Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:10 PM BST

PDB ID	:	6IV8
Title	:	the selenomethionine(SeMet)-derived Cas13d binary complex
Authors	:	Zhang, B.; Ye, Y.M.; Ye, W.W.; OuYang, S.Y.
Deposited on	:	2018-12-02
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

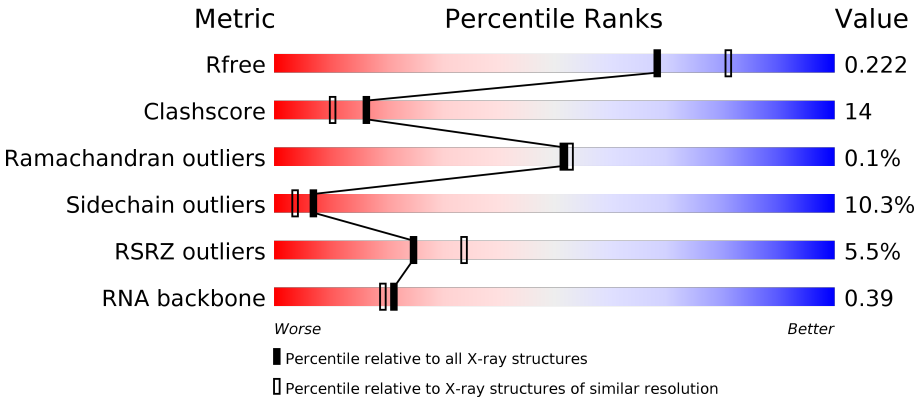
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)
RNA backbone	3102	1060 (2.60-1.72)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	930	2% 74% 16% • 7%
1	C	930	8% 61% 24% 7% • 7%
2	B	51	8% 29% 33% 20% 18%
3	D	53	8% 36% 36% 25% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16939 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 The selenomethionine (SeMet)-labeled Cas13d.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	Se	0	0	0
			7065	4494	1195	1341	10	25			
1	C	862	Total	C	N	O	S	Se	0	0	0
			7011	4465	1188	1323	10	25			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ALA	ARG	engineered mutation	UNP A0A1C5SD84
A	823	ALA	ARG	engineered mutation	UNP A0A1C5SD84
A	923	LEU	-	expression tag	UNP A0A1C5SD84
A	924	GLU	-	expression tag	UNP A0A1C5SD84
A	925	HIS	-	expression tag	UNP A0A1C5SD84
A	926	HIS	-	expression tag	UNP A0A1C5SD84
A	927	HIS	-	expression tag	UNP A0A1C5SD84
A	928	HIS	-	expression tag	UNP A0A1C5SD84
A	929	HIS	-	expression tag	UNP A0A1C5SD84
A	930	HIS	-	expression tag	UNP A0A1C5SD84
C	288	ALA	ARG	engineered mutation	UNP A0A1C5SD84
C	823	ALA	ARG	engineered mutation	UNP A0A1C5SD84
C	923	LEU	-	expression tag	UNP A0A1C5SD84
C	924	GLU	-	expression tag	UNP A0A1C5SD84
C	925	HIS	-	expression tag	UNP A0A1C5SD84
C	926	HIS	-	expression tag	UNP A0A1C5SD84
C	927	HIS	-	expression tag	UNP A0A1C5SD84
C	928	HIS	-	expression tag	UNP A0A1C5SD84
C	929	HIS	-	expression tag	UNP A0A1C5SD84
C	930	HIS	-	expression tag	UNP A0A1C5SD84

- Molecule 2 is a RNA chain called RNA (51-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	51	Total	C	N	O	P	0	0	0
			1077	484	190	352	51			

- Molecule 3 is a RNA chain called RNA (53-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	53	Total	C	N	O	P	0	0	0
			1119	503	198	365	53			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

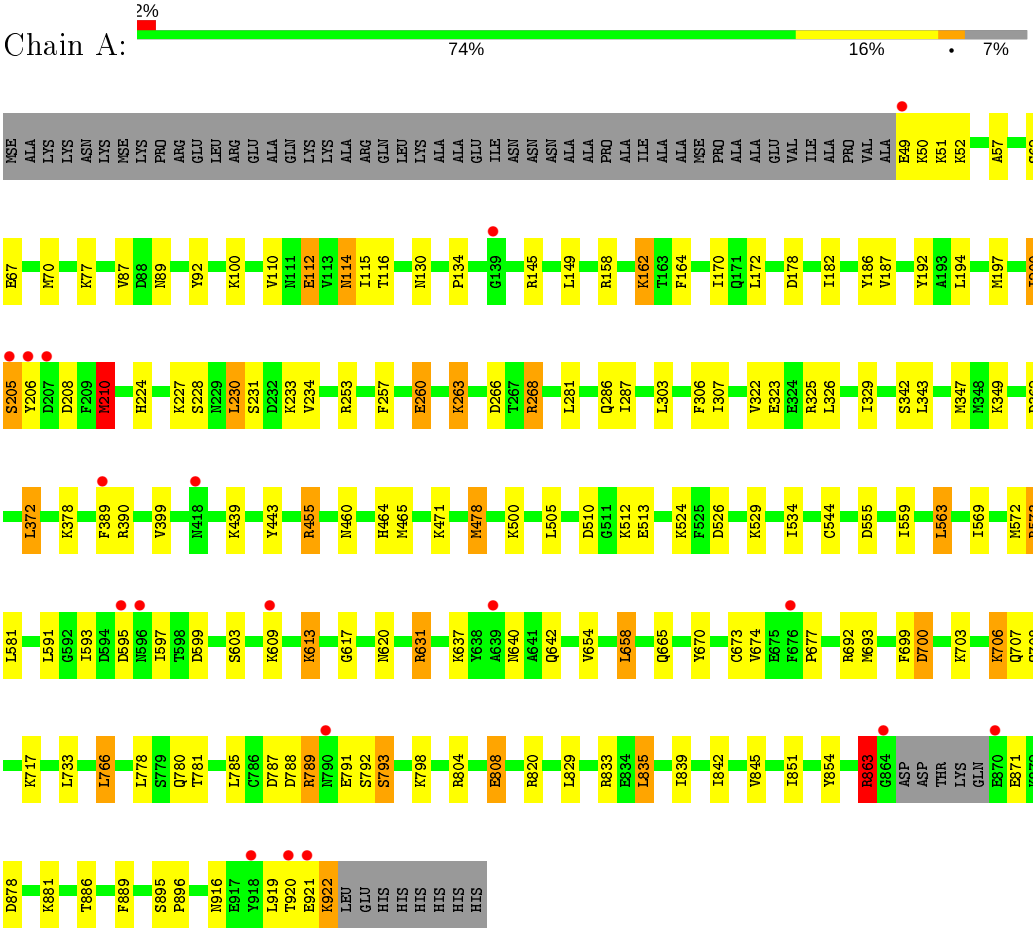
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	444	Total	O	0	0
			444	444		
5	B	106	Total	O	0	0
			106	106		
5	D	46	Total	O	0	0
			46	46		
5	C	69	Total	O	0	0
			69	69		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

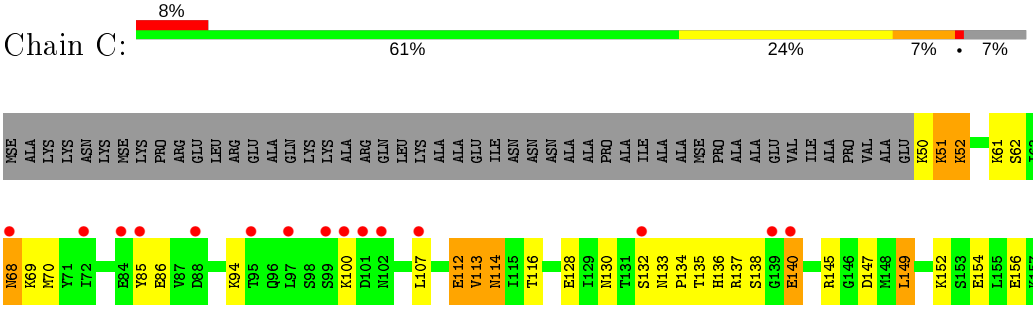
- Molecule 1: The selenomethionine (SeMet)-labeled Cas13d

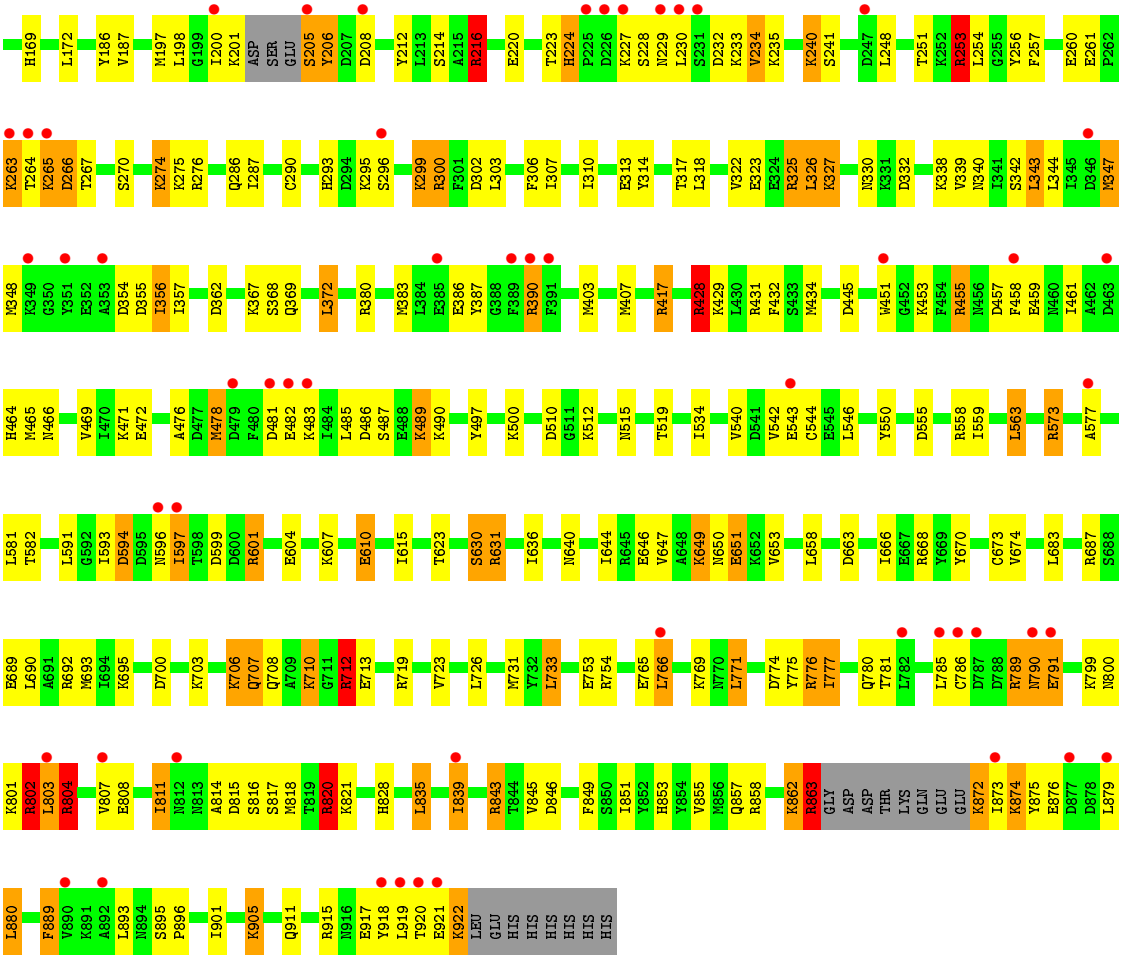
Chain A:



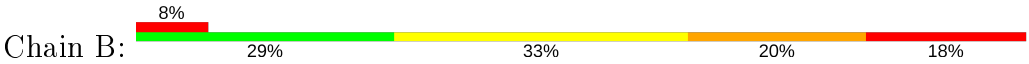
- Molecule 1: The selenomethionine (SeMet)-labeled Cas13d

Chain C:





- Molecule 2: RNA (51-MER)



- Molecule 3: RNA (53-MER)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.16Å 145.73Å 249.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.92 – 2.15 62.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (62.92-2.15) 99.6 (62.91-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.53 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.189 , 0.210 0.194 , 0.222	Depositor DCC
R_{free} test set	6600 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16939	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.93	2/7153 (0.0%)	0.82	4/9550 (0.0%)
1	C	0.71	0/7098	0.81	8/9475 (0.1%)
2	B	1.19	12/1203 (1.0%)	1.48	30/1869 (1.6%)
3	D	1.14	8/1250 (0.6%)	1.01	5/1942 (0.3%)
All	All	0.88	22/16704 (0.1%)	0.90	47/22836 (0.2%)

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	15
1	C	0	28
All	All	0	43

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	-9	G	O3'-P	-10.32	1.48	1.61
2	B	-17	U	C2'-O2'	8.80	1.53	1.41
2	B	10	A	O3'-P	-7.76	1.51	1.61
3	D	-7	C	O3'-P	-7.76	1.51	1.61
3	D	-8	U	O3'-P	-7.70	1.51	1.61
3	D	-3	A	O3'-P	-7.55	1.52	1.61
3	D	-10	A	O3'-P	-6.95	1.52	1.61
3	D	-4	A	O3'-P	-6.82	1.52	1.61
2	B	-28	C	P-OP2	-6.66	1.37	1.49
2	B	-19	A	C2'-O2'	5.96	1.49	1.41
2	B	-10	A	P-OP1	-5.64	1.39	1.49
2	B	-8	U	O3'-P	-5.62	1.54	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	-27	U	O3'-P	5.48	1.67	1.61
2	B	17	C	O5'-C5'	-5.46	1.34	1.42
1	A	513	GLU	CD-OE2	-5.45	1.19	1.25
3	D	10	A	O3'-P	-5.36	1.54	1.61
2	B	13	U	P-OP2	-5.35	1.39	1.49
2	B	-16	U	P-OP2	-5.29	1.40	1.49
3	D	-5	A	O3'-P	-5.21	1.54	1.61
1	A	808	GLU	CD-OE1	-5.15	1.20	1.25
2	B	12	A	O3'-P	-5.10	1.55	1.61
2	B	-14	C	P-OP1	-5.05	1.40	1.49

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	-17	U	O5'-P-OP1	-16.73	90.62	110.70
2	B	-22	C	O5'-P-OP1	12.10	125.22	110.70
3	D	18	A	O5'-P-OP2	-10.55	96.21	105.70
2	B	-24	U	O5'-P-OP2	-9.58	97.08	105.70
2	B	-17	U	O5'-P-OP2	9.31	121.87	110.70
2	B	-23	G	O5'-P-OP2	9.06	121.58	110.70
3	D	10	A	O5'-P-OP2	8.88	121.36	110.70
2	B	-23	G	O5'-P-OP1	-8.71	97.86	105.70
2	B	-30	C	O5'-P-OP2	8.47	120.86	110.70
2	B	-22	C	O5'-P-OP2	-8.33	98.21	105.70
2	B	1	U	O5'-P-OP2	-8.13	98.38	105.70
2	B	20	A	O5'-P-OP1	-8.06	98.45	105.70
1	C	266	ASP	CB-CA-C	-8.05	94.31	110.40
2	B	3	C	O5'-P-OP2	-7.98	98.52	105.70
2	B	-1	C	O5'-P-OP2	-7.97	98.53	105.70
1	A	210	MSE	CG-SE-CE	-7.73	81.89	98.90
2	B	-6	U	O5'-P-OP1	-7.70	98.77	105.70
3	D	-27	U	O5'-P-OP2	-6.86	99.53	105.70
2	B	-3	A	O5'-P-OP2	-6.80	99.58	105.70
2	B	-24	U	O5'-P-OP1	6.69	118.73	110.70
2	B	15	C	O5'-P-OP2	-6.53	99.82	105.70
2	B	-19	A	O5'-P-OP2	6.44	118.42	110.70
2	B	-18	U	O5'-P-OP2	-6.28	100.05	105.70
2	B	-17	U	N1-C1'-C2'	6.19	122.05	114.00
1	C	347	MSE	CB-CG-SE	-6.10	94.40	112.70
2	B	-5	A	O5'-P-OP2	-6.09	100.22	105.70
1	C	818	MSE	N-CA-CB	-6.06	99.70	110.60
2	B	9	U	C2'-C3'-O3'	5.86	123.08	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	-16	U	O5'-P-OP1	5.84	117.71	110.70
1	A	210	MSE	CA-CB-CG	-5.83	103.38	113.30
2	B	17	C	C2'-C3'-O3'	5.79	122.96	113.70
2	B	-14	C	O5'-P-OP2	5.59	117.41	110.70
1	C	265	LYS	CB-CA-C	5.57	121.54	110.40
3	D	-16	U	O5'-P-OP1	5.56	117.38	110.70
2	B	-16	U	O5'-P-OP2	-5.54	100.71	105.70
2	B	-14	C	C2'-C3'-O3'	5.45	122.42	113.70
2	B	-1	C	OP2-P-O3'	5.42	117.13	105.20
3	D	19	A	C2'-C3'-O3'	5.37	122.29	113.70
2	B	17	C	O5'-P-OP1	-5.34	100.89	105.70
2	B	-26	G	O5'-P-OP2	-5.33	100.91	105.70
1	C	186	TYR	CB-CA-C	5.23	120.86	110.40
1	C	347	MSE	CB-CA-C	-5.13	100.13	110.40
1	A	347	MSE	N-CA-CB	-5.06	101.50	110.60
1	C	354	ASP	CB-CA-C	5.05	120.51	110.40
1	A	186	TYR	CB-CA-C	5.04	120.48	110.40
2	B	-15	G	O5'-P-OP1	5.03	116.73	110.70
1	C	497	TYR	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ARG	Sidechain
1	A	158	ARG	Sidechain
1	A	253	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	325	ARG	Sidechain
1	A	390	ARG	Sidechain
1	A	455	ARG	Sidechain
1	A	573	ARG	Sidechain
1	A	631	ARG	Sidechain
1	A	692	ARG	Sidechain
1	A	789	ARG	Sidechain
1	A	804	ARG	Sidechain
1	A	820	ARG	Sidechain
1	A	833	ARG	Sidechain
1	A	863	ARG	Sidechain
1	C	145	ARG	Sidechain
1	C	158	ARG	Sidechain
1	C	216	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	253	ARG	Sidechain
1	C	300	ARG	Sidechain
1	C	325	ARG	Sidechain
1	C	380	ARG	Sidechain
1	C	390	ARG	Sidechain
1	C	417	ARG	Sidechain
1	C	428	ARG	Sidechain
1	C	455	ARG	Sidechain
1	C	558	ARG	Sidechain
1	C	573	ARG	Sidechain
1	C	601	ARG	Sidechain
1	C	631	ARG	Sidechain
1	C	668	ARG	Sidechain
1	C	692	ARG	Sidechain
1	C	712	ARG	Sidechain
1	C	719	ARG	Sidechain
1	C	754	ARG	Sidechain
1	C	776	ARG	Sidechain
1	C	789	ARG	Sidechain
1	C	802	ARG	Sidechain
1	C	804	ARG	Sidechain
1	C	820	ARG	Sidechain
1	C	843	ARG	Sidechain
1	C	863	ARG	Sidechain
1	C	915	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	7065	0	7131	113	0
1	C	7011	0	7094	290	0
2	B	1077	0	549	34	0
3	D	1119	0	571	39	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	444	0	0	5	0
5	B	106	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	69	0	0	0	0
5	D	46	0	0	1	0
All	All	16939	0	15345	452	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 14.

All (452) 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:C:876:GLU:HG3	1:C:880:LEU:HD11	1.20	1.14
1:C:137:ARG:NH2	1:C:140:GLU:HG2	1.65	1.10
1:C:342:SER:HB3	1:C:478:MSE:HE3	1.31	1.08
2:B:-30:C:H4'	2:B:-29:A:H5'	1.33	1.07
1:C:263:LYS:HE3	1:C:263:LYS:H	1.15	1.07
1:C:876:GLU:O	1:C:880:LEU:HD12	1.55	1.06
1:C:70:MSE:CE	1:C:135:THR:HG23	1.85	1.05
1:C:70:MSE:HE3	1:C:135:THR:CG2	1.86	1.04
1:C:342:SER:HB3	1:C:478:MSE:CE	1.88	1.03
1:C:597:ILE:HD11	1:C:601:ARG:HG2	1.40	1.02
3:D:-30:C:H4'	3:D:-29:A:H5'	1.42	1.01
1:A:792:SER:CB	1:A:798:LYS:HE3	1.92	0.99
1:C:670:TYR:O	1:C:674:VAL:HG22	1.63	0.98
1:C:70:MSE:HE3	1:C:135:THR:HG23	1.00	0.98
3:D:-18:U:H4'	3:D:-17:U:OP1	1.63	0.98
1:C:876:GLU:HG3	1:C:880:LEU:CD1	1.95	0.96
1:C:113:VAL:HG12	1:C:136:HIS:CD2	2.00	0.96
1:C:789:ARG:HE	1:C:791:GLU:HG2	1.28	0.96
1:C:651:GLU:OE2	1:C:695:LYS:HD3	1.64	0.96
1:C:70:MSE:HE2	1:C:134:PRO:HG2	1.47	0.95
1:C:70:MSE:HE1	1:C:133:ASN:OD1	1.64	0.95
1:C:342:SER:CB	1:C:478:MSE:CE	2.44	0.95
1:C:874:LYS:HD2	1:C:874:LYS:H	1.31	0.94
2:B:-22:C:H5"	2:B:-22:C:H6	1.32	0.92
3:D:-22:C:H5"	3:D:-22:C:H6	1.33	0.91
1:A:922:LYS:HD2	2:B:-30:C:H2'	1.54	0.90
1:C:653:VAL:HG21	1:C:839:ILE:HD12	1.52	0.89
1:C:137:ARG:HH21	1:C:140:GLU:HG2	1.27	0.89
1:C:113:VAL:CG1	1:C:136:HIS:NE2	2.35	0.89
1:C:876:GLU:CG	1:C:880:LEU:HD11	2.02	0.89
1:C:263:LYS:CE	1:C:263:LYS:H	1.87	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:GLU:OE1	1:C:765:GLU:N	2.05	0.88
1:A:329:ILE:HD11	1:A:572:MSE:SE	2.23	0.88
1:C:113:VAL:CG1	1:C:136:HIS:CD2	2.58	0.87
1:C:803:LEU:HD12	1:C:901:ILE:HG21	1.58	0.86
1:C:137:ARG:NH2	1:C:140:GLU:CG	2.39	0.86
1:C:712:ARG:HG2	1:C:712:ARG:NH1	1.88	0.86
1:C:803:LEU:CD1	1:C:901:ILE:HG21	2.06	0.85
1:C:347:MSE:HE1	1:C:461:ILE:HG13	1.59	0.85
1:C:113:VAL:HG13	1:C:136:HIS:CE1	2.12	0.85
1:C:650:ASN:HD22	1:C:653:VAL:H	1.23	0.85
1:A:792:SER:HB2	1:A:798:LYS:HE3	1.57	0.84
1:C:251:THR:HB	1:C:253:ARG:HD2	1.59	0.83
1:C:597:ILE:CD1	1:C:601:ARG:HG2	2.08	0.83
1:C:807:VAL:O	1:C:811:ILE:HG12	1.77	0.83
1:A:70:MSE:HE1	1:A:115:ILE:HD11	1.61	0.83
1:C:607:LYS:HB3	1:C:610:GLU:HG3	1.61	0.83
1:C:263:LYS:HE3	1:C:263:LYS:N	1.94	0.82
3:D:-16:U:H4'	3:D:-16:U:OP1	1.76	0.82
1:C:338:LYS:HB2	1:C:478:MSE:HG3	1.60	0.82
1:C:807:VAL:HG12	1:C:811:ILE:HD11	1.61	0.81
1:C:835:LEU:HD21	1:C:839:ILE:HG13	1.61	0.81
1:C:808:GLU:HA	1:C:811:ILE:HG13	1.61	0.81
3:D:10:A:N1	1:C:630:SER:HB2	1.96	0.80
1:C:786:CYS:HB3	1:C:804:ARG:CZ	2.11	0.80
1:A:706:LYS:HE3	1:A:708:GLN:H	1.45	0.80
1:C:293:HIS:ND1	1:C:753:GLU:HB3	1.98	0.78
1:C:857:GLN:HB3	1:C:879:LEU:CD2	2.13	0.78
1:C:228:SER:OG	1:C:230:LEU:HD13	1.83	0.78
1:C:197:MSE:HE1	1:C:257:PHE:CZ	2.19	0.78
1:A:863:ARG:NH1	1:A:863:ARG:HG2	1.98	0.77
1:C:200:ILE:HD12	1:C:200:ILE:O	1.84	0.77
1:C:789:ARG:HE	1:C:791:GLU:CG	1.96	0.77
1:A:197:MSE:HE1	1:A:257:PHE:CE2	2.20	0.77
1:C:786:CYS:HB3	1:C:804:ARG:NH1	2.01	0.76
1:C:113:VAL:HG13	1:C:136:HIS:NE2	1.99	0.76
3:D:-19:A:C2	3:D:-18:U:H5"	2.21	0.76
1:A:200:ILE:HG23	1:A:202:ASP:H	1.51	0.76
1:C:874:LYS:H	1:C:874:LYS:CD	1.94	0.76
1:A:362:ASP:HA	1:A:366:LEU:HD23	1.68	0.75
1:C:342:SER:CB	1:C:478:MSE:HE1	2.17	0.74
1:A:670:TYR:O	1:A:674:VAL:HG22	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:-30:C:C4'	2:B:-29:A:H5'	2.16	0.74
1:C:785:LEU:HB3	1:C:791:GLU:O	1.87	0.73
3:D:-19:A:H2'	3:D:-19:A:N3	2.02	0.73
1:A:921:GLU:OE1	2:B:-30:C:N4	2.21	0.73
1:C:781:THR:O	1:C:785:LEU:HD13	1.87	0.73
1:C:403:MSE:HG3	1:C:465:MSE:HG3	1.70	0.72
1:C:646:GLU:OE1	1:C:649:LYS:NZ	2.21	0.72
1:C:789:ARG:C	1:C:791:GLU:H	1.94	0.71
1:C:653:VAL:CG2	1:C:839:ILE:CD1	2.68	0.71
1:A:785:LEU:HB3	1:A:791:GLU:HB2	1.73	0.71
1:C:338:LYS:HE2	1:C:476:ALA:O	1.91	0.71
1:C:835:LEU:O	1:C:839:ILE:HB	1.91	0.71
1:C:403:MSE:O	1:C:407:MSE:HG3	1.90	0.71
1:C:876:GLU:O	1:C:880:LEU:CD1	2.37	0.71
1:C:857:GLN:HB3	1:C:879:LEU:HD22	1.71	0.70
1:C:922:LYS:N	1:C:922:LYS:HE2	2.06	0.70
1:C:786:CYS:HB2	1:C:804:ARG:HD3	1.72	0.70
1:C:889:PHE:CE1	1:C:893:LEU:HD11	2.27	0.70
1:A:260:GLU:HG3	1:A:577:ALA:HB1	1.74	0.69
1:C:187:VAL:HG11	1:C:287:ILE:HG22	1.75	0.69
1:C:653:VAL:CG2	1:C:839:ILE:HD12	2.22	0.69
3:D:-22:C:H5"	3:D:-22:C:C6	2.24	0.68
1:C:650:ASN:ND2	1:C:653:VAL:H	1.91	0.68
2:B:-22:C:C5'	2:B:-22:C:H6	2.06	0.68
1:C:653:VAL:HG21	1:C:839:ILE:CD1	2.24	0.67
1:C:152:LYS:O	1:C:156:GLU:HG3	1.95	0.67
1:A:792:SER:CA	1:A:798:LYS:HE3	2.24	0.67
1:C:789:ARG:C	1:C:791:GLU:N	2.46	0.67
1:C:94:LYS:CD	1:C:107:LEU:HD23	2.25	0.67
3:D:-22:C:C5'	3:D:-22:C:H6	2.06	0.67
1:C:51:LYS:HB2	1:C:51:LYS:NZ	2.09	0.67
1:C:791:GLU:OE1	1:C:791:GLU:HA	1.94	0.66
1:C:428:ARG:HD3	1:C:432:PHE:CZ	2.30	0.66
1:C:290:CYS:O	1:C:299:LYS:HD2	1.96	0.66
1:C:835:LEU:CD2	1:C:839:ILE:HB	2.25	0.66
1:A:569:ILE:O	1:A:572:MSE:HB2	1.97	0.64
1:C:650:ASN:ND2	1:C:653:VAL:HG23	2.12	0.64
1:C:803:LEU:CD1	1:C:901:ILE:CG2	2.76	0.64
1:C:466:ASN:HD21	1:C:469:VAL:HG23	1.63	0.64
3:D:-26:G:H8	3:D:-26:G:H5"	1.62	0.64
1:C:70:MSE:HE2	1:C:134:PRO:CG	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:HB2	1:C:216:ARG:NH1	2.12	0.63
1:A:257:PHE:HE1	1:A:637:LYS:HD2	1.63	0.63
3:D:-19:A:N3	3:D:-18:U:H5"	2.13	0.63
2:B:17:C:H6	2:B:17:C:H5"	1.63	0.63
1:A:70:MSE:HG3	1:A:89:ASN:OD1	1.98	0.63
1:A:613:LYS:HG3	1:A:613:LYS:O	1.96	0.62
1:C:789:ARG:NE	1:C:791:GLU:HG2	2.09	0.62
2:B:-30:C:H1'	5:B:286:HOH:O	1.99	0.62
1:C:224:HIS:HB3	1:C:227:LYS:HB2	1.81	0.62
1:C:260:GLU:HG3	1:C:577:ALA:HB1	1.81	0.62
1:C:116:THR:HG23	1:C:128:GLU:HG2	1.81	0.62
1:C:835:LEU:CD2	1:C:839:ILE:HG13	2.29	0.62
1:C:653:VAL:HG22	1:C:839:ILE:HD11	1.82	0.61
1:A:70:MSE:HE1	1:A:115:ILE:CD1	2.30	0.61
1:C:228:SER:OG	1:C:230:LEU:CD1	2.47	0.61
2:B:9:U:OP2	2:B:10:A:C4'	2.49	0.61
2:B:-22:C:H5"	2:B:-22:C:C6	2.25	0.61
1:C:70:MSE:CE	1:C:134:PRO:HG2	2.27	0.61
1:C:270:SER:O	1:C:274:LYS:HG3	2.01	0.61
1:A:366:LEU:HD22	1:A:366:LEU:N	2.17	0.60
1:C:342:SER:HB2	1:C:478:MSE:CE	2.31	0.60
1:A:707:GLN:NE2	1:A:707:GLN:HA	2.16	0.60
1:C:67:GLU:C	1:C:68:ASN:HD22	2.05	0.60
1:C:920:THR:HG22	1:C:920:THR:O	2.01	0.60
1:A:674:VAL:HG23	1:A:677:PRO:HB3	1.83	0.60
3:D:-22:C:C5'	3:D:-22:C:C6	2.84	0.60
1:A:329:ILE:CD1	1:A:572:MSE:SE	2.99	0.59
1:C:230:LEU:HB3	1:C:234:VAL:HG11	1.84	0.59
1:C:876:GLU:CG	1:C:880:LEU:CD1	2.74	0.59
3:D:10:A:N1	1:C:630:SER:CB	2.64	0.59
1:C:212:TYR:HE2	1:C:240:LYS:HD2	1.68	0.59
1:A:194:LEU:HD13	1:A:210:MSE:HE1	1.84	0.58
1:A:789:ARG:HB3	1:A:789:ARG:HH21	1.68	0.58
1:C:248:LEU:HD21	1:C:254:LEU:HD21	1.85	0.58
1:C:390:ARG:HH11	1:C:390:ARG:CG	2.16	0.58
3:D:-23:G:H5"	3:D:-23:G:H8	1.67	0.58
1:C:771:LEU:CD2	1:C:775:TYR:HA	2.34	0.58
1:C:342:SER:CA	1:C:478:MSE:HE1	2.34	0.57
1:A:286:GLN:HG2	1:A:306:PHE:CE2	2.40	0.57
1:C:647:VAL:HG12	1:C:731:MSE:HE1	1.85	0.57
3:D:9:U:OP2	3:D:10:A:O4'	2.21	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:LEU:HD13	1:A:781:THR:HG21	1.86	0.57
1:C:253:ARG:HG2	1:C:253:ARG:NH2	2.19	0.57
1:A:114:ASN:HD21	1:A:130:ASN:HB3	1.69	0.57
1:C:544:CYS:O	1:C:544:CYS:SG	2.62	0.57
1:C:863:ARG:NH2	1:C:863:ARG:HG2	2.19	0.57
1:A:792:SER:HA	1:A:798:LYS:HE3	1.85	0.57
1:C:863:ARG:HH21	1:C:863:ARG:HG2	1.69	0.57
1:C:872:LYS:HD3	1:C:873:ILE:O	2.05	0.57
1:A:842:ILE:HG12	1:A:854:TYR:CD2	2.39	0.57
1:C:52:LYS:O	1:C:434:MSE:HE1	2.05	0.57
1:C:857:GLN:HB3	1:C:879:LEU:HD21	1.84	0.57
1:C:483:LYS:HA	1:C:486:ASP:OD1	2.05	0.56
3:D:-30:C:H2'	3:D:-30:C:O2	2.04	0.56
1:C:653:VAL:HG22	1:C:839:ILE:CD1	2.35	0.56
1:C:807:VAL:O	1:C:811:ILE:CG1	2.50	0.56
1:C:451:TRP:CE2	1:C:455:ARG:HB2	2.40	0.56
1:A:62:SER:HB2	5:B:250:HOH:O	2.05	0.56
1:A:707:GLN:HE21	1:A:707:GLN:HA	1.71	0.56
1:C:201:LYS:O	1:C:205:SER:OG	2.20	0.56
1:C:94:LYS:HD2	1:C:107:LEU:HD23	1.87	0.55
1:C:789:ARG:HE	1:C:791:GLU:CB	2.19	0.55
1:A:573:ARG:CZ	2:B:12:A:H2	2.20	0.55
1:C:789:ARG:O	1:C:791:GLU:N	2.39	0.55
3:D:-26:G:C8	3:D:-26:G:H5"	2.41	0.55
1:A:162:LYS:HD2	1:A:164:PHE:CE1	2.41	0.55
1:A:581:LEU:HD21	1:A:599:ASP:HB3	1.89	0.55
1:C:594:ASP:HB3	1:C:596:ASN:OD1	2.07	0.55
1:C:601:ARG:HH11	1:C:604:GLU:CD	2.10	0.55
1:C:858:ARG:HH21	1:C:862:LYS:HE3	1.72	0.55
1:C:113:VAL:HG13	1:C:136:HIS:CD2	2.36	0.54
1:A:389:PHE:CZ	1:C:445:ASP:HB3	2.42	0.54
1:C:835:LEU:HD23	1:C:839:ILE:HB	1.88	0.54
1:C:540:VAL:HG12	1:C:542:VAL:HG13	1.90	0.54
1:C:68:ASN:N	1:C:68:ASN:HD22	2.05	0.54
1:A:791:GLU:OE2	1:A:791:GLU:HA	2.07	0.54
1:C:390:ARG:HH11	1:C:390:ARG:HG2	1.72	0.54
1:C:461:ILE:O	1:C:465:MSE:HG2	2.08	0.54
1:A:835:LEU:HD21	1:A:839:ILE:HD12	1.88	0.54
1:C:369:GLN:HA	1:C:372:LEU:HD22	1.89	0.54
1:A:780:GLN:NE2	5:A:1009:HOH:O	2.42	0.53
1:A:792:SER:HB2	1:A:798:LYS:CE	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:NH1	1:C:582:THR:CG2	2.71	0.53
1:C:197:MSE:HG2	1:C:253:ARG:HB2	1.91	0.53
1:C:646:GLU:O	1:C:649:LYS:HB2	2.09	0.53
3:D:-21:A:H2'	3:D:-20:A:C4	2.43	0.53
1:A:603:SER:OG	1:A:609:LYS:HG2	2.08	0.53
1:C:114:ASN:ND2	1:C:130:ASN:HB3	2.24	0.53
1:C:789:ARG:CD	1:C:791:GLU:HB2	2.38	0.53
1:A:366:LEU:HD22	1:A:366:LEU:H	1.74	0.53
2:B:10:A:N6	5:B:202:HOH:O	2.42	0.53
1:C:789:ARG:NE	1:C:791:GLU:CB	2.71	0.53
1:A:210:MSE:HE1	1:A:281:LEU:HD22	1.91	0.52
1:A:788:ASP:OD1	1:A:789:ARG:N	2.41	0.52
1:C:785:LEU:N	1:C:785:LEU:CD1	2.72	0.52
1:C:206:TYR:CD2	1:C:828:HIS:CG	2.96	0.52
1:C:918:TYR:O	1:C:921:GLU:HG2	2.10	0.52
1:C:390:ARG:NH1	1:C:390:ARG:CG	2.73	0.52
1:C:51:LYS:CB	1:C:51:LYS:NZ	2.72	0.52
1:C:708:GLN:O	1:C:710:LYS:HE3	2.10	0.52
1:C:256:TYR:CE2	1:C:636:ILE:HG21	2.44	0.52
1:C:922:LYS:N	1:C:922:LYS:CE	2.73	0.52
1:C:212:TYR:HB2	1:C:241:SER:HB3	1.91	0.52
1:C:362:ASP:OD1	1:C:368:SER:HB2	2.10	0.52
1:C:338:LYS:CE	1:C:476:ALA:O	2.57	0.52
1:A:878:ASP:HB2	5:A:1043:HOH:O	2.09	0.52
3:D:22:C:C6	3:D:22:C:H5'	2.45	0.52
1:A:785:LEU:HB3	1:A:791:GLU:CB	2.39	0.52
1:A:172:LEU:C	1:A:172:LEU:HD23	2.31	0.51
1:C:802:ARG:NH1	1:C:802:ARG:HG2	2.24	0.51
1:C:707:GLN:NE2	1:C:707:GLN:HA	2.24	0.51
3:D:-23:G:H5"	3:D:-23:G:C8	2.44	0.51
1:C:771:LEU:HD22	1:C:775:TYR:HA	1.92	0.51
1:A:895:SER:N	1:A:896:PRO:CD	2.74	0.51
1:C:214:SER:OG	1:C:216:ARG:NH1	2.43	0.51
1:C:839:ILE:HD13	1:C:839:ILE:O	2.10	0.51
1:C:251:THR:CB	1:C:253:ARG:HD2	2.37	0.51
1:C:800:ASN:HB3	1:C:803:LEU:HB2	1.93	0.51
1:C:872:LYS:CB	1:C:872:LYS:NZ	2.72	0.51
2:B:-19:A:O5'	2:B:-19:A:H8	1.94	0.51
1:C:293:HIS:CD2	1:C:299:LYS:HB3	2.46	0.51
1:C:693:MSE:HE1	1:C:723:VAL:HG22	1.93	0.51
1:A:544:CYS:O	1:A:544:CYS:SG	2.68	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:-8:U:O4	1:C:61:LYS:HE3	2.11	0.51
1:C:800:ASN:CG	1:C:803:LEU:HB2	2.31	0.51
1:A:919:LEU:HD12	1:A:919:LEU:H	1.77	0.50
1:C:895:SER:N	1:C:896:PRO:CD	2.73	0.50
1:C:64:LEU:CD1	1:C:534:ILE:HG21	2.40	0.50
1:C:845:VAL:CG1	1:C:851:ILE:HD11	2.42	0.50
1:C:85:TYR:CE2	1:C:107:LEU:HB2	2.46	0.50
1:C:710:LYS:O	1:C:713:GLU:HB2	2.11	0.50
3:D:12:A:H2	1:C:573:ARG:CZ	2.25	0.50
1:A:192:TYR:HA	1:A:206:TYR:OH	2.11	0.50
1:C:187:VAL:HG11	1:C:287:ILE:CG2	2.40	0.50
1:C:889:PHE:CD1	1:C:893:LEU:HD11	2.47	0.50
1:C:607:LYS:CB	1:C:610:GLU:HG3	2.38	0.50
1:C:803:LEU:HD13	1:C:901:ILE:CG2	2.42	0.50
1:C:230:LEU:HB3	1:C:234:VAL:CG1	2.41	0.50
1:C:808:GLU:CA	1:C:811:ILE:HG13	2.37	0.50
1:C:323:GLU:O	1:C:327:LYS:HB2	2.12	0.50
1:C:51:LYS:HB2	1:C:51:LYS:HZ2	1.75	0.50
1:C:355:ASP:OD2	1:C:417:ARG:NH2	2.24	0.49
1:C:889:PHE:O	1:C:893:LEU:HD12	2.12	0.49
2:B:-18:U:H1'	2:B:-17:U:O4'	2.11	0.49
1:C:789:ARG:HG3	1:C:791:GLU:HB2	1.94	0.49
2:B:-20:A:H3'	2:B:-19:A:C8	2.47	0.49
2:B:-22:C:C5'	2:B:-22:C:C6	2.90	0.49
1:A:205:SER:HB3	1:A:208:ASP:CG	2.33	0.49
2:B:8:U:C3'	2:B:9:U:H5'	2.43	0.49
1:C:230:LEU:HD23	1:C:234:VAL:HG11	1.95	0.49
1:C:766:LEU:HA	1:C:769:LYS:HG3	1.93	0.48
1:A:194:LEU:CD1	1:A:210:MSE:HE1	2.43	0.48
1:A:916:ASN:O	1:A:919:LEU:HD11	2.13	0.48
1:C:112:GLU:O	1:C:136:HIS:HB2	2.13	0.48
1:C:275:LYS:NZ	1:C:313:GLU:OE1	2.43	0.48
3:D:21:G:N2	1:C:577:ALA:O	2.45	0.48
1:C:69:LYS:HD2	1:C:86:GLU:OE2	2.13	0.48
2:B:9:U:OP2	2:B:10:A:O4'	2.32	0.48
1:C:307:ILE:HD11	1:C:318:LEU:HD11	1.95	0.48
1:C:673:CYS:HB3	1:C:693:MSE:HE1	1.95	0.48
1:C:223:THR:C	1:C:224:HIS:ND1	2.67	0.48
1:C:347:MSE:CE	1:C:457:ASP:O	2.62	0.48
3:D:21:G:C6	1:C:623:THR:HG21	2.49	0.48
1:A:224:HIS:HB3	1:A:227:LYS:HD3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ASN:OD1	1:A:464:HIS:CE1	2.67	0.48
1:C:253:ARG:HH11	1:C:582:THR:CG2	2.27	0.48
1:C:276:ARG:HG2	1:C:317:THR:HG23	1.95	0.48
1:C:302:ASP:OD1	1:C:302:ASP:N	2.37	0.48
1:C:776:ARG:HD3	1:C:814:ALA:HB3	1.94	0.48
1:A:187:VAL:HG11	1:A:287:ILE:HG22	1.96	0.48
3:D:-19:A:H2'	3:D:-18:U:O5'	2.13	0.48
1:A:260:GLU:HG3	1:A:577:ALA:CB	2.43	0.48
1:C:197:MSE:HG2	1:C:253:ARG:CB	2.44	0.48
1:C:607:LYS:HD2	1:C:615:ILE:O	2.14	0.48
1:A:835:LEU:HD22	1:A:839:ILE:HB	1.96	0.47
1:A:399:VAL:HG21	1:A:465:MSE:HB3	1.96	0.47
1:A:613:LYS:HE2	1:A:613:LYS:HB2	1.50	0.47
1:C:286:GLN:HG2	1:C:306:PHE:CE1	2.49	0.47
1:C:383:MSE:HE2	1:C:458:PHE:CE2	2.49	0.47
1:A:640:ASN:OD1	1:A:642:GLN:N	2.46	0.47
2:B:9:U:OP2	2:B:10:A:H5"	2.14	0.47
1:C:690:LEU:HD22	1:C:726:LEU:CD2	2.44	0.47
1:C:348:MSE:HB2	1:C:356:ILE:HD11	1.97	0.47
1:C:597:ILE:HD12	1:C:597:ILE:HA	1.77	0.47
1:C:789:ARG:CG	1:C:791:GLU:HB2	2.44	0.47
1:C:922:LYS:H	1:C:922:LYS:HE2	1.79	0.47
1:A:230:LEU:HG	1:A:234:VAL:HG11	1.97	0.47
1:C:114:ASN:HD21	1:C:130:ASN:HB3	1.79	0.47
1:C:835:LEU:CD2	1:C:839:ILE:CG1	2.93	0.47
1:A:322:VAL:HG21	1:A:500:LYS:HG2	1.96	0.47
1:C:922:LYS:HA	1:C:922:LYS:HD3	1.48	0.47
1:C:835:LEU:CD2	1:C:839:ILE:CB	2.92	0.47
1:C:918:TYR:HB3	1:C:921:GLU:HG3	1.97	0.47
1:C:776:ARG:HD3	1:C:814:ALA:CB	2.45	0.46
1:A:673:CYS:HB3	1:A:693:MSE:HE1	1.96	0.46
1:A:845:VAL:CG1	1:A:851:ILE:HD11	2.45	0.46
3:D:-26:G:OP1	1:C:799:LYS:HD3	2.15	0.46
1:C:601:ARG:NH1	1:C:604:GLU:OE2	2.48	0.46
1:A:559:ILE:HG22	1:A:563:LEU:HD22	1.97	0.46
1:C:546:LEU:HD13	1:C:550:TYR:O	2.15	0.46
1:C:149:LEU:HA	1:C:149:LEU:HD12	1.78	0.46
1:C:874:LYS:HD2	1:C:874:LYS:N	2.13	0.46
1:A:342:SER:HB2	1:A:478:MSE:HE3	1.97	0.46
1:A:787:ASP:OD2	1:A:808:GLU:OE2	2.33	0.46
1:C:700:ASP:OD1	1:C:703:LYS:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ASN:O	1:C:344:LEU:HG	2.16	0.46
1:C:347:MSE:HE1	1:C:461:ILE:CG1	2.36	0.46
1:A:620:ASN:HD22	2:B:19:A:P	2.39	0.46
1:A:792:SER:HB3	1:A:798:LYS:HE3	1.93	0.46
1:C:265:LYS:HA	1:C:265:LYS:HD3	1.50	0.46
1:A:263:LYS:H	1:A:263:LYS:HG2	1.35	0.46
1:A:654:VAL:HG12	1:A:658:LEU:HD22	1.98	0.46
1:C:147:ASP:N	1:C:147:ASP:OD1	2.49	0.46
3:D:10:A:C2	1:C:630:SER:HB3	2.51	0.46
2:B:-16:U:C6	2:B:-16:U:H5"	2.51	0.45
1:A:665:GLN:OE1	2:B:9:U:H4'	2.16	0.45
1:A:389:PHE:HZ	1:C:445:ASP:HB3	1.81	0.45
1:A:791:GLU:OE1	1:A:793:SER:HB2	2.16	0.45
1:C:785:LEU:HD13	1:C:785:LEU:H	1.82	0.45
1:A:197:MSE:CE	1:A:257:PHE:CE2	2.96	0.45
1:A:369:GLN:HA	1:A:372:LEU:HD22	1.99	0.45
1:A:178:ASP:HB2	1:A:524:LYS:HD2	1.99	0.45
1:A:710:LYS:HA	1:A:710:LYS:HD3	1.75	0.45
2:B:9:U:P	2:B:10:A:H5"	2.57	0.45
1:C:197:MSE:CG	1:C:253:ARG:HB3	2.47	0.45
1:C:172:LEU:C	1:C:172:LEU:HD23	2.37	0.45
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.31	0.45
1:A:526:ASP:O	1:A:529:LYS:HG3	2.16	0.45
1:A:792:SER:CB	1:A:798:LYS:CE	2.82	0.45
3:D:-20:A:OP2	3:D:-20:A:C8	2.69	0.45
1:A:194:LEU:HD13	1:A:210:MSE:CE	2.47	0.44
1:C:673:CYS:O	1:C:693:MSE:HE1	2.17	0.44
1:C:785:LEU:H	1:C:785:LEU:CD1	2.30	0.44
1:C:922:LYS:H	1:C:922:LYS:CE	2.30	0.44
3:D:-13:A:H2'	3:D:-12:C:O4'	2.17	0.44
1:C:70:MSE:HE1	1:C:134:PRO:HD2	1.99	0.44
1:C:407:MSE:HB3	1:C:458:PHE:CZ	2.52	0.44
1:C:911:GLN:HA	1:C:918:TYR:CE2	2.52	0.44
3:D:-19:A:C8	3:D:-19:A:OP2	2.70	0.44
1:A:512:LYS:HE3	2:B:8:U:P	2.57	0.44
1:C:453:LYS:O	1:C:453:LYS:HG2	2.18	0.44
1:A:593:ILE:CD1	1:A:699:PHE:HB3	2.48	0.44
1:C:863:ARG:H	1:C:863:ARG:HG3	1.40	0.44
2:B:-15:G:H2'	2:B:-15:G:N3	2.33	0.44
1:C:322:VAL:HG21	1:C:500:LYS:HG2	1.99	0.44
1:A:182:ILE:HA	1:A:182:ILE:HD12	1.88	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:LEU:HD12	1:C:326:LEU:HA	1.78	0.44
1:C:774:ASP:OD2	1:C:776:ARG:NH2	2.51	0.43
1:C:693:MSE:CE	1:C:723:VAL:HG22	2.47	0.43
1:C:712:ARG:NH1	1:C:712:ARG:CG	2.72	0.43
1:A:707:GLN:HA	1:A:717:LYS:HE3	2.00	0.43
1:A:780:GLN:CD	5:A:1009:HOH:O	2.56	0.43
1:C:581:LEU:HD21	1:C:599:ASP:HB3	2.00	0.43
1:C:116:THR:CG2	1:C:128:GLU:HG2	2.46	0.43
1:C:483:LYS:HZ3	1:C:483:LYS:HB2	1.83	0.43
3:D:8:U:P	1:C:512:LYS:HE3	2.59	0.43
1:A:116:THR:OG1	1:A:130:ASN:OD1	2.32	0.43
1:C:357:ILE:HG22	1:C:485:LEU:HD21	1.99	0.43
1:A:378:LYS:HD3	1:A:443:TYR:CG	2.53	0.43
1:C:342:SER:HA	1:C:478:MSE:HE1	1.99	0.43
1:C:482:GLU:H	1:C:482:GLU:HG3	1.46	0.43
1:C:663:ASP:HB3	1:C:683:LEU:HD11	2.01	0.43
2:B:9:U:OP2	2:B:10:A:C5'	2.67	0.43
1:C:666:ILE:HD12	1:C:687:ARG:HG2	2.00	0.43
1:C:835:LEU:HD21	1:C:839:ILE:CG1	2.42	0.43
3:D:-30:C:O2	3:D:-30:C:C2'	2.65	0.43
1:A:87:VAL:HG11	1:A:110:VAL:HG11	2.01	0.42
1:C:140:GLU:OE2	1:C:140:GLU:HA	2.18	0.42
1:C:733:LEU:HA	1:C:733:LEU:HD12	1.83	0.42
1:A:573:ARG:NH2	2:B:12:A:C2	2.87	0.42
1:C:212:TYR:CE2	1:C:240:LYS:HD2	2.51	0.42
1:C:777:ILE:HD12	1:C:777:ILE:HA	1.69	0.42
1:C:785:LEU:HD12	1:C:785:LEU:N	2.34	0.42
2:B:-22:C:H2'	2:B:-21:A:O4'	2.18	0.42
2:B:-30:C:H2'	2:B:-30:C:O2	2.18	0.42
1:C:849:PHE:CZ	1:C:853:HIS:CD2	3.07	0.42
3:D:-29:A:O3'	1:C:905:LYS:NZ	2.52	0.42
1:A:192:TYR:CD2	1:A:829:LEU:HD22	2.54	0.42
1:A:922:LYS:CD	2:B:-30:C:H2'	2.35	0.42
1:C:559:ILE:HG22	1:C:563:LEU:HD22	2.01	0.42
1:C:644:ILE:HD13	1:C:644:ILE:HA	1.89	0.42
1:C:640:ASN:O	1:C:644:ILE:HG12	2.20	0.42
1:C:849:PHE:CE1	1:C:853:HIS:HD2	2.38	0.42
1:C:862:LYS:HD2	1:C:862:LYS:HA	1.82	0.42
1:C:515:ASN:O	1:C:519:THR:HG23	2.20	0.42
1:A:228:SER:OG	1:A:230:LEU:HB2	2.20	0.42
1:C:164:PHE:CD2	1:C:169:HIS:CE1	3.08	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:TYR:CE2	1:C:828:HIS:CG	3.07	0.42
1:A:92:TYR:OH	1:A:112:GLU:HB2	2.19	0.42
1:C:70:MSE:CE	1:C:133:ASN:OD1	2.53	0.42
1:C:310:ILE:HD12	1:C:314:TYR:CG	2.55	0.42
3:D:-27:U:H2'	3:D:-26:G:H5"	2.02	0.42
1:A:389:PHE:HZ	1:C:445:ASP:CB	2.33	0.41
1:C:874:LYS:N	1:C:874:LYS:CD	2.73	0.41
1:A:52:LYS:HE2	2:B:-1:C:O3'	2.19	0.41
1:C:800:ASN:CB	1:C:803:LEU:HB2	2.50	0.41
1:A:77:LYS:HE2	5:A:1397:HOH:O	2.19	0.41
1:A:873:ILE:HG22	1:A:875:TYR:H	1.84	0.41
2:B:-20:A:O2'	2:B:-19:A:H5'	2.21	0.41
2:B:20:A:H2'	2:B:21:G:C8	2.55	0.41
1:C:343:LEU:HD11	1:C:464:HIS:HD2	1.85	0.41
1:A:64:LEU:CD1	1:A:534:ILE:HG21	2.50	0.41
1:A:886:THR:HG22	1:A:889:PHE:H	1.86	0.41
1:A:52:LYS:HD2	1:A:57:ALA:HB2	2.02	0.41
1:A:573:ARG:NH2	2:B:12:A:H2	2.17	0.41
1:C:817:SER:HA	1:C:820:ARG:NH2	2.34	0.41
1:C:863:ARG:HD3	1:C:863:ARG:O	2.21	0.41
1:C:873:ILE:HG22	1:C:875:TYR:H	1.86	0.41
1:A:170:ILE:HA	1:A:170:ILE:HD12	1.92	0.41
1:A:617:GLY:O	1:A:707:GLN:HG2	2.20	0.41
1:C:224:HIS:N	1:C:224:HIS:ND1	2.67	0.41
1:C:286:GLN:HG2	1:C:306:PHE:CZ	2.56	0.41
1:C:766:LEU:HD12	1:C:766:LEU:HA	1.92	0.41
1:C:851:ILE:O	1:C:855:VAL:HG23	2.20	0.41
3:D:10:A:C2	1:C:630:SER:CB	3.03	0.41
1:A:700:ASP:O	1:A:703:LYS:HG2	2.21	0.41
1:C:789:ARG:HH21	1:C:789:ARG:HG2	1.85	0.41
3:D:-15:G:H2'	3:D:-14:C:H6	1.86	0.41
1:C:362:ASP:O	1:C:367:LYS:N	2.50	0.41
1:C:706:LYS:NZ	1:C:708:GLN:H	2.19	0.41
1:A:307:ILE:HD12	1:A:307:ILE:HA	1.88	0.41
3:D:-13:A:H2'	3:D:-12:C:C6	2.56	0.41
1:C:338:LYS:HG2	1:C:339:VAL:N	2.35	0.41
1:C:807:VAL:HG12	1:C:811:ILE:CD1	2.42	0.41
3:D:10:A:C5'	3:D:10:A:H8	2.34	0.41
1:C:789:ARG:O	1:C:790:ASN:C	2.59	0.41
1:A:63:ILE:HG21	1:A:134:PRO:HG3	2.02	0.40
1:A:372:LEU:HA	1:A:372:LEU:HD12	1.92	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:GLU:OE2	1:C:695:LYS:CD	2.52	0.40
1:C:889:PHE:CD1	1:C:893:LEU:CD1	3.03	0.40
3:D:-19:A:C2'	3:D:-18:U:O5'	2.69	0.40
1:C:330:ASN:HB3	1:C:489:LYS:HE3	2.03	0.40
1:C:372:LEU:HD12	1:C:372:LEU:HA	1.85	0.40
1:C:387:TYR:HB3	1:C:451:TRP:NE1	2.35	0.40
1:C:387:TYR:CD2	1:C:451:TRP:CG	3.10	0.40
1:C:774:ASP:CG	1:C:776:ARG:HH21	2.25	0.40
1:A:323:GLU:HG2	5:A:1404:HOH:O	2.21	0.40
1:C:325:ARG:HD3	1:C:325:ARG:HA	1.92	0.40
5:D:231:HOH:O	1:C:431:ARG:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	865/930 (93%)	855 (99%)	10 (1%)	0	100	100
1	C	856/930 (92%)	840 (98%)	15 (2%)	1 (0%)	51	53
All	All	1721/1860 (92%)	1695 (98%)	25 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	790	ASN

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	783/802 (98%)	728 (93%)	55 (7%)	15 10
1	C	777/802 (97%)	671 (86%)	106 (14%)	3 1
All	All	1560/1604 (97%)	1399 (90%)	161 (10%)	7 4

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	50	LYS
1	A	51	LYS
1	A	66	SER
1	A	67	GLU
1	A	100	LYS
1	A	112	GLU
1	A	114	ASN
1	A	149	LEU
1	A	162	LYS
1	A	200	ILE
1	A	201	LYS
1	A	203	SER
1	A	204	GLU
1	A	205	SER
1	A	210	MSE
1	A	230	LEU
1	A	231	SER
1	A	233	LYS
1	A	260	GLU
1	A	263	LYS
1	A	266	ASP
1	A	268	ARG
1	A	303	LEU
1	A	326	LEU
1	A	343	LEU
1	A	349	LYS
1	A	372	LEU
1	A	439	LYS
1	A	455	ARG
1	A	471	LYS
1	A	478	MSE
1	A	505	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	510	ASP
1	A	555	ASP
1	A	563	LEU
1	A	578	SER
1	A	591	LEU
1	A	595	ASP
1	A	597	ILE
1	A	613	LYS
1	A	631	ARG
1	A	658	LEU
1	A	700	ASP
1	A	706	LYS
1	A	733	LEU
1	A	766	LEU
1	A	778	LEU
1	A	793	SER
1	A	835	LEU
1	A	863	ARG
1	A	871	GLU
1	A	881	LYS
1	A	920	THR
1	A	922	LYS
1	C	50	LYS
1	C	51	LYS
1	C	52	LYS
1	C	62	SER
1	C	66	SER
1	C	68	ASN
1	C	100	LYS
1	C	112	GLU
1	C	113	VAL
1	C	114	ASN
1	C	132	SER
1	C	138	SER
1	C	140	GLU
1	C	149	LEU
1	C	154	GLU
1	C	158	ARG
1	C	198	LEU
1	C	205	SER
1	C	206	TYR
1	C	208	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	216	ARG
1	C	220	GLU
1	C	224	HIS
1	C	229	ASN
1	C	232	ASP
1	C	233	LYS
1	C	234	VAL
1	C	235	LYS
1	C	240	LYS
1	C	253	ARG
1	C	261	GLU
1	C	263	LYS
1	C	264	THR
1	C	266	ASP
1	C	267	THR
1	C	274	LYS
1	C	295	LYS
1	C	296	SER
1	C	299	LYS
1	C	300	ARG
1	C	303	LEU
1	C	326	LEU
1	C	327	LYS
1	C	332	ASP
1	C	343	LEU
1	C	356	ILE
1	C	372	LEU
1	C	386	GLU
1	C	428	ARG
1	C	429	LYS
1	C	459	GLU
1	C	471	LYS
1	C	472	GLU
1	C	478	MSE
1	C	481	ASP
1	C	487	SER
1	C	489	LYS
1	C	490	LYS
1	C	510	ASP
1	C	543	GLU
1	C	555	ASP
1	C	563	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	591	LEU
1	C	593	ILE
1	C	594	ASP
1	C	597	ILE
1	C	610	GLU
1	C	630	SER
1	C	631	ARG
1	C	649	LYS
1	C	651	GLU
1	C	658	LEU
1	C	689	GLU
1	C	706	LYS
1	C	707	GLN
1	C	710	LYS
1	C	712	ARG
1	C	733	LEU
1	C	766	LEU
1	C	771	LEU
1	C	777	ILE
1	C	780	GLN
1	C	791	GLU
1	C	801	LYS
1	C	802	ARG
1	C	803	LEU
1	C	804	ARG
1	C	811	ILE
1	C	815	ASP
1	C	816	SER
1	C	820	ARG
1	C	821	LYS
1	C	835	LEU
1	C	839	ILE
1	C	843	ARG
1	C	846	ASP
1	C	862	LYS
1	C	863	ARG
1	C	872	LYS
1	C	874	LYS
1	C	880	LEU
1	C	889	PHE
1	C	905	LYS
1	C	917	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	919	LEU
1	C	922	LYS

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	102	ASN
1	A	114	ASN
1	A	217	ASN
1	A	707	GLN
1	A	714	ASN
1	A	790	ASN
1	A	828	HIS
1	C	68	ASN
1	C	102	ASN
1	C	114	ASN
1	C	337	ASN
1	C	395	GLN
1	C	464	HIS
1	C	466	ASN
1	C	650	ASN
1	C	707	GLN
1	C	773	ASN
1	C	882	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	51/51 (100%)	14 (27%)	6 (11%)
3	D	52/53 (98%)	15 (28%)	4 (7%)
All	All	103/104 (99%)	29 (28%)	10 (9%)

All (29) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-29	A
2	B	-22	C
2	B	-18	U
2	B	-17	U
2	B	-16	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	-15	G
2	B	-14	C
2	B	-4	A
2	B	7	A
2	B	9	U
2	B	10	A
2	B	13	U
2	B	17	C
2	B	21	G
3	D	-26	G
3	D	-23	G
3	D	-22	C
3	D	-21	A
3	D	-20	A
3	D	-19	A
3	D	-17	U
3	D	-16	U
3	D	-4	A
3	D	7	A
3	D	9	U
3	D	10	A
3	D	13	U
3	D	22	C
3	D	23	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	-30	C
2	B	-20	A
2	B	-16	U
2	B	-10	A
2	B	-4	A
2	B	9	U
3	D	-18	U
3	D	-17	U
3	D	-4	A
3	D	9	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	844/930 (90%)	0.22	21 (2%)	57	65	13, 29, 71, 179	0
1	C	837/930 (90%)	0.58	70 (8%)	11	15	26, 57, 104, 168	0
2	B	51/51 (100%)	-0.08	4 (7%)	13	18	18, 38, 140, 169	0
3	D	53/53 (100%)	-0.06	4 (7%)	14	19	30, 51, 167, 200	0
All	All	1785/1964 (90%)	0.37	99 (5%)	25	34	13, 44, 99, 200	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	803	LEU	8.0
1	C	264	THR	6.8
1	C	791	GLU	6.2
1	C	353	ALA	6.2
1	C	920	THR	5.5
1	A	790	ASN	5.0
1	C	229	ASN	4.7
1	C	787	ASP	4.4
1	C	349	LYS	4.1
1	A	596	ASN	4.0
1	C	263	LYS	4.0
1	C	390	ARG	3.9
1	C	807	VAL	3.8
1	C	543	GLU	3.7
1	C	230	LEU	3.7
1	C	165	ASP	3.6
1	C	873	ILE	3.5
3	D	-20	A	3.5
1	A	206	TYR	3.5
1	A	920	THR	3.4
1	A	205	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	918	TYR	3.4
1	A	921	GLU	3.4
1	C	877	ASP	3.4
1	C	879	LEU	3.3
1	C	67	GLU	3.3
1	C	481	ASP	3.3
1	A	139	GLY	3.2
1	C	812	ASN	3.2
2	B	-17	U	3.2
1	C	99	SER	3.1
1	C	97	LEU	3.1
1	A	202	ASP	3.1
1	A	49	GLU	3.1
1	C	463	ASP	3.1
1	C	85	TYR	3.0
1	C	451	TRP	3.0
1	C	482	GLU	3.0
1	C	766	LEU	3.0
2	B	-19	A	3.0
1	C	596	ASN	2.9
1	C	227	LYS	2.9
3	D	-17	U	2.9
1	C	391	PHE	2.9
1	C	139	GLY	2.9
1	A	918	TYR	2.8
1	C	479	ASP	2.8
1	C	458	PHE	2.8
3	D	-19	A	2.6
1	C	101	ASP	2.6
1	C	839	ILE	2.6
1	C	95	THR	2.5
1	C	890	VAL	2.5
1	C	921	GLU	2.5
1	C	597	ILE	2.5
1	C	892	ALA	2.5
1	C	919	LEU	2.5
1	A	639	ALA	2.5
1	C	577	ALA	2.5
2	B	21	G	2.5
1	A	870	GLU	2.5
1	C	72	ILE	2.5
1	C	296	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	785	LEU	2.4
1	C	483	LYS	2.4
1	C	265	LYS	2.4
1	C	226	ASP	2.4
1	C	786	CYS	2.4
1	A	864	GLY	2.4
1	C	346	ASP	2.4
1	A	418	ASN	2.3
1	C	107	LEU	2.3
1	A	712	ARG	2.3
1	C	68	ASN	2.3
1	C	102	ASN	2.3
1	A	709	ALA	2.3
1	A	609	LYS	2.2
1	C	88	ASP	2.2
1	C	389	PHE	2.2
1	C	208	ASP	2.2
1	C	790	ASN	2.2
1	A	207	ASP	2.2
1	C	200	ILE	2.2
1	A	595	ASP	2.2
1	C	351	TYR	2.2
1	C	225	PRO	2.2
1	C	205	SER	2.1
2	B	-20	A	2.1
1	C	132	SER	2.1
1	C	84	GLU	2.1
1	A	676	PHE	2.1
1	C	231	SER	2.1
1	C	140	GLU	2.1
1	A	389	PHE	2.1
1	C	100	LYS	2.0
1	C	782	LEU	2.0
3	D	-18	U	2.0
1	C	247	ASP	2.0
1	C	385	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	D	101	1/1	0.97	0.05	36,36,36,36	0
4	MG	B	101	1/1	0.98	0.12	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.