



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:53 PM EDT

PDB ID : 6IV8 / pdb_00006iv8
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 types of validation reports are described at

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

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

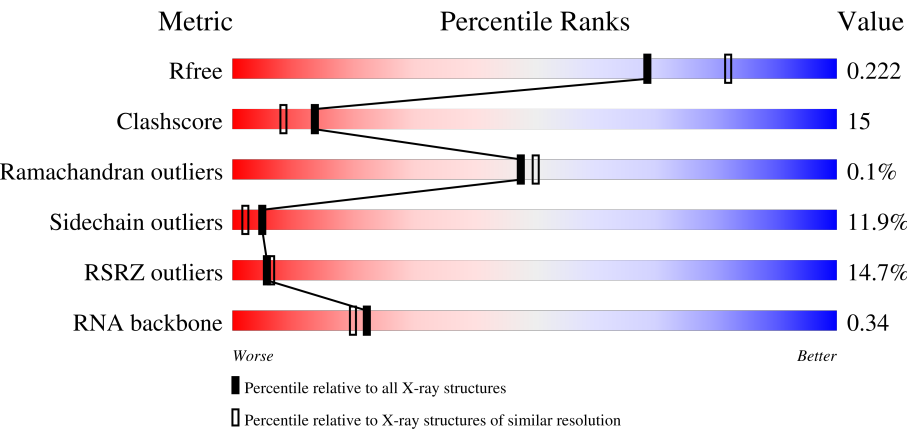
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)
RNA backbone	3983	1112 (2.50-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	930	7% 72%19%7%
1	C	930	21% 58%26%8%7%
2	B	51	6% 41%27%16%16%
3	D	53	4% 38%32%21%9%

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 (CCD ID: 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		

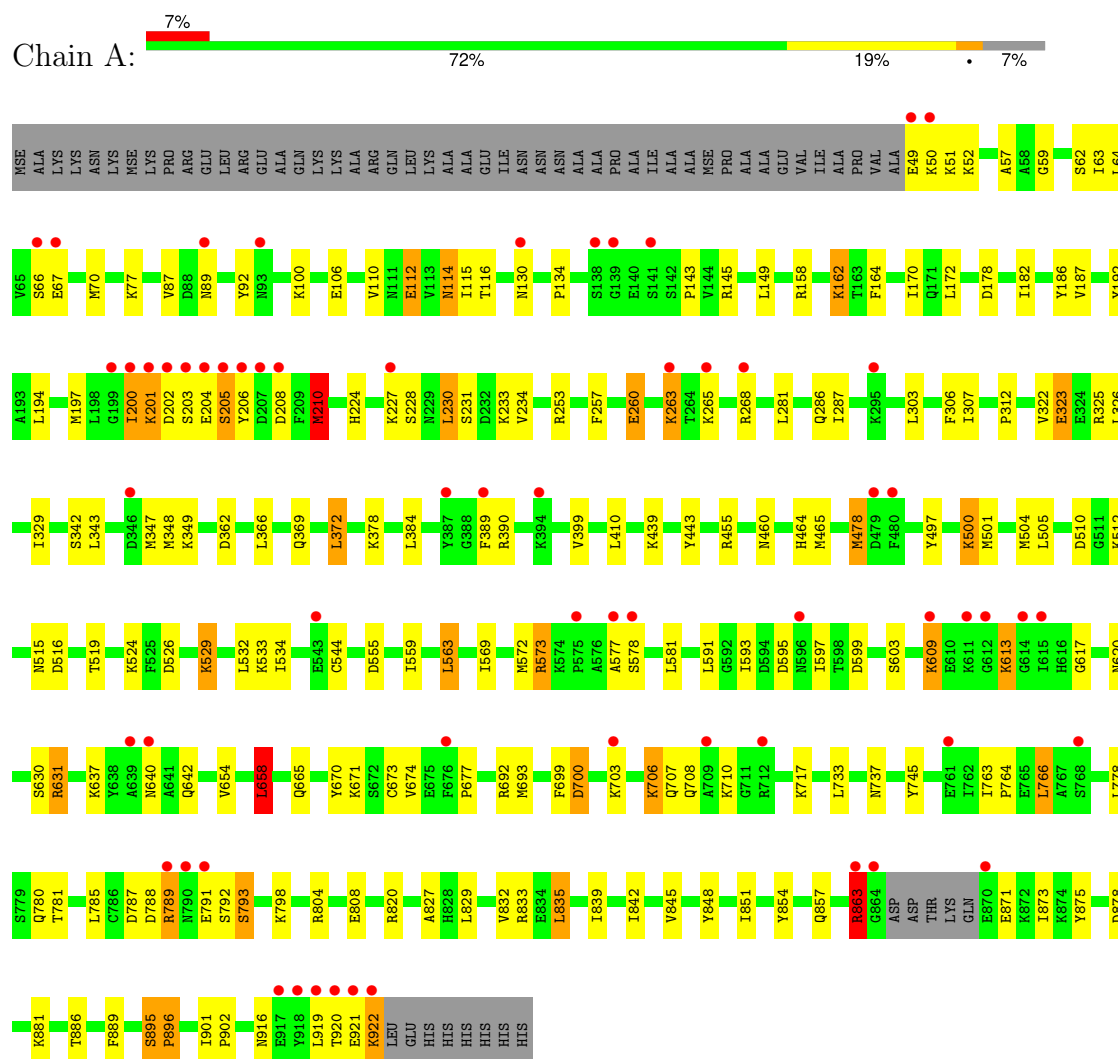
- Molecule 5 is water.

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		

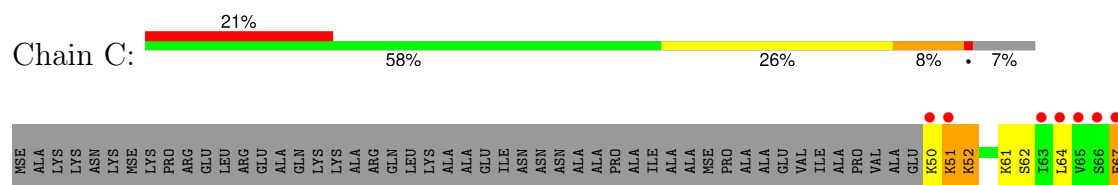
3 Residue-property plots

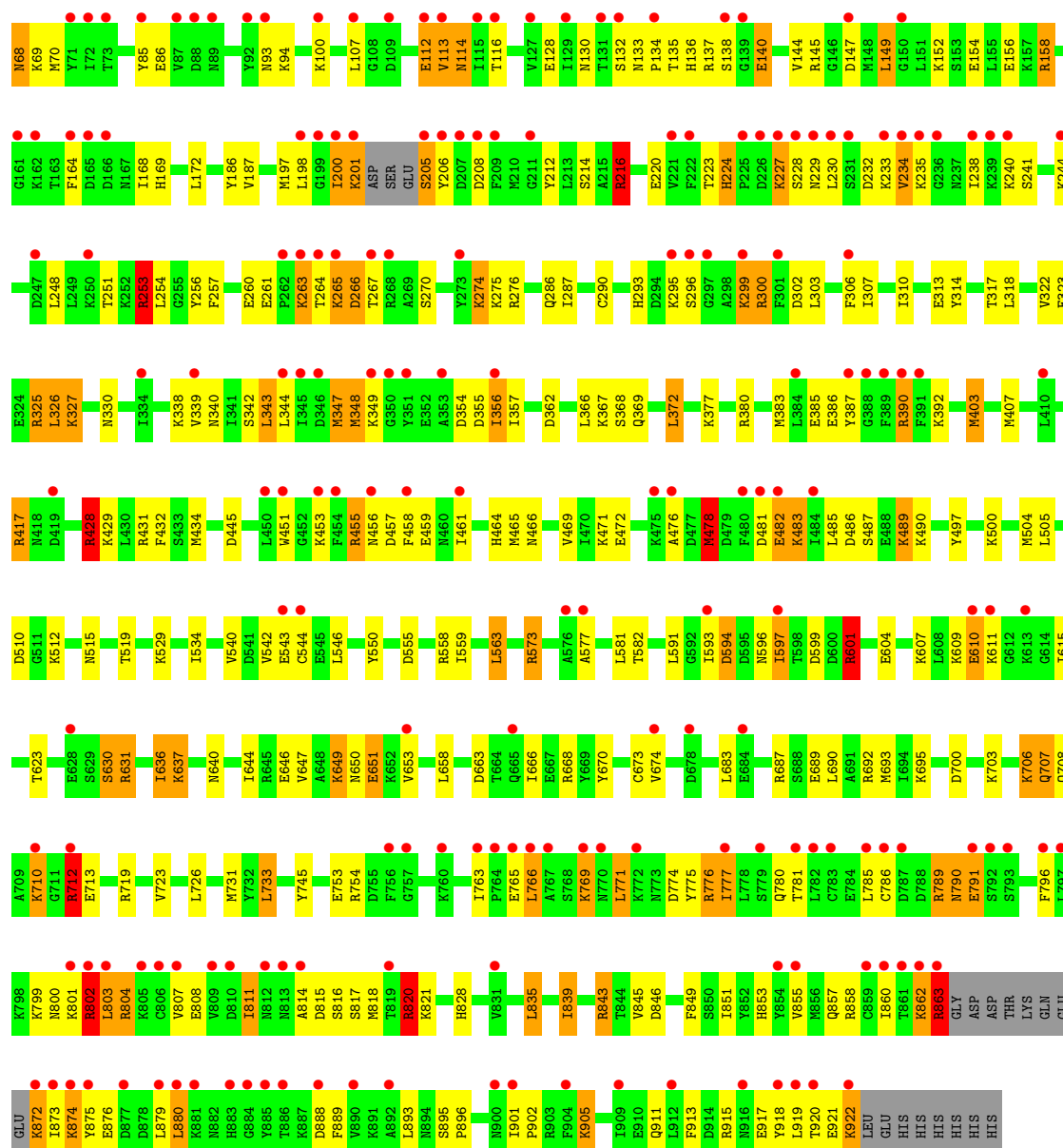
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

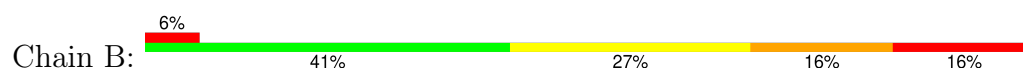


- Molecule 1: The selenomethionine (SeMet)-labeled Cas13d





• Molecule 2: RNA (51-MER)



• Molecule 3: RNA (53-MER)



4 Data and refinement statistics

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 62.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (62.92-2.15) 99.6 (62.92-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.08%)	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)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	1.42	21/7153 (0.3%)	1.38	13/9550 (0.1%)
1	C	1.08	3/7098 (0.0%)	1.35	14/9475 (0.1%)
2	B	1.00	5/1203 (0.4%)	1.36	21/1869 (1.1%)
3	D	0.96	6/1250 (0.5%)	1.10	10/1942 (0.5%)
All	All	1.22	35/16704 (0.2%)	1.34	58/22836 (0.3%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	-9	G	O3'-P	-8.25	1.48	1.61
2	B	-17	U	C2'-O2'	7.63	1.53	1.41
1	A	895	SER	C-O	-7.21	1.18	1.24
1	C	478	MSE	CA-C	-6.72	1.44	1.52
1	A	519	THR	C-O	-6.54	1.16	1.24
3	D	-7	C	O3'-P	-6.21	1.51	1.61
2	B	10	A	O3'-P	-6.21	1.51	1.61
3	D	-8	U	O3'-P	-6.16	1.51	1.61
3	D	-3	A	O3'-P	-6.04	1.52	1.61
1	A	827	ALA	C-O	-5.96	1.16	1.24
1	A	896	PRO	C-O	-5.77	1.16	1.24
1	A	312	PRO	C-O	-5.76	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	901	ILE	C-O	-5.72	1.19	1.24
2	B	-28	C	P-OP2	-5.66	1.37	1.49
2	B	17	C	O5'-C5'	-5.56	1.34	1.42
3	D	-10	A	O3'-P	-5.56	1.52	1.61
1	A	764	PRO	C-O	-5.48	1.17	1.24
3	D	-4	A	O3'-P	-5.45	1.52	1.61
1	A	516	ASP	C-O	-5.43	1.17	1.24
1	A	737	ASN	C-O	-5.43	1.17	1.24
1	A	857	GLN	C-O	-5.40	1.17	1.24
1	A	902	PRO	C-O	-5.38	1.17	1.24
1	A	323	GLU	C-O	-5.31	1.18	1.24
1	A	515	ASN	C-O	-5.31	1.18	1.24
1	A	59	GLY	C-O	-5.27	1.18	1.24
1	A	410	LEU	C-O	-5.23	1.18	1.24
1	C	348	MSE	CA-C	-5.21	1.47	1.53
1	A	630	SER	C-O	-5.18	1.17	1.24
1	A	848	TYR	C-O	-5.18	1.18	1.24
1	A	501	MSE	C-O	-5.17	1.18	1.24
1	A	532	LEU	C-O	-5.17	1.18	1.24
2	B	-19	A	C2'-O2'	5.17	1.49	1.41
1	A	348	MSE	CA-C	-5.17	1.46	1.53
1	C	902	PRO	C-O	-5.14	1.17	1.24
1	A	832	VAL	C-O	-5.02	1.18	1.24

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	ASP	CB-CA-C	-10.36	94.31	109.84
1	A	347	MSE	N-CA-C	9.28	121.47	111.36
3	D	-17	U	C4'-C3'-O3'	7.86	121.19	109.40
1	A	210	MSE	CG-SE-CE	-7.74	81.89	98.92
2	B	-17	U	C2'-C3'-O3'	7.47	120.71	109.50
1	C	347	MSE	N-CA-C	7.20	119.12	111.28
1	C	818	MSE	N-CA-CB	-7.11	99.70	110.01
2	B	20	A	C4'-C3'-O3'	-7.11	102.33	113.00
2	B	10	A	C3'-C2'-O2'	7.10	121.35	110.70
2	B	-17	U	C4'-C3'-O3'	-6.99	98.91	109.40
3	D	-9	G	C4'-C3'-O3'	-6.84	102.74	113.00
1	C	265	LYS	CB-CA-C	6.43	121.54	110.94
1	C	347	MSE	CB-CA-C	-6.42	100.13	110.79
3	D	-10	A	C4'-C3'-O3'	-6.37	103.45	113.00
2	B	9	U	C2'-C3'-O3'	6.25	123.08	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	-30	C	C1'-C2'-O2'	-6.20	102.50	111.80
2	B	17	C	C2'-C3'-O3'	6.17	122.96	113.70
1	C	347	MSE	CB-CG-SE	-6.10	94.40	112.70
3	D	9	U	C4'-C3'-O3'	6.02	122.04	113.00
2	B	-17	U	C3'-C2'-O2'	-6.00	105.59	114.60
3	D	-18	U	C2'-C3'-O3'	5.95	118.43	109.50
1	C	478	MSE	N-CA-C	-5.89	98.91	108.52
1	C	186	TYR	CB-CA-C	5.89	120.86	110.85
1	A	347	MSE	N-CA-CB	-5.85	101.50	110.16
1	C	497	TYR	CB-CA-C	5.82	120.44	110.79
2	B	-14	C	C2'-C3'-O3'	5.81	122.42	113.70
2	B	-17	U	O5'-P-OP1	-5.79	90.62	108.00
2	B	13	U	C1'-C2'-O2'	-5.76	99.77	108.40
2	B	-22	C	O5'-P-OP1	5.74	125.22	108.00
3	D	19	A	C2'-C3'-O3'	5.73	122.29	113.70
3	D	4	U	C4'-C3'-O3'	-5.73	104.41	113.00
3	D	-15	G	C4'-C3'-O3'	-5.70	104.45	113.00
3	D	-23	G	C4'-C3'-O3'	-5.68	104.47	113.00
1	A	186	TYR	CB-CA-C	5.66	120.48	110.85
2	B	-12	C	C3'-C2'-O2'	5.63	119.15	110.70
1	A	497	TYR	CB-CA-C	5.62	120.12	110.79
1	A	745	TYR	CB-CA-C	5.53	120.25	110.85
1	C	456	ASN	CB-CA-C	5.48	120.17	110.85
1	C	913	PHE	N-CA-C	5.41	116.86	111.07
2	B	-17	U	N1-C1'-C2'	5.36	122.05	114.00
1	A	210	MSE	CA-CB-CG	-5.36	103.38	114.10
1	C	745	TYR	CB-CA-C	5.35	119.95	110.85
1	C	354	ASP	CB-CA-C	5.34	120.51	110.63
1	A	143	PRO	N-CA-C	-5.29	107.24	113.86
1	C	796	PHE	CB-CA-C	-5.26	102.86	110.96
1	A	763	ILE	CA-C-N	5.24	124.87	119.05
1	A	763	ILE	C-N-CA	5.24	124.87	119.05
1	A	500	LYS	CB-CA-C	5.22	119.45	110.79
2	B	14	A	C1'-C2'-O2'	-5.20	104.00	111.80
2	B	-23	G	C4'-C3'-O3'	-5.14	105.28	113.00
2	B	-16	U	C3'-C2'-O2'	5.09	118.33	110.70
2	B	-19	A	C3'-C2'-O2'	5.08	122.22	114.60
2	B	13	U	C3'-C2'-O2'	5.06	118.29	110.70
2	B	17	C	C5'-C4'-C3'	-5.04	108.44	116.00
3	D	-26	G	C1'-C2'-O2'	5.03	115.95	108.40
2	B	-7	C	C4'-C3'-O3'	-5.03	105.46	113.00
1	A	658	LEU	CA-C-N	5.02	125.55	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	658	LEU	C-N-CA	5.02	125.55	119.98

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
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

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Mol	Chain	Res	Type	Group
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	114	0
1	C	7011	0	7094	296	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
5	C	69	0	0	1	0
5	D	46	0	0	1	0
All	All	16939	0	15345	459	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 15.

All (459) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:C:874:LYS:HD2	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:H	1:C:263:LYS:CE	1.87	0.88
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:NH1	1:C:712:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:200:ILE:HD12	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:789:ARG:C	1:C:791:GLU:H	1.94	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
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:N	2.46	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H6	2:B:-22:C:C5'	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:94:LYS:CD	1:C:107:LEU:HD23	2.25	0.67
3:D:-22:C:H6	3:D:-22:C:C5'	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:C:67:GLU:C	1:C:68:ASN:HD22	2.05	0.65
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:H5''	3:D:-26:G:H8	1.62	0.64
1:C:70:MSE:HE2	1:C:134:PRO:CG	2.26	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:366:LEU:HD22	2.17	0.60
1:C:342:SER:HB2	1:C:478:MSE:CE	2.31	0.60
1:C:920:THR:HG22	1:C:920:THR:O	2.01	0.60
1:C:637:LYS:NZ	5:C:1003:HOH:O	2.35	0.60
1:A:674:VAL:HG23	1:A:677:PRO:HB3	1.83	0.60
3:D:-22:C:C6	3:D:-22:C:C5'	2.84	0.60
1:A:329:ILE:CD1	1:A:572:MSE:SE	2.99	0.59
1:C:601:ARG:HH11	1:C:604:GLU:CD	2.10	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
1:A:707:GLN:HA	1:A:707:GLN:NE2	2.16	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:HH21	1:A:789:ARG:HB3	1.68	0.58
1:C:248:LEU:HD21	1:C:254:LEU:HD21	1.85	0.58
3:D:-23:G:H5''	3:D:-23:G:H8	1.67	0.58
1:C:390:ARG:HH11	1:C:390:ARG:CG	2.16	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
3:D:9:U:OP2	3:D:10:A:O4'	2.21	0.57
1:C:647:VAL:HG12	1:C:731:MSE:HE1	1.85	0.57
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:SG	1:C:544:CYS:O	2.62	0.57
1:C:863:ARG:HG2	1:C:863:ARG:NH2	2.19	0.57
1:A:792:SER:HA	1:A:798:LYS:HE3	1.85	0.57
1:C:863:ARG:HG2	1:C:863:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:807:VAL:O	1:C:811:ILE:CG1	2.50	0.56
1:A:172:LEU:C	1:A:172:LEU:HD23	2.31	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:HA	1:A:707:GLN:HE21	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:C:800:ASN:CG	1:C:803:LEU:HB2	2.31	0.55
1:A:573:ARG:CZ	2:B:12:A:H2	2.20	0.55
3:D:-26:G:H5''	3:D:-26:G:C8	2.41	0.55
1:C:789:ARG:O	1:C:791:GLU:N	2.39	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:858:ARG:HH21	1:C:862:LYS:HE3	1.72	0.55
1:A:389:PHE:CZ	1:C:445:ASP:HB3	2.42	0.54
1:C:113:VAL:HG13	1:C:136:HIS:CD2	2.36	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:HD22	1:C:68:ASN:N	2.05	0.54
1:A:791:GLU:HA	1:A:791:GLU:OE2	2.07	0.54
1:A:205:SER:HB3	1:A:208:ASP:CG	2.33	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
1:C:253:ARG:NH1	1:C:582:THR:CG2	2.71	0.53
3:D:-21:A:H2'	3:D:-20:A:C4	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:TYR:CD2	1:C:828:HIS:CG	2.96	0.52
1:C:223:THR:C	1:C:224:HIS:ND1	2.67	0.52
1:C:785:LEU:N	1:C:785:LEU:CD1	2.72	0.52
1:C:918:TYR:O	1:C:921:GLU:HG2	2.10	0.52
1:C:51:LYS:NZ	1:C:51:LYS:CB	2.72	0.52
1:C:390:ARG:CG	1:C:390:ARG:NH1	2.73	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:H5'	3:D:22:C:C6	2.45	0.52
1:A:785:LEU:HB3	1:A:791:GLU:CB	2.39	0.52
1:C:802:ARG:NH1	1:C:802:ARG:HG2	2.24	0.51
3:D:-23:G:H5''	3:D:-23:G:C8	2.44	0.51
1:C:707:GLN:HA	1:C:707:GLN:NE2	2.24	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:NZ	1:C:872:LYS:CB	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:SG	1:A:544:CYS:O	2.68	0.51
3:D:-8:U:O4	1:C:61:LYS:HE3	2.11	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
3:D:12:A:H2	1:C:573:ARG:CZ	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:51:LYS:HB2	1:C:51:LYS:HZ2	1.75	0.50
1:C:323:GLU:O	1:C:327:LYS:HB2	2.12	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
1:C:172:LEU:HD23	1:C:172:LEU:C	2.37	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
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
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
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
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
3:D:21:G:C6	1:C:623:THR:HG21	2.49	0.48
1:C:347:MSE:CE	1:C:457:ASP:O	2.62	0.48
1:A:224:HIS:HB3	1:A:227:LYS:HD3	1.96	0.48
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:A:780:GLN:CD	5:A:1009:HOH:O	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:C:922:LYS:H	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:HD12	1:C:149:LEU:HA	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
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:HD3	1:C:265:LYS:HA	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
3:D:10:A:C2	1:C:630:SER:HB3	2.51	0.46
1:C:147:ASP:OD1	1:C:147:ASP:N	2.49	0.46
1:A:389:PHE:HZ	1:C:445:ASP:HB3	1.81	0.45
1:A:665:GLN:OE1	2:B:9:U:H4'	2.16	0.45
2:B:-16:U:C6	2:B:-16:U:H5''	2.51	0.45
1:A:791:GLU:OE1	1:A:793:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:ARG:O	1:C:790:ASN:C	2.59	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:C:774:ASP:CG	1:C:776:ARG:HH21	2.25	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:A:201:LYS:HD3	1:A:201:LYS:HA	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:C8	3:D:-20:A:OP2	2.69	0.45
1:A:194:LEU:HD13	1:A:210:MSE:CE	2.47	0.44
3:D:-13:A:H2'	3:D:-12:C:O4'	2.17	0.44
1:C:504:MSE:C	1:C:504:MSE:SE	3.10	0.44
1:C:673:CYS:O	1:C:693:MSE:HE1	2.17	0.44
1:C:785:LEU:CD1	1:C:785:LEU:H	2.30	0.44
1:C:922:LYS:CE	1:C:922:LYS:H	2.30	0.44
1:C:70:MSE:HE1	1:C:134:PRO:HD2	1.99	0.44
1:C:483:LYS:HZ3	1:C:483:LYS:HB2	1.82	0.44
1:C:407:MSE:HB3	1:C:458:PHE:CZ	2.52	0.44
3:D:-19:A:C8	3:D:-19:A:OP2	2.70	0.44
1:C:911:GLN:HA	1:C:918:TYR:CE2	2.52	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:N3	2:B:-15:G:H2'	2.33	0.44
1:C:322:VAL:HG21	1:C:500:LYS:HG2	1.99	0.44
1:A:182:ILE:HD12	1:A:182:ILE:HA	1.88	0.44
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:C:581:LEU:HD21	1:C:599:ASP:HB3	2.00	0.43
3:D:8:U:P	1:C:512:LYS:HE3	2.59	0.43
1:C:116:THR:CG2	1:C:128:GLU:HG2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:-30:C:O2	3:D:-30:C:C2'	2.65	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
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:HD12	1:C:733:LEU:HA	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:706:LYS:HD3	1:C:706:LYS:C	2.44	0.42
1:C:777:ILE:HA	1:C:777:ILE:HD12	1.69	0.42
1:C:785:LEU:N	1:C:785:LEU:HD12	2.34	0.42
2:B:-30:C:H2'	2:B:-30:C:O2	2.18	0.42
2:B:-22:C:H2'	2:B:-21:A:O4'	2.18	0.42
3:D:-29:A:O3'	1:C:905:LYS:NZ	2.52	0.42
1:C:849:PHE:CZ	1:C:853:HIS:CD2	3.07	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:640:ASN:O	1:C:644:ILE:HG12	2.20	0.42
1:C:644:ILE:HD13	1:C:644:ILE:HA	1.89	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
1:C:200:ILE:HD12	1:C:200:ILE:C	2.44	0.42
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
3:D:-27:U:H2'	3:D:-26:G:H5''	2.02	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
1:A:389:PHE:HZ	1:C:445:ASP:CB	2.33	0.41
1:C:874:LYS:CD	1:C:874:LYS:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:646:GLU:CD	1:C:649:LYS:NZ	2.77	0.41
1:C:817:SER:HA	1:C:820:ARG:NH2	2.34	0.41
1:C:863:ARG:O	1:C:863:ARG:HD3	2.21	0.41
1:C:873:ILE:HG22	1:C:875:TYR:H	1.86	0.41
1:A:170:ILE:HD12	1:A:170:ILE:HA	1.92	0.41
1:A:617:GLY:O	1:A:707:GLN:HG2	2.20	0.41
3:D:10:A:C2	1:C:630:SER:CB	3.03	0.41
1:C:224:HIS:ND1	1:C:224:HIS:N	2.67	0.41
1:C:286:GLN:HG2	1:C:306:PHE:CZ	2.56	0.41
1:C:766:LEU:HA	1:C:766:LEU:HD12	1.92	0.41
1:C:851:ILE:O	1:C:855:VAL:HG23	2.20	0.41
1:A:700:ASP:O	1:A:703:LYS:HG2	2.21	0.41
3:D:-15:G:H2'	3:D:-14:C:H6	1.86	0.41
1:C:789:ARG:HG2	1:C:789:ARG:HH21	1.85	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
3:D:10:A:C5'	3:D:10:A:H8	2.34	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
1:C:835:LEU:CD2	1:C:835:LEU:C	2.93	0.41
1:A:504:MSE:SE	1:A:504:MSE:C	3.14	0.40
1:A:63:ILE:HG21	1:A:134:PRO:HG3	2.02	0.40
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.92	0.40
3:D:-19:A:C2'	3:D:-18:U:O5'	2.69	0.40
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
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:A:323:GLU:HG2	5:A:1404:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:231:HOH:O	1:C:431:ARG:HG2	2.20	0.40
1:C:325:ARG:HA	1:C:325:ARG:HD3	1.92	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%)	48	50
All	All	1721/1860 (92%)	1695 (98%)	25 (2%)	1 (0%)	48	50

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%)	725 (93%)	58 (7%)	13	8
1	C	777/802 (97%)	649 (84%)	128 (16%)	2	1
All	All	1560/1604 (97%)	1374 (88%)	186 (12%)	5	2

All (186) 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	106	GLU
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	265	LYS
1	A	303	LEU
1	A	326	LEU
1	A	343	LEU
1	A	349	LYS
1	A	372	LEU
1	A	384	LEU
1	A	439	LYS
1	A	478	MSE
1	A	505	LEU
1	A	510	ASP
1	A	529	LYS
1	A	533	LYS
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	609	LYS

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Mol	Chain	Res	Type
1	A	613	LYS
1	A	631	ARG
1	A	658	LEU
1	A	671	LYS
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	67	GLU
1	C	68	ASN
1	C	93	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	144	VAL
1	C	149	LEU
1	C	154	GLU
1	C	158	ARG
1	C	168	ILE
1	C	198	LEU
1	C	200	ILE
1	C	201	LYS
1	C	205	SER
1	C	208	ASP
1	C	216	ARG
1	C	220	GLU

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Mol	Chain	Res	Type
1	C	224	HIS
1	C	227	LYS
1	C	229	ASN
1	C	232	ASP
1	C	233	LYS
1	C	234	VAL
1	C	235	LYS
1	C	238	ILE
1	C	244	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	343	LEU
1	C	349	LYS
1	C	356	ILE
1	C	366	LEU
1	C	372	LEU
1	C	377	LYS
1	C	385	GLU
1	C	386	GLU
1	C	392	LYS
1	C	403	MSE
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	482	GLU
1	C	483	LYS

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Mol	Chain	Res	Type
1	C	487	SER
1	C	489	LYS
1	C	490	LYS
1	C	505	LEU
1	C	510	ASP
1	C	529	LYS
1	C	543	GLU
1	C	555	ASP
1	C	563	LEU
1	C	591	LEU
1	C	593	ILE
1	C	594	ASP
1	C	597	ILE
1	C	601	ARG
1	C	609	LYS
1	C	610	GLU
1	C	611	LYS
1	C	630	SER
1	C	631	ARG
1	C	636	ILE
1	C	637	LYS
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	763	ILE
1	C	766	LEU
1	C	769	LYS
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	811	ILE
1	C	815	ASP

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Mol	Chain	Res	Type
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	860	ILE
1	C	862	LYS
1	C	863	ARG
1	C	872	LYS
1	C	874	LYS
1	C	880	LEU
1	C	888	ASP
1	C	905	LYS
1	C	917	GLU
1	C	919	LEU
1	C	922	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	114	ASN
1	A	217	ASN
1	A	224	HIS
1	A	289	GLN
1	A	308	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	104	ASN
1	C	195	ASN
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%)	18 (35%)	6 (11%)
3	D	52/53 (98%)	16 (30%)	4 (7%)
All	All	103/104 (99%)	34 (33%)	10 (9%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-29	A
2	B	-22	C
2	B	-20	A
2	B	-19	A
2	B	-18	U
2	B	-17	U
2	B	-16	U
2	B	-15	G
2	B	-14	C
2	B	-10	A
2	B	-9	G
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	-3	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	844/930 (90%)	0.28	61 (7%) 21 25	13, 29, 71, 179	0
1	C	837/930 (90%)	1.36	196 (23%) 2 2	26, 57, 104, 168	0
2	B	51/51 (100%)	-0.08	3 (5%) 28 32	18, 38, 134, 160	0
3	D	53/53 (100%)	0.18	2 (3%) 44 49	30, 51, 161, 193	0
All	All	1785/1964 (90%)	0.77	262 (14%) 6 6	13, 44, 99, 193	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	803	LEU	9.0
1	C	200	ILE	7.8
1	A	922	LYS	6.3
1	C	201	LYS	5.7
1	A	206	TYR	5.6
1	A	864	GLY	5.5
1	A	205	SER	5.4
1	C	919	LEU	5.4
1	C	206	TYR	5.3
1	A	200	ILE	5.2
1	C	807	VAL	5.1
1	C	205	SER	5.0
1	C	230	LEU	4.8
1	C	264	THR	4.6
1	C	132	SER	4.6
1	A	919	LEU	4.6
1	C	875	TYR	4.4
1	A	676	PHE	4.3
1	C	208	ASP	4.3
1	C	792	SER	4.2
1	C	766	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	107	LEU	4.1
1	C	890	VAL	4.0
1	C	809	VAL	4.0
1	C	207	ASP	4.0
1	C	873	ILE	3.9
1	C	451	TRP	3.9
1	C	301	PHE	3.9
1	C	389	PHE	3.9
1	C	922	LYS	3.8
1	C	221	VAL	3.8
1	C	880	LEU	3.7
1	C	227	LYS	3.7
1	C	920	THR	3.7
1	A	203	SER	3.7
1	C	883	HIS	3.7
1	A	263	LYS	3.6
1	A	790	ASN	3.6
1	C	209	PHE	3.6
1	C	71	TYR	3.6
1	C	613	LYS	3.6
1	C	862	LYS	3.6
1	A	389	PHE	3.5
1	C	819	THR	3.5
1	C	353	ALA	3.5
1	C	863	ARG	3.5
1	C	892	ALA	3.5
1	C	879	LEU	3.5
1	C	234	VAL	3.5
1	C	796	PHE	3.4
1	A	49	GLU	3.4
1	C	233	LYS	3.4
1	C	50	LYS	3.4
1	C	772	LYS	3.4
1	A	207	ASP	3.3
1	C	782	LEU	3.3
1	C	139	GLY	3.3
1	C	884	GLY	3.3
1	C	387	TYR	3.3
1	C	265	LYS	3.3
1	C	296	SER	3.2
1	C	475	LYS	3.2
1	C	198	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	199	GLY	3.2
1	A	791	GLU	3.2
1	C	802	ARG	3.2
1	C	757	GLY	3.2
1	C	872	LYS	3.2
1	A	768	SER	3.1
1	C	480	PHE	3.1
1	C	72	ILE	3.1
1	C	138	SER	3.1
1	A	918	TYR	3.0
1	C	854	TYR	3.0
1	C	874	LYS	3.0
1	C	127	VAL	3.0
1	C	247	ASP	3.0
1	C	785	LEU	3.0
1	C	116	THR	3.0
1	C	67	GLU	3.0
1	C	610	GLU	2.9
1	C	295	LYS	2.9
1	A	208	ASP	2.9
1	C	134	PRO	2.9
1	A	201	LYS	2.9
1	C	64	LEU	2.9
1	C	806	CYS	2.9
1	C	225	PRO	2.9
1	C	240	LYS	2.9
1	C	886	THR	2.9
1	C	226	ASP	2.8
1	C	916	ASN	2.8
1	C	356	ILE	2.8
1	C	813	ASN	2.8
1	C	92	TYR	2.8
1	C	476	ALA	2.8
1	C	576	ALA	2.8
1	C	767	ALA	2.8
1	C	860	ILE	2.8
1	A	138	SER	2.8
1	C	165	ASP	2.8
2	B	-30	C	2.8
1	C	250	LYS	2.8
1	C	228	SER	2.7
1	A	917	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	912	LEU	2.7
1	A	863	ARG	2.7
1	C	786	CYS	2.7
1	C	543	GLU	2.7
1	C	350	GLY	2.7
1	A	50	LYS	2.7
1	A	640	ASN	2.7
1	A	921	GLU	2.7
1	A	227	LYS	2.7
1	C	881	LYS	2.7
1	C	888	ASP	2.6
1	A	295	LYS	2.6
1	A	268	ARG	2.6
1	C	131	THR	2.6
1	A	202	ASP	2.6
1	C	793	SER	2.6
1	C	65	VAL	2.6
1	C	814	ALA	2.6
1	C	263	LYS	2.6
1	C	710	LYS	2.6
1	C	787	ASP	2.6
1	C	877	ASP	2.6
1	C	66	SER	2.6
1	C	904	PHE	2.6
1	C	238	ILE	2.6
1	C	597	ILE	2.6
1	C	901	ILE	2.6
1	A	609	LYS	2.6
1	C	909	ILE	2.5
1	C	235	LYS	2.5
1	C	760	LYS	2.5
1	C	129	ILE	2.5
1	C	211	GLY	2.5
1	C	89	ASN	2.5
1	C	481	ASP	2.5
1	A	575	PRO	2.5
1	A	639	ALA	2.5
3	D	-20	A	2.5
1	C	299	LYS	2.5
1	C	334	ILE	2.5
1	C	461	ILE	2.5
2	B	-22	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	346	ASP	2.4
1	C	885	TYR	2.4
1	C	267	THR	2.4
1	A	577	ALA	2.4
1	C	765	GLU	2.4
1	C	810	ASP	2.4
1	C	85	TYR	2.4
1	C	390	ARG	2.4
1	A	612	GLY	2.4
1	C	456	ASN	2.4
1	C	900	ASN	2.4
1	A	611	LYS	2.4
1	C	239	LYS	2.4
1	C	781	THR	2.4
1	A	709	ALA	2.4
1	C	797	LEU	2.4
1	A	870	GLU	2.4
1	C	458	PHE	2.4
1	A	615	ILE	2.4
1	C	593	ILE	2.4
1	C	611	LYS	2.4
1	C	262	PRO	2.4
1	C	801	LYS	2.3
1	A	204	GLU	2.3
1	C	859	CYS	2.3
1	C	351	TYR	2.3
1	C	918	TYR	2.3
1	A	199	GLY	2.3
1	A	712	ARG	2.3
1	A	789	ARG	2.3
1	C	391	PHE	2.3
1	C	763	ILE	2.3
1	C	791	GLU	2.3
1	C	831	VAL	2.3
1	C	577	ALA	2.3
1	C	109	ASP	2.3
1	C	147	ASP	2.3
1	A	265	LYS	2.3
1	C	805	LYS	2.3
1	A	480	PHE	2.3
1	C	113	VAL	2.3
1	C	783	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	166	ASP	2.3
1	C	150	GLY	2.3
1	A	67	GLU	2.2
1	C	684	GLU	2.2
1	C	231	SER	2.2
1	C	222	PHE	2.2
1	C	339	VAL	2.2
1	C	653	VAL	2.2
1	C	764	PRO	2.2
1	C	812	ASN	2.2
1	C	419	ASP	2.2
1	C	388	GLY	2.2
1	C	164	PHE	2.2
1	C	712	ARG	2.2
1	C	756	PHE	2.2
1	C	93	ASN	2.2
1	C	349	LYS	2.2
1	A	139	GLY	2.2
1	C	769	LYS	2.2
1	A	596	ASN	2.2
1	C	770	ASN	2.2
1	C	454	PHE	2.2
1	C	88	ASP	2.2
1	A	543	GLU	2.2
1	C	410	LEU	2.2
1	A	141	SER	2.2
3	D	22	C	2.2
1	C	678	ASP	2.2
1	C	345	ILE	2.1
1	C	855	VAL	2.1
1	A	614	GLY	2.1
1	C	344	LEU	2.1
1	C	229	ASN	2.1
1	C	861	THR	2.1
1	C	63	ILE	2.1
1	C	297	GLY	2.1
1	C	384	LEU	2.1
1	C	779	SER	2.1
1	C	628	GLU	2.1
1	A	479	ASP	2.1
1	C	346	ASP	2.1
1	C	273	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	-21	A	2.1
1	C	665	GLN	2.1
1	C	161	GLY	2.1
1	C	306	PHE	2.1
1	C	453	LYS	2.1
1	A	578	SER	2.1
1	A	387	TYR	2.1
1	A	394	LYS	2.1
1	C	484	ILE	2.1
1	C	87	VAL	2.1
1	C	482	GLU	2.0
1	C	450	LEU	2.0
1	A	89	ASN	2.0
1	A	93	ASN	2.0
1	C	544	CYS	2.0
1	C	268	ARG	2.0
1	A	920	THR	2.0
1	C	73	THR	2.0
1	C	51	LYS	2.0
1	C	162	LYS	2.0
1	C	244	LYS	2.0
1	C	236	GLY	2.0
1	C	115	ILE	2.0
1	C	777	ILE	2.0
1	A	761	GLU	2.0
1	C	112	GLU	2.0
1	C	674	VAL	2.0
1	A	66	SER	2.0
1	A	130	ASN	2.0
1	A	703	LYS	2.0
1	C	100	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	101	1/1	0.99	0.02	16,16,16,16	0
4	MG	D	101	1/1	0.99	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.