
3	I	256	NO3	O1-N	3.47	1.38	1.24
5	G	302	SAM	C2-N3	3.55	1.38	1.32
3	M	255	NO3	O1-N	3.62	1.39	1.24
5	K	302	SAM	C2-N3	3.62	1.38	1.32
3	F	148	NO3	O1-N	3.69	1.39	1.24
5	C	302	SAM	C2-N3	3.82	1.38	1.32
5	O	302	SAM	C2-N3	3.89	1.39	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	256	SAH	N3-C2-N1	-15.56	116.98	128.89
6	M	256	SAH	N3-C2-N1	-14.67	117.67	128.89
6	I	259	SAH	N3-C2-N1	-13.25	118.75	128.89
5	K	302	SAM	N3-C2-N1	-13.21	118.78	128.89
5	O	302	SAM	N3-C2-N1	-13.10	118.86	128.89
6	A	258	SAH	N3-C2-N1	-13.00	118.94	128.89
5	C	302	SAM	N3-C2-N1	-12.51	119.32	128.89
5	G	302	SAM	N3-C2-N1	-11.87	119.81	128.89
8	F	149	2MM	CB-CA-C	-4.16	105.94	111.59
8	M	257	2MM	CB-CA-C	-3.76	106.48	111.59
6	M	256	SAH	C5'-SD-CG	-3.06	93.23	102.41
6	A	258	SAH	C5'-SD-CG	-3.01	93.36	102.41
6	I	259	SAH	C5'-SD-CG	-2.51	94.87	102.41
5	K	302	SAM	C1'-N9-C4	-2.48	123.19	126.94
5	O	302	SAM	C4-C5-N7	-2.43	107.24	109.48
8	F	149	2MM	CG-CB-CA	-2.43	109.49	113.22
5	C	302	SAM	O4'-C4'-C5'	-2.04	103.45	108.90
6	E	256	SAH	C5'-SD-CG	-2.02	96.34	102.41
8	B	149	2MM	CB-CA-C	2.18	114.55	111.59
6	E	256	SAH	C2-N1-C6	2.38	123.02	118.77
8	J	148	2MM	CB-CA-C	2.42	114.87	111.59
8	F	149	2MM	CB-CA-N	2.45	117.15	113.36
8	B	149	2MM	CG-CB-CA	2.64	117.28	113.22
8	M	257	2MM	CE-SD-CG	2.90	110.25	100.37
8	F	149	2MM	CE-SD-CG	3.32	111.71	100.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	259	EDO	1	0
8	B	149	2MM	2	0
5	C	302	SAM	3	0
3	F	148	NO3	1	0
8	F	149	2MM	4	0
5	G	302	SAM	2	0
8	J	148	2MM	1	0
5	K	302	SAM	4	0
8	M	257	2MM	9	0
5	O	302	SAM	5	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	254/254 (100%)	0.42	1 (0%) 93 95	19, 28, 43, 56	1 (0%)
1	C	250/254 (98%)	0.90	16 (6%) 23 31	23, 32, 67, 70	2 (0%)
1	E	254/254 (100%)	0.54	4 (1%) 74 80	20, 29, 45, 59	0
1	G	251/254 (98%)	0.71	11 (4%) 38 47	22, 32, 66, 70	2 (0%)
1	I	254/254 (100%)	0.31	0 100 100	25, 32, 45, 57	0
1	K	250/254 (98%)	0.88	34 (13%) 4 6	28, 38, 81, 83	2 (0%)
1	M	254/254 (100%)	0.27	1 (0%) 93 95	25, 33, 48, 62	0
1	O	250/254 (98%)	0.85	35 (14%) 4 6	28, 37, 78, 81	2 (0%)
2	B	126/147 (85%)	0.84	16 (12%) 5 8	22, 39, 80, 92	0
2	D	72/147 (48%)	1.81	27 (37%) 0 0	62, 70, 86, 90	2 (2%)
2	F	130/147 (88%)	1.02	18 (13%) 4 6	23, 48, 92, 98	0
2	H	71/147 (48%)	1.17	7 (9%) 9 14	62, 68, 85, 90	2 (2%)
2	J	127/147 (86%)	0.80	14 (11%) 7 11	25, 42, 83, 92	0
2	L	72/147 (48%)	2.58	40 (55%) 0 0	76, 84, 100, 100	2 (2%)
2	N	130/147 (88%)	0.80	20 (15%) 3 4	27, 50, 91, 100	0
2	P	72/147 (48%)	2.66	35 (48%) 0 0	78, 82, 98, 100	2 (2%)
All	All	2817/3208 (87%)	0.80	279 (9%) 9 14	19, 35, 83, 100	17 (0%)

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	10	LEU	9.9
2	P	4	VAL	9.8
2	P	71	THR	9.0
2	B	125	ARG	8.9
2	B	126	MET	8.0

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Mol	Chain	Res	Type	RSRZ
2	P	49	GLY	7.8
1	O	12	ALA	7.8
2	F	126	MET	7.5
2	L	37	PHE	7.4
1	K	12	ALA	7.4
1	O	10	LEU	7.1
2	N	113	PRO	7.0
2	J	126	MET	6.9
2	L	1	MET	6.9
1	C	10	LEU	6.8
2	P	38	VAL	6.7
1	K	44	ASP	6.6
2	N	125	ARG	6.5
1	O	17	LEU	6.3
2	L	41	PHE	6.2
2	F	139	VAL	6.0
2	P	1	MET	5.7
1	O	35	VAL	5.7
2	P	43	ALA	5.7
1	K	13	LEU	5.7
2	D	1	MET	5.7
2	P	37	PHE	5.6
1	K	7	LYS	5.6
2	L	19	PRO	5.5
2	F	120	LEU	5.5
2	P	47	ASN	5.5
1	K	19	GLY	5.4
2	F	105	LEU	5.3
2	L	14	ALA	5.3
2	P	41	PHE	5.2
1	G	10	LEU	5.1
1	O	13	LEU	5.1
2	N	121	GLU	5.1
2	D	67	PHE	5.0
2	L	65	PHE	5.0
2	P	54	PRO	5.0
2	L	50	ASP	5.0
2	D	71	THR	5.0
2	F	104	VAL	5.0
2	F	138	VAL	5.0
2	P	53	VAL	5.0
2	F	128	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
2	F	141	ALA	4.9
2	F	109	LYS	4.9
2	P	65	PHE	4.9
1	C	19	GLY	4.6
2	P	14	ALA	4.5
2	P	13	PRO	4.5
2	L	21	PRO	4.5
1	C	44	ASP	4.5
2	H	1	MET	4.5
2	D	72	PRO	4.5
2	B	139	VAL	4.5
2	L	52	ILE	4.4
2	P	10	LEU	4.4
2	H	71	THR	4.4
1	K	31	ARG	4.3
1	A	55	GLY	4.3
1	O	62	ALA	4.3
2	N	126	MET	4.3
2	L	34	ILE	4.3
2	J	123	ALA	4.3
2	P	19	PRO	4.3
1	C	35	VAL	4.3
1	G	17	LEU	4.3
2	H	65	PHE	4.3
2	J	108	ALA	4.2
2	F	122	ALA	4.2
2	L	49	GLY	4.2
2	J	139	VAL	4.2
2	L	8	VAL	4.2
2	L	72	PRO	4.2
2	P	12	LEU	4.2
1	O	51	TRP	4.1
1	K	20	LEU	4.1
2	L	13	PRO	4.1
1	K	26	ARG	4.1
2	L	71	THR	4.1
2	N	109	LYS	4.1
2	P	7	VAL	4.1
2	N	122	ALA	4.1
2	J	125	ARG	4.1
1	O	61	GLU	4.1
2	L	15	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	57	ILE	4.0
1	O	18	PRO	3.9
2	D	55	VAL	3.9
2	P	44	ALA	3.9
2	L	38	VAL	3.9
1	O	44	ASP	3.8
2	D	28	GLY	3.8
2	L	47	ASN	3.7
2	B	121	GLU	3.7
2	L	45	THR	3.7
2	B	35	MET	3.7
2	B	120	LEU	3.7
2	N	132	ARG	3.7
2	L	25	PRO	3.7
1	E	55	GLY	3.6
2	D	4	VAL	3.6
1	K	35	VAL	3.6
1	K	55	GLY	3.6
2	F	125	ARG	3.6
2	N	139	VAL	3.6
1	O	55	GLY	3.6
2	L	61	ALA	3.5
2	P	48	MET	3.5
2	F	103	GLN	3.5
2	P	18	THR	3.5
1	M	239	LEU	3.4
2	N	105	LEU	3.4
1	K	40	PRO	3.4
2	L	18	THR	3.4
1	O	59	TRP	3.3
2	N	108	ALA	3.3
2	L	48	MET	3.3
2	N	120	LEU	3.3
2	P	52	ILE	3.3
1	O	101	THR	3.3
2	P	20	ALA	3.3
2	L	12	LEU	3.3
2	L	11	GLN	3.3
2	L	4	VAL	3.3
1	K	45	LEU	3.2
1	K	46	PRO	3.2
1	K	17	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	122	ALA	3.2
1	O	26	ARG	3.2
2	J	127	ILE	3.2
1	C	18	PRO	3.2
1	O	58	ASP	3.2
2	P	34	ILE	3.2
1	K	15	PRO	3.2
2	L	32	ALA	3.2
2	P	63	ARG	3.2
1	G	26	ARG	3.1
2	B	122	ALA	3.1
2	D	66	THR	3.1
2	L	42	ASN	3.1
1	K	24	GLY	3.1
1	O	65	ARG	3.0
1	O	46	PRO	3.0
1	O	38	PHE	3.0
1	K	57	GLU	3.0
2	D	65	PHE	3.0
2	P	67	PHE	3.0
1	C	30	GLU	3.0
1	K	65	ARG	2.9
1	G	55	GLY	2.9
2	D	46	ALA	2.9
2	N	112	MET	2.9
1	K	38	PHE	2.9
2	L	63	ARG	2.9
2	L	10	LEU	2.9
1	O	54	VAL	2.9
2	B	140	GLY	2.8
2	D	3	LYS	2.8
2	H	7	VAL	2.8
1	C	50	VAL	2.8
1	K	239	LEU	2.8
2	J	109	LYS	2.8
1	K	224	ALA	2.8
2	F	113	PRO	2.8
2	N	89	HIS	2.8
2	D	39	LYS	2.8
2	P	45	THR	2.8
1	K	6	LEU	2.8
2	D	41	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	36	TRP	2.8
2	N	137	GLU	2.8
2	L	9	LYS	2.7
2	L	54	PRO	2.7
2	D	5	VAL	2.7
1	C	13	LEU	2.7
2	L	67	PHE	2.7
1	K	33	GLY	2.7
2	D	7	VAL	2.7
2	D	8	VAL	2.7
2	L	68	VAL	2.6
2	B	88	ALA	2.6
2	F	92	GLY	2.6
2	P	16	LYS	2.6
1	O	21	PHE	2.6
1	O	30	GLU	2.6
1	O	63	TRP	2.6
2	J	86	LYS	2.6
1	K	85	GLU	2.6
2	H	17	ALA	2.6
2	P	61	ALA	2.6
1	O	6	LEU	2.6
2	N	96	VAL	2.6
1	G	61	GLU	2.5
1	K	47	TYR	2.5
2	L	7	VAL	2.5
2	J	128	ALA	2.5
2	B	109	LYS	2.5
2	N	140	GLY	2.5
2	B	137	GLU	2.5
2	L	53	VAL	2.5
2	P	42	ASN	2.5
1	O	11	GLU	2.5
2	D	14	ALA	2.5
2	L	3	LYS	2.5
1	K	21	PHE	2.5
2	N	138	VAL	2.4
2	F	132	ARG	2.4
1	E	43	VAL	2.4
1	O	157	GLN	2.4
2	N	98	ARG	2.4
1	G	44	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	20	LEU	2.4
2	D	60	TYR	2.4
1	C	57	GLU	2.4
2	P	25	PRO	2.4
1	O	119	ARG	2.4
1	G	101	THR	2.4
2	F	98	ARG	2.4
1	C	59	TRP	2.4
2	D	13	PRO	2.4
2	L	46	ALA	2.4
1	O	19	GLY	2.3
2	P	5	VAL	2.3
2	P	70	LYS	2.3
2	D	18	THR	2.3
2	D	37	PHE	2.3
1	O	36	TRP	2.3
2	H	10	LEU	2.3
1	G	42	PRO	2.3
1	O	47	TYR	2.3
2	H	4	VAL	2.3
1	G	49	GLY	2.3
1	O	64	ARG	2.3
2	F	107	ILE	2.3
2	B	98	ARG	2.3
2	B	135	GLY	2.3
1	O	31	ARG	2.3
1	K	16	ILE	2.2
2	L	51	ALA	2.2
2	L	70	LYS	2.2
1	O	29	TRP	2.2
1	K	50	VAL	2.2
1	O	4	TYR	2.2
1	O	39	PHE	2.2
1	O	33	GLY	2.2
2	D	58	THR	2.2
1	K	51	TRP	2.2
2	J	133	SER	2.2
1	K	119	ARG	2.2
1	C	67	LEU	2.2
2	B	112	MET	2.2
2	B	108	ALA	2.2
2	D	6	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	21	PRO	2.2
1	C	17	LEU	2.2
2	F	124	ALA	2.2
1	C	1	MET	2.2
1	K	61	GLU	2.2
2	P	2	LYS	2.1
1	K	240	GLU	2.1
2	P	11	GLN	2.1
1	E	1	MET	2.1
1	C	33	GLY	2.1
2	J	113	PRO	2.1
1	C	246	GLU	2.1
2	D	50	ASP	2.1
2	N	123	ALA	2.1
2	D	49	GLY	2.1
1	E	60	LEU	2.0
2	J	84	LEU	2.0
1	C	60	LEU	2.0
1	G	65	ARG	2.0
2	B	123	ALA	2.0
2	J	120	LEU	2.0
2	N	128	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NO3	N	148	4/4	0.92	0.30	6.46	38,39,39,39	0
3	NO3	M	255	4/4	0.94	0.20	5.31	30,30,31,33	0
7	EDO	B	150	4/4	0.39	0.24	4.87	81,81,82,82	0
8	2MM	M	257	10/11	0.92	0.21	3.20	37,39,40,43	0
5	SAM	K	302	27/27	0.92	0.18	1.98	34,41,54,57	0
3	NO3	E	255	4/4	0.95	0.23	1.88	23,24,25,27	0
5	SAM	O	302	27/27	0.85	0.18	1.74	36,39,56,58	0
3	NO3	I	256	4/4	0.92	0.17	1.58	25,26,26,27	0
5	SAM	C	302	27/27	0.85	0.19	0.45	31,35,56,57	0
6	SAH	M	256	26/26	0.94	0.14	0.11	21,27,28,29	0
8	2MM	J	148	10/11	0.91	0.15	-0.01	27,30,38,39	0
5	SAM	G	302	27/27	0.88	0.16	-0.23	30,33,54,55	0
3	NO3	I	255	4/4	0.95	0.14	-0.33	32,32,32,32	0
6	SAH	I	259	26/26	0.91	0.13	-0.73	22,25,28,29	0
3	NO3	A	255	4/4	0.96	0.15	-0.88	27,27,28,29	0
3	NO3	F	148	4/4	0.91	0.15	-1.01	37,38,38,38	0
8	2MM	B	149	10/11	0.92	0.14	-1.22	23,25,37,37	0
4	CL	I	257	1/1	0.84	0.10	-1.31	53,53,53,53	0
3	NO3	B	148	4/4	0.97	0.15	-1.38	30,30,31,31	0
8	2MM	F	149	10/11	0.88	0.14	-1.95	26,28,38,38	0
6	SAH	E	256	26/26	0.94	0.11	-2.35	18,22,24,24	0
6	SAH	A	258	26/26	0.96	0.08	-4.84	17,21,23,25	0
4	CL	A	257	1/1	0.93	0.06	-7.08	47,47,47,47	0
4	CL	A	256	1/1	0.96	0.09	-	47,47,47,47	0
4	CL	I	258	1/1	0.87	0.12	-	48,48,48,48	0
7	EDO	A	259	4/4	0.83	0.29	-	74,74,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.