



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:06 AM BST

PDB ID : 6IFN
Title : Crystal structure of Type III-A CRISPR Csm complex
Authors : You, L.; Wang, J.; Wang, Y.
Deposited on : 2018-09-20
Resolution : 2.90 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
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

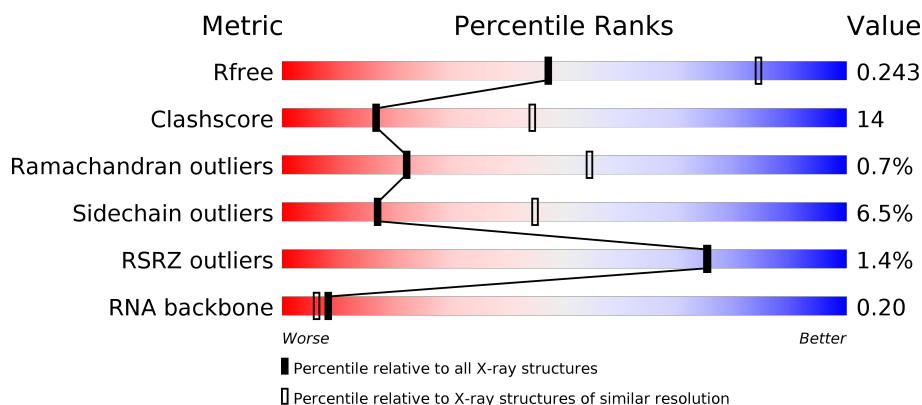
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 $\leq 5\%$. 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	758	<div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
2	E	220	<div> <div>%</div> <div>72%</div> <div>25%</div> <div>•</div> </div>
2	F	220	<div> <div>70%</div> <div>29%</div> <div>•</div> </div>
2	G	220	<div> <div>%</div> <div>78%</div> <div>21%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	B	299	<div><div></div><div>69%27%<div><div></div><div></div></div></div></div>
4	C	126	<div><div></div><div>67%25%6%<div><div></div><div></div></div></div></div>
4	D	126	<div><div>4%</div><div></div><div>67%29%<div><div></div><div></div></div></div></div>
5	H	357	<div><div>6%</div><div></div><div>62%31%<div><div></div><div></div></div></div></div>
6	N	40	<div><div></div><div>8%45%23%5%20%<div><div></div><div></div></div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18048 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 Type III-A CRISPR-associated protein Csm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5726	3675	959	1076	16			

- Molecule 2 is a protein called Type III-A CRISPR-associated RAMP protein Csm3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	220	Total	C	N	O	S	0	0	0
			1681	1063	287	328	3			
2	E	219	Total	C	N	O	S	0	0	0
			1675	1059	286	327	3			
2	G	220	Total	C	N	O	S	0	0	0
			1621	1022	281	316	2			

- Molecule 3 is a protein called Type III-A CRISPR-associated RAMP protein Csm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	297	Total	C	N	O	S	0	0	0
			2311	1482	383	441	5			

- Molecule 4 is a protein called Type III-A CRISPR-associated protein Csm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	124	Total	C	N	O	S	0	0	0
			959	622	160	175	2			
4	D	123	Total	C	N	O	S	0	0	0
			904	588	149	165	2			

- Molecule 5 is a protein called Type III-A CRISPR-associated RAMP protein Csm5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	345	Total	C	N	O	S	0	0	0
			2499	1600	433	462	4			

- Molecule 6 is a RNA chain called RNA (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	32	Total	C	N	O	P	0	0	0
			670	302	115	222	31			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

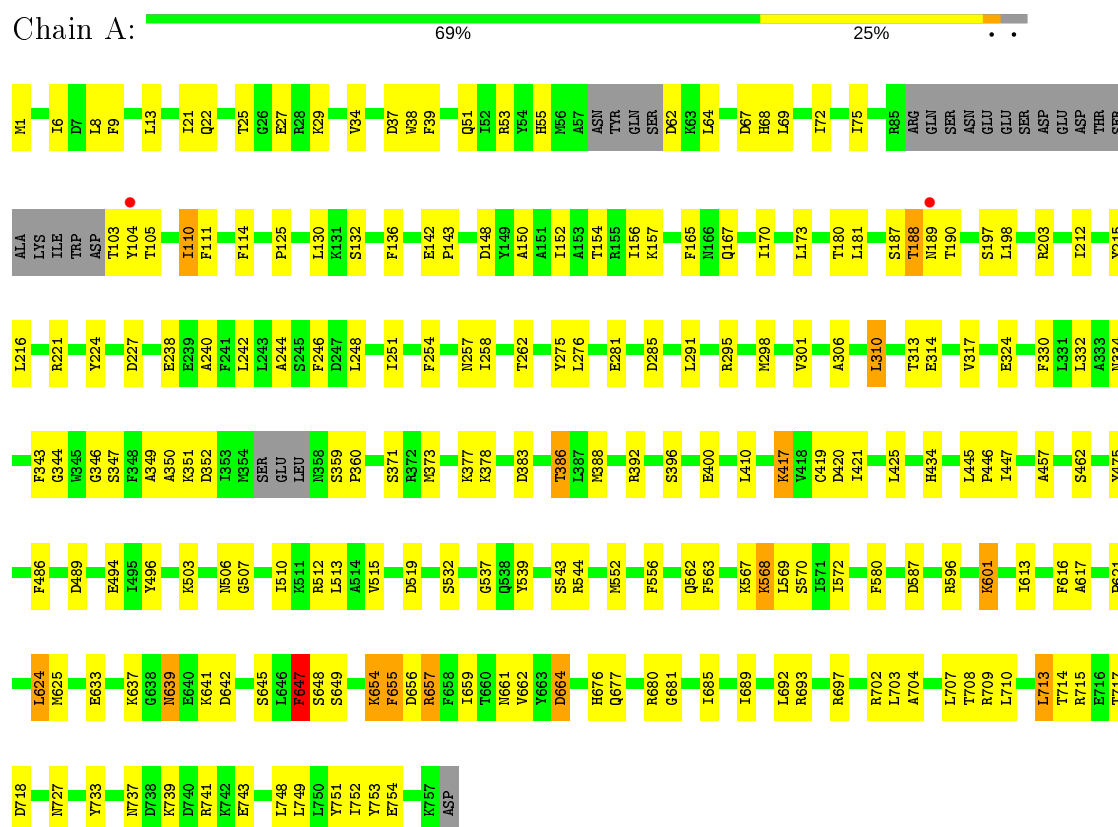
- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mn	0	0
			1	1		

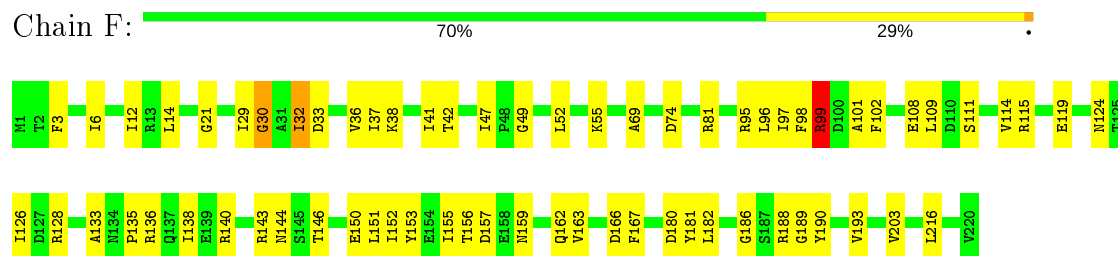
3 Residue-property plots

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.

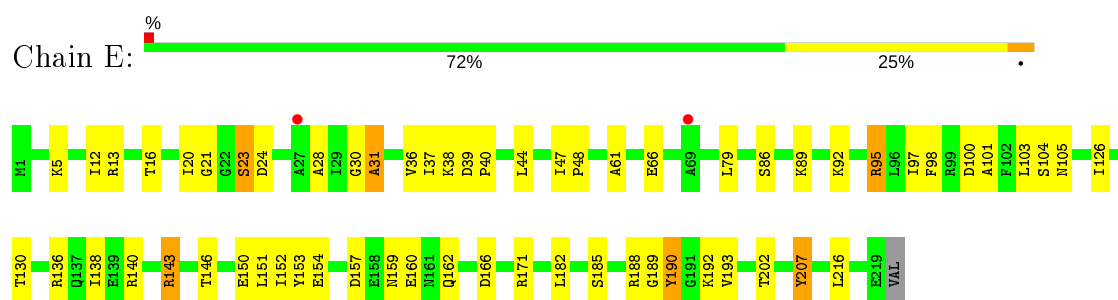
- Molecule 1: Type III-A CRISPR-associated protein Csm1



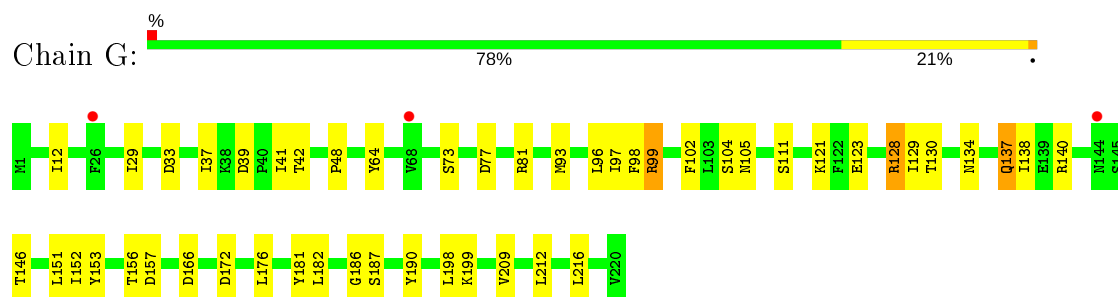
- Molecule 2: Type III-A CRISPR-associated RAMP protein Csm3



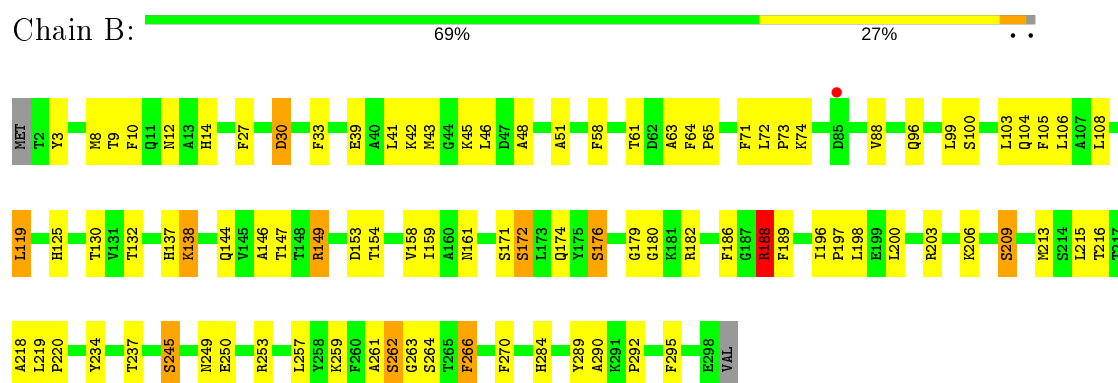
- Molecule 2: Type III-A CRISPR-associated RAMP protein Csm3



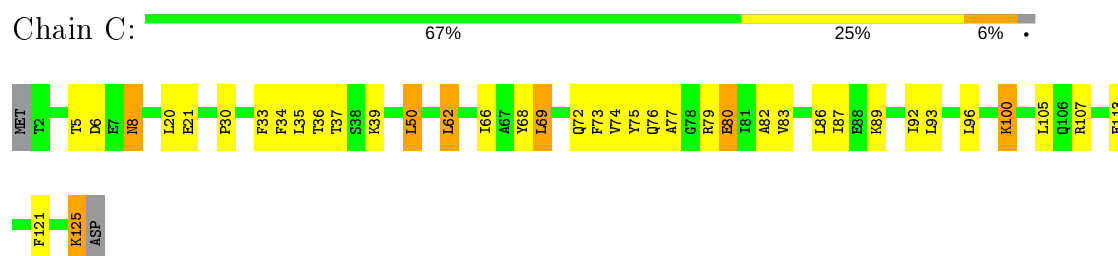
- Molecule 2: Type III-A CRISPR-associated RAMP protein Csm3



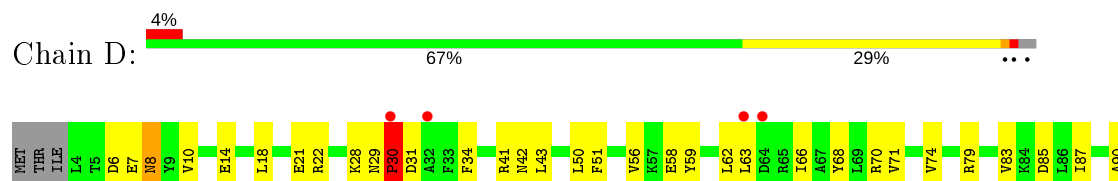
- Molecule 3: Type III-A CRISPR-associated RAMP protein Csm4

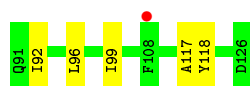


- Molecule 4: Type III-A CRISPR-associated protein Csm2

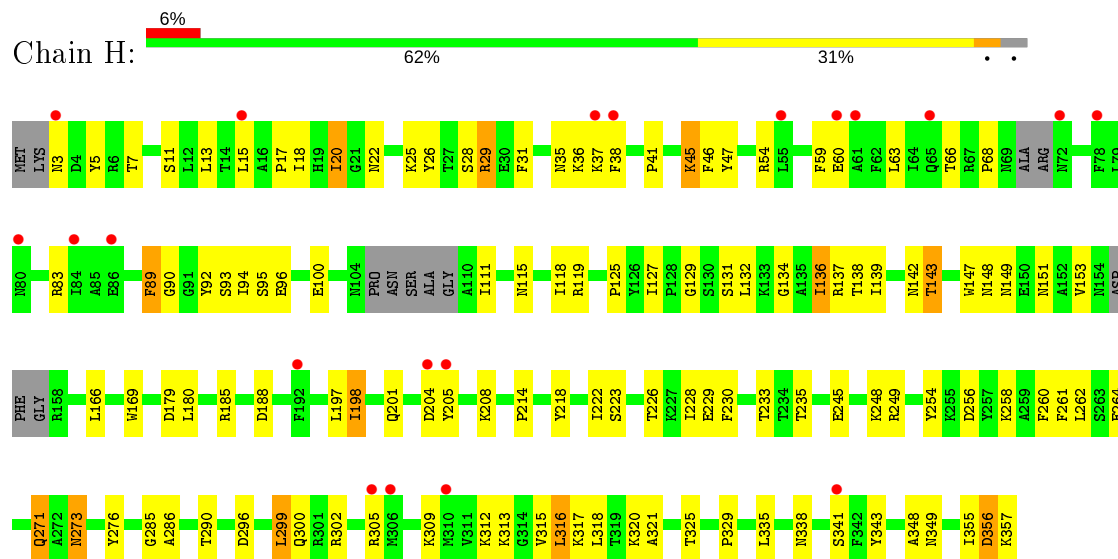


- Molecule 4: Type III-A CRISPR-associated protein Csm2

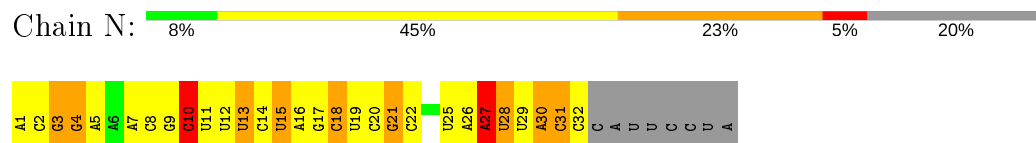




- Molecule 5: Type III-A CRISPR-associated RAMP protein Csm5



- Molecule 6: RNA (32-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.54Å 82.33Å 161.36Å 90.00° 99.32° 90.00°	Depositor
Resolution (Å)	48.68 – 2.90 48.64 – 2.88	Depositor EDS
% Data completeness (in resolution range)	83.8 (48.68-2.90) 83.8 (48.64-2.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.201 , 0.244 0.203 , 0.243	Depositor DCC
R_{free} test set	3053 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18048	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN

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	0.58	0/5846	0.73	2/7909 (0.0%)
2	E	0.55	0/1699	0.73	0/2295
2	F	0.52	0/1706	0.69	1/2304 (0.0%)
2	G	0.47	0/1644	0.67	0/2228
3	B	0.66	0/2363	0.76	1/3202 (0.0%)
4	C	0.53	0/973	0.69	2/1316 (0.2%)
4	D	0.50	0/918	0.72	1/1250 (0.1%)
5	H	0.55	0/2551	0.76	0/3464
6	N	0.68	1/747 (0.1%)	1.15	10/1160 (0.9%)
All	All	0.57	1/18447 (0.0%)	0.75	17/25128 (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	A	0	1
2	E	0	1
2	F	0	2
2	G	0	1
3	B	0	3
4	C	0	1
4	D	0	1
5	H	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	10	C	O3'-P	-5.23	1.54	1.61

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	SER	N-CA-CB	9.01	124.01	110.50
6	N	21	G	O4'-C1'-N9	7.04	113.83	108.20
6	N	10	C	O5'-P-OP1	-6.91	99.48	105.70
6	N	4	G	O5'-P-OP2	-6.90	99.49	105.70
4	C	8	ASN	N-CA-C	6.77	129.28	111.00
6	N	21	G	N9-C1'-C2'	6.37	122.28	114.00
6	N	8	C	O5'-P-OP2	-5.98	100.32	105.70
6	N	31	C	N1-C1'-C2'	5.93	121.71	114.00
6	N	11	U	O5'-P-OP1	5.86	117.74	110.70
4	D	30	PRO	N-CA-C	-5.63	97.47	112.10
2	F	33	ASP	CB-CA-C	-5.56	99.28	110.40
1	A	647	PHE	CB-CA-C	-5.39	99.62	110.40
6	N	16	A	C2'-C3'-O3'	5.27	122.14	113.70
6	N	27	A	N9-C1'-C2'	5.15	120.69	114.00
4	C	8	ASN	CB-CA-C	-5.12	100.17	110.40
3	B	188	ARG	NE-CZ-NH2	-5.05	117.78	120.30
6	N	27	A	C3'-C2'-C1'	-5.01	97.49	101.50

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	680	ARG	Sidechain
3	B	179	GLY	Peptide
3	B	182	ARG	Sidechain
3	B	262	SER	Peptide
4	C	100	LYS	Peptide
4	D	62	LEU	Peptide
2	E	190	TYR	Peptide
2	F	128	ARG	Sidechain
2	F	99	ARG	Sidechain
2	G	128	ARG	Sidechain
5	H	309	LYS	Peptide
5	H	66	THR	Peptide

5.2 Too-close contacts ⓘ

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	5726	0	5388	139	0
2	E	1675	0	1642	57	0
2	F	1681	0	1632	61	0
2	G	1621	0	1528	41	0
3	B	2311	0	2213	61	1
4	C	959	0	926	39	0
4	D	904	0	819	32	0
5	H	2499	0	2227	106	0
6	N	670	0	345	36	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
All	All	18048	0	16720	494	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 14.

All (494) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:198:ILE:HD11	5:H:223:SER:CB	1.23	1.57
5:H:198:ILE:CD1	5:H:223:SER:CB	2.17	1.23
5:H:38:PHE:N	5:H:94:ILE:O	1.76	1.17
1:A:1:MET:N	1:A:167:GLN:OE1	1.77	1.17
5:H:37:LYS:HA	5:H:95:SER:HA	1.28	1.14
1:A:22:GLN:HA	1:A:25:THR:HG22	1.33	1.09
5:H:198:ILE:HD11	5:H:223:SER:CA	1.85	1.07
2:E:95:ARG:HH22	2:E:162:GLN:HE21	1.01	0.97
5:H:36:LYS:O	5:H:96:GLU:N	1.97	0.97
1:A:103:THR:O	1:A:189:ASN:ND2	1.98	0.95
5:H:46:PHE:HA	5:H:89:PHE:CD2	2.01	0.95
1:A:22:GLN:HA	1:A:25:THR:CG2	1.97	0.94
2:F:99:ARG:NH1	2:E:192:LYS:HG3	1.88	0.88
1:A:67:ASP:OD1	1:A:224:TYR:N	2.06	0.87
3:B:39:GLU:OE2	3:B:172:SER:OG	1.92	0.87
5:H:38:PHE:O	5:H:93:SER:CB	2.24	0.86
5:H:317:LYS:NZ	6:N:31:C:OP2	2.10	0.85
1:A:708:THR:HG21	4:C:121:PHE:HA	1.60	0.84
5:H:204:ASP:HB3	5:H:315:VAL:HG11	1.59	0.83
2:E:95:ARG:NH2	2:E:162:GLN:HE21	1.76	0.83
5:H:198:ILE:CD1	5:H:223:SER:HA	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:ARG:NH2	6:N:13:U:O2'	2.13	0.82
4:C:72:GLN:HE21	4:C:76:GLN:HE21	1.28	0.81
5:H:29:ARG:NH2	5:H:63:LEU:O	2.13	0.81
3:B:42:LYS:NZ	2:E:154:GLU:OE2	2.14	0.80
1:A:221:ARG:HH22	1:A:238:GLU:CD	1.84	0.79
2:E:95:ARG:HH22	2:E:162:GLN:NE2	1.79	0.79
2:G:212:LEU:O	2:G:216:LEU:HD12	1.81	0.79
5:H:285:GLY:HA2	6:N:30:A:OP1	1.83	0.79
1:A:677:GLN:HG2	1:A:681:GLY:HA3	1.66	0.78
5:H:198:ILE:CD1	5:H:223:SER:CA	2.55	0.77
5:H:46:PHE:HA	5:H:89:PHE:CE2	2.20	0.77
1:A:221:ARG:NH2	1:A:238:GLU:OE1	2.18	0.76
2:E:16:THR:OG1	2:E:190:TYR:O	2.04	0.76
3:B:125:HIS:HB3	3:B:154:THR:HG21	1.67	0.76
2:G:138:ILE:HD11	2:G:190:TYR:OH	1.85	0.76
5:H:18:ILE:HD11	5:H:348:ALA:HB2	1.68	0.76
1:A:104:TYR:HD2	1:A:188:THR:HB	1.51	0.75
3:B:188:ARG:NH2	2:E:150:GLU:OE2	2.20	0.75
3:B:12:ASN:ND2	2:E:100:ASP:OD2	2.20	0.75
2:G:212:LEU:O	2:G:216:LEU:CD1	2.33	0.75
5:H:198:ILE:HD11	5:H:223:SER:HA	1.67	0.74
1:A:685:ILE:HG23	1:A:748:LEU:HD22	1.70	0.74
2:E:21:GLY:HA2	2:E:36:VAL:HA	1.70	0.74
2:F:138:ILE:HD11	2:F:190:TYR:OH	1.88	0.73
1:A:702:ARG:NH1	4:C:113:GLU:OE2	2.21	0.73
1:A:22:GLN:CA	1:A:25:THR:HG22	2.16	0.72
1:A:624:LEU:HD21	3:B:130:THR:HG21	1.70	0.72
6:N:15:U:H2'	6:N:15:U:O2	1.88	0.72
4:D:79:ARG:HH12	5:H:25:LYS:HG3	1.55	0.72
4:D:41:ARG:NH1	2:G:137:GLN:OE1	2.23	0.72
1:A:563:PHE:O	1:A:567:LYS:HE3	1.88	0.72
2:F:29:ILE:O	2:F:30:GLY:O	2.09	0.71
5:H:46:PHE:CA	5:H:89:PHE:CD2	2.75	0.70
3:B:171:SER:O	3:B:174:GLN:HG2	1.92	0.70
2:G:105:ASN:CG	2:G:146:THR:HG22	2.12	0.69
5:H:29:ARG:HH21	5:H:63:LEU:HA	1.57	0.69
5:H:37:LYS:CA	5:H:95:SER:HA	2.17	0.69
4:C:62:LEU:O	4:C:66:ILE:HD12	1.93	0.69
5:H:20:ILE:O	6:N:28:U:OP2	2.10	0.69
1:A:1:MET:HG3	1:A:167:GLN:OE1	1.92	0.69
4:C:6:ASP:OD1	4:C:107:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:286:ALA:HB1	5:H:299:LEU:HD21	1.75	0.68
1:A:657:ARG:NE	1:A:743:GLU:OE1	2.27	0.67
1:A:445:LEU:HD23	1:A:446:PRO:HD2	1.77	0.67
1:A:8:LEU:HA	1:A:51:GLN:HE22	1.60	0.67
5:H:139:ILE:O	5:H:143:THR:HG22	1.95	0.67
5:H:169:TRP:CB	5:H:179:ASP:OD2	2.40	0.67
2:E:138:ILE:HD11	2:E:190:TYR:OH	1.94	0.66
5:H:325:THR:HA	5:H:335:LEU:HG	1.77	0.66
2:F:21:GLY:HA2	2:F:37:ILE:N	2.09	0.66
2:E:92:LYS:O	6:N:5:A:O2'	2.14	0.66
1:A:281:GLU:OE2	1:A:295:ARG:NH2	2.29	0.66
5:H:169:TRP:HB2	5:H:179:ASP:OD2	1.96	0.66
4:C:87:ILE:HD12	4:C:93:LEU:HD11	1.79	0.65
2:E:153:TYR:OH	2:E:166:ASP:OD2	2.14	0.65
5:H:22:ASN:HD22	5:H:118:ILE:HA	1.62	0.65
1:A:37:ASP:OD1	1:A:53:ARG:NH2	2.29	0.65
4:C:20:LEU:HD22	4:C:33:PHE:HD2	1.62	0.65
2:E:171:ARG:HG2	2:E:216:LEU:HD23	1.79	0.65
5:H:245:GLU:HG3	5:H:249:ARG:HH11	1.63	0.64
2:F:3:PHE:HD1	2:F:156:THR:HG22	1.62	0.64
1:A:657:ARG:O	1:A:661:ASN:HB2	1.97	0.64
1:A:689:ILE:HG21	2:E:31:ALA:HB1	1.79	0.64
2:F:115:ARG:HD2	4:C:68:TYR:CE2	2.32	0.64
4:C:37:THR:H	4:C:125:LYS:HB2	1.63	0.63
5:H:355:ILE:O	5:H:356:ASP:HB2	1.99	0.63
5:H:214:PRO:HG3	5:H:320:LYS:HZ1	1.64	0.62
1:A:621:PRO:HD3	3:B:144:GLN:HE22	1.64	0.62
1:A:187:SER:HB3	1:A:190:THR:HG22	1.82	0.62
4:D:29:ASN:O	4:D:30:PRO:O	2.18	0.62
1:A:313:THR:O	1:A:317:VAL:HG23	2.01	0.61
5:H:5:TYR:CE1	5:H:235:THR:HG22	2.36	0.61
1:A:739:LYS:O	1:A:743:GLU:HG3	1.99	0.61
2:G:187:SER:HA	5:H:185:ARG:HG3	1.81	0.61
5:H:254:TYR:HE1	5:H:262:LEU:HD12	1.66	0.61
1:A:136:PHE:CE1	1:A:601:LYS:HG2	2.36	0.61
4:C:87:ILE:CD1	4:C:93:LEU:HD11	2.31	0.61
5:H:28:SER:HA	5:H:31:PHE:CE1	2.36	0.60
1:A:13:LEU:HD23	1:A:173:LEU:HD22	1.82	0.60
1:A:1:MET:HB2	1:A:6:ILE:CD1	2.32	0.60
3:B:14:HIS:HB3	3:B:180:GLY:HA2	1.82	0.60
1:A:552:MET:HE3	1:A:556:PHE:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:159:ASN:O	2:E:162:GLN:N	2.33	0.60
2:F:126:ILE:HD12	6:N:20:C:C2	2.37	0.60
4:C:36:THR:HG23	4:C:125:LYS:HG3	1.83	0.60
1:A:662:VAL:HG22	1:A:743:GLU:HB3	1.83	0.60
2:F:41:ILE:HG23	2:F:42:THR:HG23	1.84	0.60
4:D:59:TYR:OH	4:D:99:ILE:O	2.17	0.59
2:F:144:ASN:HB2	2:G:41:ILE:HD13	1.85	0.59
5:H:131:SER:HA	6:N:26:A:H1'	1.83	0.59
5:H:111:ILE:CD1	5:H:218:TYR:CD2	2.85	0.59
1:A:693:ARG:NH2	2:E:31:ALA:HB2	2.18	0.59
2:E:37:ILE:HD13	2:E:48:PRO:HG3	1.84	0.59
2:F:55:LYS:NZ	2:F:180:ASP:OD1	2.35	0.59
1:A:69:LEU:H	1:A:69:LEU:HD12	1.68	0.59
3:B:74:LYS:HE2	3:B:100:SER:O	2.01	0.59
2:G:198:LEU:HG	2:G:216:LEU:HD23	1.83	0.59
4:C:72:GLN:HE21	4:C:76:GLN:NE2	1.97	0.59
2:G:129:ILE:HG13	5:H:151:ASN:HB3	1.84	0.59
3:B:203:ARG:HD3	3:B:295:PHE:CZ	2.38	0.58
3:B:132:THR:HB	2:E:23:SER:HB3	1.84	0.58
1:A:212:ILE:O	1:A:216:LEU:HD12	2.03	0.58
2:F:115:ARG:NH1	4:C:68:TYR:CZ	2.72	0.58
2:F:159:ASN:O	2:F:162:GLN:N	2.35	0.58
1:A:693:ARG:HH22	2:E:31:ALA:HB2	1.69	0.58
1:A:105:THR:OG1	1:A:142:GLU:HG3	2.03	0.58
1:A:330:PHE:O	1:A:334:ASN:ND2	2.31	0.58
4:C:20:LEU:HD22	4:C:33:PHE:CD2	2.38	0.58
1:A:710:LEU:O	1:A:714:THR:HG23	2.03	0.58
1:A:519:ASP:HB2	1:A:633:GLU:OE2	2.03	0.57
5:H:119:ARG:HA	5:H:125:PRO:HA	1.85	0.57
3:B:33:PHE:CD2	3:B:289:TYR:HB2	2.40	0.57
3:B:71:PHE:O	3:B:72:LEU:HD23	2.03	0.57
2:F:136:ARG:NH1	6:N:19:U:C2	2.73	0.57
2:E:126:ILE:HG13	6:N:14:C:C5	2.39	0.57
2:F:143:ARG:NH2	2:G:39:ASP:CG	2.58	0.57
4:C:39:LYS:HD3	4:C:80:GLU:HG2	1.85	0.57
1:A:709:ARG:O	1:A:713:LEU:HD12	2.04	0.57
3:B:245:SER:HB2	3:B:284:HIS:NE2	2.20	0.57
1:A:539:TYR:O	1:A:544:ARG:HD2	2.05	0.57
1:A:616:PHE:CD1	1:A:625:MET:HG2	2.39	0.57
3:B:103:LEU:HD21	3:B:106:LEU:HD21	1.86	0.57
4:C:76:GLN:OE1	4:C:79:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:44:LEU:HD13	2:E:103:LEU:HD23	1.85	0.57
2:F:108:GLU:O	2:F:111:SER:OG	2.20	0.57
5:H:89:PHE:N	5:H:89:PHE:CD1	2.73	0.57
5:H:258:LYS:HA	5:H:262:LEU:HB2	1.87	0.56
4:D:14:GLU:O	4:D:18:LEU:HD12	2.05	0.56
4:D:56:VAL:O	4:D:56:VAL:CG1	2.52	0.56
2:F:143:ARG:HH21	2:G:39:ASP:CG	2.09	0.56
2:E:138:ILE:HD11	2:E:190:TYR:CZ	2.41	0.56
2:F:21:GLY:HA3	2:F:36:VAL:HA	1.88	0.56
3:B:48:ALA:O	3:B:51:ALA:HB3	2.06	0.55
5:H:111:ILE:HD13	5:H:218:TYR:CE2	2.41	0.55
4:D:58:GLU:OE1	4:D:58:GLU:N	2.37	0.55
4:C:34:PHE:HB3	4:C:82:ALA:HB2	1.89	0.55
4:D:74:VAL:HG12	5:H:63:LEU:HB3	1.89	0.55
4:C:72:GLN:NE2	4:C:76:GLN:HE21	2.02	0.55
4:D:21:GLU:CB	4:D:85:ASP:OD2	2.55	0.55
1:A:132:SER:O	1:A:562:GLN:HG3	2.06	0.55
2:E:171:ARG:HG2	2:E:216:LEU:CD2	2.36	0.55
2:E:185:SER:HB3	2:E:188:ARG:NH2	2.22	0.55
1:A:1:MET:HB2	1:A:6:ILE:HD11	1.89	0.55
4:C:92:ILE:O	4:C:96:LEU:HD12	2.07	0.55
2:F:49:GLY:HA2	2:F:52:LEU:HD12	1.89	0.55
1:A:275:TYR:CD2	1:A:425:LEU:HD21	2.41	0.54
1:A:685:ILE:HG22	1:A:752:ILE:HD11	1.88	0.54
2:E:185:SER:HB3	2:E:188:ARG:HH21	1.71	0.54
5:H:26:TYR:OH	5:H:119:ARG:NH1	2.39	0.54
2:F:138:ILE:HD11	2:F:190:TYR:CZ	2.42	0.54
2:G:212:LEU:O	2:G:216:LEU:HD13	2.07	0.54
2:E:202:THR:HG21	2:E:207:TYR:O	2.08	0.54
3:B:132:THR:H	2:E:23:SER:HB2	1.72	0.54
2:E:136:ARG:HH22	6:N:13:U:C2'	2.20	0.54
2:G:77:ASP:O	2:G:81:ARG:HB2	2.08	0.54
5:H:271:GLN:HE22	5:H:343:TYR:HD2	1.55	0.54
5:H:3:ASN:HA	5:H:357:LYS:C	2.28	0.54
2:F:188:ARG:NH1	6:N:18:C:OP2	2.41	0.53
3:B:219:LEU:HD22	3:B:257:LEU:HD11	1.91	0.53
4:D:90:ALA:HB3	4:D:92:ILE:CD1	2.38	0.53
2:G:104:SER:HB2	2:G:146:THR:HG23	1.90	0.53
3:B:58:PHE:O	3:B:206:LYS:NZ	2.42	0.53
2:G:123:GLU:OE1	2:G:190:TYR:OH	2.26	0.53
2:F:189:GLY:HA2	2:G:98:PHE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:C	1:A:569:LEU:HD12	2.29	0.53
4:C:93:LEU:HA	4:C:96:LEU:HD13	1.90	0.53
3:B:216:THR:HB	3:B:292:PRO:HA	1.90	0.53
5:H:111:ILE:HD13	5:H:218:TYR:CZ	2.43	0.52
2:F:21:GLY:CA	2:F:36:VAL:HA	2.38	0.52
1:A:110:ILE:HD12	1:A:110:ILE:H	1.75	0.52
1:A:647:PHE:CD1	1:A:647:PHE:N	2.76	0.52
1:A:21:ILE:O	1:A:25:THR:HG22	2.09	0.52
4:D:7:GLU:OE1	4:D:7:GLU:HA	2.10	0.52
2:G:138:ILE:HD11	2:G:190:TYR:CZ	2.44	0.52
5:H:198:ILE:CG1	5:H:223:SER:CB	2.86	0.52
5:H:47:TYR:OH	5:H:60:GLU:OE1	2.19	0.52
3:B:132:THR:OG1	3:B:144:GLN:HG3	2.10	0.52
4:D:63:LEU:HA	4:D:66:ILE:HD13	1.91	0.52
1:A:676:HIS:ND1	1:A:718:ASP:OD2	2.41	0.52
3:B:8:MET:HG2	3:B:189:PHE:CE1	2.44	0.52
2:F:115:ARG:HD2	4:C:68:TYR:HE2	1.75	0.52
4:C:93:LEU:H	4:C:93:LEU:HD12	1.74	0.52
2:F:14:LEU:HB2	2:F:143:ARG:O	2.09	0.52
2:G:37:ILE:HD13	2:G:48:PRO:HG3	1.92	0.52
5:H:89:PHE:HD1	5:H:89:PHE:H	1.56	0.52
1:A:532:SER:HA	1:A:537:GLY:HA2	1.92	0.52
2:G:128:ARG:CZ	5:H:138:THR:HG22	2.39	0.52
5:H:127:ILE:HD12	5:H:228:ILE:HG21	1.92	0.51
1:A:111:PHE:HA	1:A:114:PHE:HB3	1.91	0.51
2:G:33:ASP:N	2:G:33:ASP:OD1	2.41	0.51
1:A:383:ASP:OD1	1:A:386:THR:OG1	2.27	0.51
3:B:43:MET:HE2	3:B:45:LYS:HE3	1.93	0.51
5:H:22:ASN:ND2	5:H:118:ILE:HA	2.24	0.51
1:A:142:GLU:HB3	1:A:143:PRO:HD3	1.93	0.51
1:A:51:GLN:O	1:A:55:HIS:HB3	2.11	0.51
6:N:15:U:O2	6:N:15:U:C2'	2.59	0.51
2:F:47:ILE:HB	2:F:101:ALA:HB3	1.93	0.51
5:H:169:TRP:HA	5:H:179:ASP:CG	2.27	0.51
5:H:261:PHE:O	5:H:264:GLU:HG2	2.11	0.51
4:D:90:ALA:HB3	4:D:92:ILE:HD12	1.92	0.51
5:H:147:TRP:HB3	5:H:166:LEU:HD21	1.93	0.50
5:H:5:TYR:CD1	5:H:235:THR:HG22	2.46	0.50
1:A:39:PHE:HE1	1:A:165:PHE:CE2	2.28	0.50
1:A:475:TYR:CE1	1:A:486:PHE:CZ	2.99	0.50
4:D:71:VAL:CG2	5:H:47:TYR:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:PRO:CD	3:B:144:GLN:HE22	2.23	0.50
1:A:8:LEU:HD13	1:A:69:LEU:HB3	1.93	0.50
3:B:61:THR:HG22	3:B:158:VAL:HG13	1.93	0.50
5:H:17:PRO:HA	5:H:222:ILE:O	2.11	0.50
1:A:359:SER:N	1:A:360:PRO:HD2	2.27	0.50
1:A:156:ILE:HD11	1:A:180:THR:OG1	2.12	0.50
2:F:109:LEU:HB3	2:F:114:VAL:HG21	1.94	0.50
5:H:276:TYR:O	5:H:349:ASN:HA	2.11	0.50
2:F:99:ARG:NH1	2:E:192:LYS:CG	2.68	0.50
5:H:36:LYS:O	5:H:96:GLU:CB	2.60	0.50
1:A:513:LEU:HD21	1:A:625:MET:HE1	1.93	0.50
3:B:64:PHE:CE1	3:B:73:PRO:HD3	2.46	0.50
5:H:46:PHE:CA	5:H:89:PHE:HD2	2.24	0.50
2:G:105:ASN:CB	2:G:146:THR:HG22	2.41	0.50
3:B:149:ARG:HH11	2:E:39:ASP:CG	2.16	0.49
2:F:188:ARG:HD2	6:N:19:U:OP2	2.12	0.49
3:B:41:LEU:HD12	3:B:46:LEU:HD22	1.95	0.49
2:E:36:VAL:O	2:E:38:LYS:HG3	2.12	0.49
1:A:510:ILE:HG13	1:A:512:ARG:HG2	1.95	0.49
1:A:9:PHE:CE2	1:A:170:ILE:HG13	2.48	0.49
2:G:105:ASN:HB3	2:G:146:THR:HG22	1.95	0.49
3:B:61:THR:CG2	3:B:159:ILE:H	2.26	0.49
2:E:20:ILE:HA	6:N:10:C:OP1	2.13	0.49
4:D:29:ASN:C	4:D:30:PRO:O	2.51	0.49
5:H:134:GLY:HA3	6:N:26:A:O4'	2.13	0.49
2:F:12:ILE:HG23	2:F:193:VAL:HG13	1.95	0.49
6:N:28:U:H2'	6:N:29:U:O2	2.13	0.49
1:A:657:ARG:HE	1:A:743:GLU:CD	2.13	0.48
3:B:96:GLN:HB2	3:B:119:LEU:HD13	1.95	0.48
1:A:25:THR:HG23	1:A:27:GLU:H	1.79	0.48
1:A:344:GLY:HA2	1:A:373:MET:SD	2.53	0.48
4:D:83:VAL:O	4:D:87:ILE:HG13	2.13	0.48
2:G:130:THR:O	5:H:302:ARG:NH2	2.41	0.48
2:F:115:ARG:NH1	4:C:68:TYR:CE2	2.82	0.48
2:G:41:ILE:HG23	2:G:42:THR:HG23	1.95	0.48
1:A:298:MET:SD	1:A:301:VAL:HG22	2.54	0.48
1:A:291:LEU:HD13	1:A:310:LEU:HD13	1.95	0.48
5:H:260:PHE:CE1	5:H:313:LYS:HE2	2.48	0.48
1:A:677:GLN:CG	1:A:681:GLY:HA3	2.40	0.48
2:F:69:ALA:HB1	2:F:74:ASP:HB2	1.96	0.48
1:A:685:ILE:CG2	1:A:752:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:VAL:HG21	5:H:47:TYR:HB2	1.96	0.48
4:D:28:LYS:O	4:D:30:PRO:HD3	2.14	0.48
2:F:36:VAL:O	2:F:38:LYS:HG3	2.13	0.47
3:B:237:THR:CG2	3:B:261:ALA:HB2	2.43	0.47
2:E:12:ILE:HG23	2:E:193:VAL:HG13	1.95	0.47
4:D:50:LEU:HD21	4:D:66:ILE:HG13	1.95	0.47
4:D:70:ARG:O	4:D:74:VAL:HG23	2.14	0.47
5:H:198:ILE:CG1	5:H:223:SER:CA	2.92	0.47
5:H:254:TYR:HE2	5:H:273:ASN:HB3	1.78	0.47
6:N:29:U:O2	6:N:29:U:O4'	2.32	0.47
6:N:31:C:O2	6:N:31:C:H2'	2.15	0.47
1:A:373:MET:HG2	1:A:377:LYS:HE3	1.97	0.47
1:A:434:HIS:NE2	1:A:457:ALA:HB2	2.30	0.47
1:A:642:ASP:HB3	1:A:654:LYS:HE2	1.96	0.47
6:N:20:C:O2	6:N:20:C:O4'	2.28	0.47
1:A:69:LEU:N	1:A:69:LEU:HD12	2.29	0.47
3:B:147:THR:HG21	3:B:186:PHE:CE1	2.49	0.47
5:H:111:ILE:CD1	5:H:218:TYR:CE2	2.98	0.47
5:H:54:ARG:HG2	5:H:54:ARG:O	2.15	0.47
1:A:125:PRO:HG2	1:A:148:ASP:HB3	1.97	0.47
1:A:639:ASN:C	1:A:641:LYS:H	2.17	0.47
3:B:234:TYR:HA	3:B:264:SER:HB3	1.97	0.47
6:N:28:U:O2	6:N:28:U:O4'	2.33	0.47
2:F:14:LEU:O	2:F:143:ARG:O	2.32	0.47
1:A:257:ASN:O	1:A:258:ILE:HD13	2.15	0.47
1:A:388:MET:HE3	1:A:388:MET:HA	1.97	0.47
2:E:105:ASN:ND2	2:E:146:THR:HG23	2.30	0.47
5:H:37:LYS:HA	5:H:95:SER:CA	2.20	0.47
2:G:12:ILE:O	2:G:146:THR:HA	2.15	0.47
1:A:285:ASP:OD2	1:A:295:ARG:NH1	2.47	0.47
2:E:104:SER:HG	2:E:146:THR:HG1	1.53	0.47
5:H:285:GLY:CA	6:N:30:A:OP1	2.58	0.47
4:D:87:ILE:HG23	4:D:92:ILE:HB	1.97	0.46
2:F:96:LEU:HD22	2:F:151:LEU:HD11	1.97	0.46
5:H:300:GLN:NE2	5:H:312:LYS:O	2.47	0.46
1:A:503:LYS:HD2	1:A:507:GLY:O	2.15	0.46
4:C:62:LEU:CD1	4:C:66:ILE:HD11	2.45	0.46
2:F:81:ARG:NH1	2:F:166:ASP:OD1	2.40	0.46
6:N:18:C:O2'	6:N:19:U:H5'	2.16	0.46
3:B:65:PRO:O	3:B:71:PHE:HB2	2.15	0.46
5:H:325:THR:HA	5:H:335:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ILE:HA	1:A:421:ILE:HD13	1.78	0.46
1:A:552:MET:HE3	1:A:556:PHE:CE2	2.49	0.46
3:B:218:ALA:HA	3:B:290:ALA:HB1	1.98	0.46
2:G:182:LEU:HD12	2:G:182:LEU:HA	1.82	0.46
2:G:156:THR:HG23	2:G:157:ASP:H	1.81	0.46
5:H:35:ASN:O	5:H:36:LYS:C	2.54	0.46
1:A:751:TYR:O	1:A:754:GLU:HB3	2.16	0.46
3:B:257:LEU:CD2	3:B:259:LYS:HD2	2.46	0.46
1:A:215:TYR:CE1	1:A:240:ALA:HA	2.51	0.45
1:A:512:ARG:HD3	1:A:617:ALA:HA	1.97	0.45
1:A:203:ARG:NH1	1:A:295:ARG:O	2.50	0.45
1:A:659:ILE:O	1:A:664:ASP:OD1	2.35	0.45
3:B:96:GLN:HA	3:B:99:LEU:HB2	1.98	0.45
5:H:131:SER:HA	6:N:26:A:C1'	2.47	0.45
5:H:132:LEU:O	5:H:136:ILE:HD13	2.17	0.45
3:B:3:TYR:HB2	3:B:161:ASN:HA	1.98	0.45
4:C:77:ALA:HA	4:C:83:VAL:HG12	1.97	0.45
1:A:692:LEU:HD22	1:A:741:ARG:HB2	1.98	0.45
5:H:229:GLU:HG3	5:H:230:PHE:N	2.32	0.45
5:H:20:ILE:CG2	6:N:28:U:OP1	2.65	0.45
1:A:1:MET:HB2	1:A:6:ILE:HD13	1.99	0.45
1:A:425:LEU:HD23	1:A:445:LEU:HD11	1.98	0.45
5:H:13:LEU:HA	5:H:226:THR:O	2.17	0.45
4:C:5:THR:H	4:C:8:ASN:HB2	1.82	0.45
1:A:221:ARG:NH1	1:A:227:ASP:OD2	2.49	0.45
4:D:14:GLU:HG2	4:D:18:LEU:HD11	1.99	0.45
3:B:33:PHE:CG	3:B:289:TYR:HB2	2.51	0.45
1:A:400:GLU:OE1	3:B:253:ARG:NH1	2.50	0.44
5:H:41:PRO:HA	5:H:90:GLY:HA3	1.98	0.44
5:H:46:PHE:CB	5:H:89:PHE:CE2	3.00	0.44
1:A:246:PHE:CE2	1:A:306:ALA:HB3	2.52	0.44
1:A:248:LEU:HD23	1:A:251:ILE:HD11	1.99	0.44
1:A:244:ALA:HB3	1:A:310:LEU:HD21	2.00	0.44
2:E:47:ILE:HB	2:E:101:ALA:HB3	1.99	0.44
3:B:61:THR:OG1	3:B:215:LEU:O	2.34	0.44
4:C:125:LYS:HE2	4:C:125:LYS:HB3	1.76	0.44
4:D:63:LEU:HD23	4:D:66:ILE:HD13	2.00	0.44
2:E:104:SER:OG	2:E:146:THR:OG1	2.24	0.44
2:F:115:ARG:CD	4:C:68:TYR:CE2	3.00	0.44
2:F:163:VAL:HG12	2:F:167:PHE:CE2	2.52	0.44
1:A:9:PHE:CZ	1:A:13:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:74:VAL:HG11	4:D:118:TYR:CE1	2.52	0.44
2:E:182:LEU:HD12	2:E:182:LEU:HA	1.83	0.44
1:A:596:ARG:HD3	1:A:655:PHE:CD1	2.52	0.44
2:F:143:ARG:HD2	2:G:102:PHE:CZ	2.52	0.44
2:F:180:ASP:O	2:G:99:ARG:NH2	2.47	0.44
1:A:519:ASP:HB3	1:A:637:LYS:HE3	1.98	0.44
2:G:105:ASN:HB3	2:G:146:THR:CG2	2.48	0.44
1:A:1:MET:CG	1:A:167:GLN:OE1	2.64	0.43
2:F:182:LEU:HA	2:F:182:LEU:HD12	1.80	0.43
2:F:98:PHE:O	2:E:189:GLY:HA2	2.18	0.43
2:G:181:TYR:CE2	2:G:186:GLY:HA3	2.53	0.43
2:G:97:ILE:HB	2:G:152:ILE:HB	1.99	0.43
1:A:703:LEU:HD22	1:A:733:TYR:CG	2.53	0.43
4:C:50:LEU:HD13	4:C:105:LEU:HD11	2.00	0.43
2:G:121:LYS:HB2	2:G:140:ARG:HD2	2.01	0.43
2:F:21:GLY:O	6:N:15:U:H2'	2.19	0.43
2:F:97:ILE:HB	2:F:152:ILE:HB	2.00	0.43
1:A:572:ILE:HB	1:A:580:PHE:HD1	1.83	0.43
3:B:108:LEU:HD22	3:B:200:LEU:HB2	2.00	0.43
4:D:7:GLU:O	4:D:8:ASN:OD1	2.36	0.43
2:F:124:ASN:HD22	2:F:133:ALA:HB1	1.82	0.43
2:F:153:TYR:OH	2:F:166:ASP:OD2	2.28	0.43
2:F:181:TYR:CE2	2:F:186:GLY:HA3	2.53	0.43
5:H:180:LEU:HD12	5:H:180:LEU:O	2.19	0.43
5:H:29:ARG:HH21	5:H:63:LEU:CA	2.28	0.43
2:F:135:PRO:HB3	6:N:21:G:C5	2.52	0.43
3:B:257:LEU:HD23	3:B:259:LYS:HD2	2.00	0.43
2:E:97:ILE:HB	2:E:152:ILE:HB	2.00	0.43
2:G:64:TYR:OH	2:G:172:ASP:OD2	2.29	0.43
5:H:46:PHE:CB	5:H:89:PHE:HE2	2.30	0.43
4:C:35:LEU:HD21	4:C:86:LEU:HD22	2.00	0.43
2:E:24:ASP:O	2:E:28:ALA:N	2.51	0.43
5:H:45:LYS:HB3	5:H:89:PHE:HB2	2.01	0.43
2:E:136:ARG:NH2	6:N:13:U:C2'	2.82	0.43
6:N:29:U:C2'	6:N:30:A:H5'	2.49	0.43
1:A:38:TRP:NE1	1:A:157:LYS:HG2	2.33	0.43
1:A:737:ASN:OD1	1:A:739:LYS:HG2	2.19	0.43
4:C:5:THR:O	4:C:8:ASN:HB2	2.19	0.43
2:E:138:ILE:HD11	2:E:190:TYR:CE2	2.54	0.43
4:C:69:LEU:HD22	4:C:73:PHE:CD2	2.54	0.43
5:H:118:ILE:O	5:H:118:ILE:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:205:TYR:C	5:H:205:TYR:CD1	2.92	0.43
5:H:3:ASN:HA	5:H:357:LYS:O	2.19	0.43
2:G:123:GLU:HA	6:N:27:A:H5''	2.00	0.43
1:A:324:GLU:HB2	1:A:343:PHE:CD1	2.54	0.42
3:B:27:PHE:CE1	3:B:63:ALA:HB2	2.54	0.42
1:A:704:ALA:HB1	4:C:121:PHE:CD1	2.54	0.42
3:B:149:ARG:NH1	2:E:39:ASP:CG	2.72	0.42
5:H:100:GLU:HA	5:H:201:GLN:NE2	2.34	0.42
5:H:46:PHE:CA	5:H:89:PHE:CE2	2.96	0.42
1:A:181:LEU:HD13	1:A:198:LEU:HD23	2.02	0.42
1:A:285:ASP:CG	1:A:295:ARG:HH11	2.21	0.42
4:D:56:VAL:HG12	4:D:56:VAL:O	2.19	0.42
5:H:7:THR:HG22	5:H:233:THR:HG22	2.01	0.42
1:A:396:SER:OG	1:A:396:SER:O	2.29	0.42
4:D:22:ARG:CB	4:D:31:ASP:O	2.67	0.42
1:A:72:ILE:O	1:A:75:ILE:HG22	2.19	0.42
3:B:213:MET:HG3	3:B:263:GLY:HA3	2.02	0.42
2:G:153:TYR:OH	2:G:166:ASP:OD2	2.27	0.42
1:A:539:TYR:HA	1:A:544:ARG:NH1	2.35	0.42
1:A:710:LEU:HA	1:A:710:LEU:HD12	1.92	0.42
3:B:130:THR:HA	3:B:146:ALA:HA	2.00	0.42
2:F:156:THR:O	2:F:157:ASP:C	2.57	0.42
5:H:312:LYS:H	5:H:312:LYS:HD2	1.85	0.42
2:F:119:GLU:CD	2:F:140:ARG:HH21	2.23	0.42
5:H:129:GLY:H	5:H:188:ASP:HA	1.85	0.42
1:A:212:ILE:HG23	1:A:216:LEU:HD11	2.00	0.42
2:F:140:ARG:HD3	2:F:190:TYR:CE2	2.55	0.42
3:B:249:ASN:OD1	2:E:89:LYS:N	2.51	0.42
2:E:61:ALA:HA	2:E:79:LEU:HD11	2.02	0.42
3:B:176:SER:OG	2:E:5:LYS:NZ	2.53	0.42
6:N:3:G:H4'	6:N:4:G:H5'	2.02	0.42
1:A:349:ALA:O	1:A:351:LYS:N	2.53	0.42
5:H:142:ASN:ND2	5:H:290:THR:O	2.50	0.42
1:A:29:LYS:HE3	1:A:34:VAL:HG22	2.01	0.41
3:B:174:GLN:HB2	3:B:189:PHE:O	2.20	0.41
4:D:7:GLU:C	4:D:8:ASN:OD1	2.58	0.41
4:D:87:ILE:HA	4:D:92:ILE:HD13	2.02	0.41
2:F:99:ARG:HH12	2:E:192:LYS:HG3	1.81	0.41
6:N:12:U:O2'	6:N:13:U:H5'	2.19	0.41
1:A:298:MET:SD	1:A:301:VAL:CG2	3.07	0.41
3:B:262:SER:HA	3:B:263:GLY:HA2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:TYR:HE1	2:E:30:GLY:HA3	1.85	0.41
2:F:109:LEU:HB3	2:F:114:VAL:CG2	2.50	0.41
5:H:198:ILE:HG13	5:H:223:SER:N	2.35	0.41
2:E:86:SER:HB2	6:N:5:A:H8	1.86	0.41
1:A:51:GLN:HE21	1:A:69:LEU:CB	2.33	0.41
1:A:709:ARG:HA	1:A:709:ARG:HD2	1.94	0.41
1:A:150:ALA:O	1:A:154:THR:HG23	2.20	0.41
3:B:196:ILE:HA	3:B:197:PRO:HD2	1.93	0.41
3:B:284:HIS:CE1	6:N:1:A:C8	3.08	0.41
5:H:245:GLU:HG3	5:H:249:ARG:NH1	2.34	0.41
2:F:135:PRO:HB3	6:N:21:G:C6	2.56	0.41
1:A:130:LEU:HD22	1:A:475:TYR:CD2	2.55	0.41
1:A:285:ASP:CG	1:A:295:ARG:NH1	2.74	0.41
1:A:410:LEU:HD13	1:A:417:LYS:HG2	2.02	0.41
3:B:266:PHE:CD1	3:B:266:PHE:N	2.88	0.41
2:E:140:ARG:HD3	2:E:190:TYR:CE2	2.54	0.41
2:F:99:ARG:HH11	2:E:192:LYS:CD	2.33	0.41
2:F:150:GLU:OE2	2:E:192:LYS:NZ	2.50	0.41
2:G:138:ILE:HD11	2:G:190:TYR:CE2	2.55	0.41
5:H:111:ILE:HD11	5:H:218:TYR:CD2	2.56	0.41
1:A:242:LEU:HA	1:A:346:GLY:O	2.21	0.41
1:A:378:LYS:HE2	1:A:378:LYS:HB3	1.91	0.41
2:G:96:LEU:HD22	2:G:151:LEU:HD11	2.02	0.41
3:B:30:ASP:OD2	3:B:259:LYS:NZ	2.39	0.41
4:D:41:ARG:HG3	4:D:42:ASN:N	2.35	0.41
2:F:102:PHE:CE1	2:E:143:ARG:HD3	2.56	0.41
2:F:6:ILE:HD11	2:F:155:ILE:HD11	2.02	0.41
1:A:62:ASP:O	1:A:64:LEU:HD23	2.21	0.41
4:D:74:VAL:HG21	5:H:60:GLU:HG2	2.02	0.41
3:B:149:ARG:NH1	2:E:39:ASP:OD1	2.53	0.41
2:F:12:ILE:O	2:F:146:THR:HA	2.20	0.41
2:F:3:PHE:CD1	2:F:156:THR:HG22	2.49	0.41
2:F:81:ARG:O	2:F:95:ARG:HG3	2.20	0.41
5:H:25:LYS:HE3	5:H:115:ASN:OD1	2.20	0.41
1:A:254:PHE:CD1	1:A:276:LEU:HD11	2.55	0.41
1:A:494:GLU:HB3	1:A:496:TYR:CE2	2.55	0.41
1:A:568:LYS:HE3	1:A:587:ASP:OD2	2.20	0.41
3:B:10:PHE:CD2	3:B:189:PHE:HB3	2.56	0.41
5:H:321:ALA:HB3	5:H:343:TYR:CD1	2.55	0.41
1:A:291:LEU:CD1	1:A:310:LEU:HD13	2.50	0.41
1:A:655:PHE:O	1:A:659:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:LEU:HA	1:A:749:LEU:HD23	1.79	0.41
5:H:204:ASP:OD2	6:N:31:C:O2'	2.28	0.41
1:A:142:GLU:N	1:A:143:PRO:CD	2.84	0.40
3:B:138:LYS:HA	3:B:138:LYS:HD3	1.68	0.40
2:G:81:ARG:NH1	2:G:166:ASP:OD1	2.54	0.40
1:A:152:ILE:HG23	1:A:180:THR:HB	2.02	0.40
1:A:707:LEU:HD23	1:A:707:LEU:HA	1.93	0.40
4:C:20:LEU:HA	4:C:89:LYS:HD3	2.03	0.40
2:E:98:PHE:CE1	2:E:151:LEU:HD13	2.57	0.40
2:F:32:ILE:H	2:F:32:ILE:HG13	1.56	0.40
5:H:46:PHE:N	5:H:89:PHE:HD2	2.20	0.40
1:A:515:VAL:O	1:A:613:ILE:HA	2.22	0.40
4:C:20:LEU:HD23	4:C:21:GLU:N	2.36	0.40
4:C:74:VAL:HG23	4:D:117:ALA:HB1	2.03	0.40
5:H:15:LEU:O	5:H:271:GLN:NE2	2.54	0.40
3:B:104:GLN:HB3	3:B:105:PHE:CD2	2.55	0.40
5:H:316:LEU:HD23	5:H:318:LEU:HG	2.04	0.40
1:A:447:ILE:HD12	1:A:447:ILE:HA	1.96	0.40
3:B:220:PRO:HG3	3:B:270:PHE:CE1	2.57	0.40
4:C:62:LEU:HD13	4:C:66:ILE:HD11	2.03	0.40
4:C:75:TYR:CD2	2:G:29:ILE:HG23	2.57	0.40
2:G:128:ARG:HH12	5:H:137:ARG:HG2	1.87	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)
3:B:209:SER:OG	3:B:250:GLU:OE1[2_557]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/758 (96%)	688 (95%)	34 (5%)	3 (0%)	34	66
2	E	217/220 (99%)	206 (95%)	9 (4%)	2 (1%)	17	48
2	F	218/220 (99%)	208 (95%)	9 (4%)	1 (0%)	29	61
2	G	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
3	B	295/299 (99%)	282 (96%)	13 (4%)	0	100	100
4	C	122/126 (97%)	118 (97%)	3 (2%)	1 (1%)	19	51
4	D	121/126 (96%)	112 (93%)	8 (7%)	1 (1%)	19	51
5	H	337/357 (94%)	291 (86%)	39 (12%)	7 (2%)	7	26
All	All	2253/2326 (97%)	2115 (94%)	123 (6%)	15 (1%)	22	54

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	30	GLY
4	D	30	PRO
5	H	68	PRO
5	H	329	PRO
2	E	207	TYR
5	H	356	ASP
1	A	350	ALA
1	A	639	ASN
1	A	647	PHE
2	E	31	ALA
5	H	92	TYR
5	H	149	ASN
5	H	296	ASP
5	H	305	ARG
4	C	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/651 (87%)	527 (93%)	37 (7%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	173/188 (92%)	164 (95%)	9 (5%)	23	55
2	F	172/188 (92%)	168 (98%)	4 (2%)	50	80
2	G	156/188 (83%)	147 (94%)	9 (6%)	20	50
3	B	243/263 (92%)	228 (94%)	15 (6%)	18	47
4	C	91/112 (81%)	85 (93%)	6 (7%)	16	44
4	D	77/112 (69%)	69 (90%)	8 (10%)	7	21
5	H	217/312 (70%)	195 (90%)	22 (10%)	7	23
All	All	1693/2014 (84%)	1583 (94%)	110 (6%)	17	45

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

Mol	Chain	Res	Type
1	A	68	HIS
1	A	110	ILE
1	A	188	THR
1	A	197	SER
1	A	262	THR
1	A	310	LEU
1	A	314	GLU
1	A	332	LEU
1	A	347	SER
1	A	352	ASP
1	A	371	SER
1	A	386	THR
1	A	392	ARG
1	A	417	LYS
1	A	419	CYS
1	A	420	ASP
1	A	462	SER
1	A	489	ASP
1	A	506	ASN
1	A	543	SER
1	A	568	LYS
1	A	570	SER
1	A	601	LYS
1	A	624	LEU
1	A	645	SER
1	A	647	PHE
1	A	649	SER
1	A	654	LYS

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Mol	Chain	Res	Type
1	A	655	PHE
1	A	656	ASP
1	A	657	ARG
1	A	664	ASP
1	A	697	ARG
1	A	713	LEU
1	A	715	ARG
1	A	717	THR
1	A	727	ASN
2	F	32	ILE
2	F	99	ARG
2	F	203	VAL
2	F	216	LEU
3	B	9	THR
3	B	30	ASP
3	B	88	VAL
3	B	119	LEU
3	B	137	HIS
3	B	138	LYS
3	B	149	ARG
3	B	153	ASP
3	B	172	SER
3	B	176	SER
3	B	188	ARG
3	B	198	LEU
3	B	209	SER
3	B	245	SER
3	B	266	PHE
2	E	13	ARG
2	E	23	SER
2	E	40	PRO
2	E	66	GLU
2	E	95	ARG
2	E	130	THR
2	E	143	ARG
2	E	157	ASP
2	E	160	GLU
4	C	50	LEU
4	C	62	LEU
4	C	69	LEU
4	C	80	GLU
4	C	100	LYS

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Mol	Chain	Res	Type
4	C	125	LYS
4	D	6	ASP
4	D	8	ASN
4	D	10	VAL
4	D	34	PHE
4	D	43	LEU
4	D	51	PHE
4	D	68	TYR
4	D	96	LEU
2	G	73	SER
2	G	93	MET
2	G	99	ARG
2	G	111	SER
2	G	134	ASN
2	G	137	GLN
2	G	176	LEU
2	G	199	LYS
2	G	209	VAL
5	H	11	SER
5	H	20	ILE
5	H	29	ARG
5	H	45	LYS
5	H	59	PHE
5	H	83	ARG
5	H	89	PHE
5	H	136	ILE
5	H	143	THR
5	H	148	ASN
5	H	153	VAL
5	H	197	LEU
5	H	198	ILE
5	H	208	LYS
5	H	248	LYS
5	H	256	ASP
5	H	271	GLN
5	H	273	ASN
5	H	299	LEU
5	H	316	LEU
5	H	338	ASN
5	H	341	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
3	B	83	GLN
3	B	144	GLN
2	E	162	GLN
4	C	72	GLN
5	H	148	ASN
5	H	201	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	N	31/40 (77%)	12 (38%)	3 (9%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	N	2	C
6	N	3	G
6	N	9	G
6	N	10	C
6	N	15	U
6	N	17	G
6	N	18	C
6	N	22	C
6	N	27	A
6	N	28	U
6	N	30	A
6	N	32	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	N	7	A
6	N	13	U
6	N	25	U

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

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

5.5 Carbohydrates [i](#)

There are no 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, 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	733/758 (96%)	-0.56	2 (0%) 94 94	22, 43, 79, 113	0
2	E	219/220 (99%)	-0.41	2 (0%) 84 84	26, 43, 85, 135	0
2	F	220/220 (100%)	-0.28	0 100 100	34, 55, 84, 129	0
2	G	220/220 (100%)	-0.03	3 (1%) 75 75	41, 65, 96, 122	0
3	B	297/299 (99%)	-0.59	1 (0%) 94 94	18, 32, 61, 119	0
4	C	124/126 (98%)	-0.44	0 100 100	35, 55, 80, 101	0
4	D	123/126 (97%)	0.08	5 (4%) 37 32	49, 72, 101, 127	0
5	H	345/357 (96%)	0.10	20 (5%) 23 19	40, 70, 106, 129	0
6	N	32/40 (80%)	-0.35	0 100 100	20, 43, 79, 118	0
All	All	2313/2366 (97%)	-0.33	33 (1%) 75 75	18, 52, 93, 135	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	30	PRO	5.4
5	H	3	ASN	5.1
5	H	310	MET	4.6
3	B	85	ASP	4.3
5	H	78	PHE	4.1
2	G	26	PHE	3.5
2	G	68	VAL	3.3
1	A	104	TYR	3.2
1	A	189	ASN	2.9
4	D	32	ALA	2.8
5	H	305	ARG	2.8
5	H	204	ASP	2.7
5	H	192	PHE	2.7
4	D	63	LEU	2.7
5	H	80	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
5	H	60	GLU	2.7
5	H	65	GLN	2.6
2	E	27	ALA	2.6
5	H	84	ILE	2.4
5	H	37	LYS	2.3
5	H	61	ALA	2.3
2	G	144	ASN	2.3
4	D	64	ASP	2.3
5	H	306	MET	2.2
5	H	15	LEU	2.2
4	D	108	PHE	2.2
5	H	205	TYR	2.1
2	E	69	ALA	2.1
5	H	38	PHE	2.1
5	H	86	GLU	2.1
5	H	72	ASN	2.1
5	H	55	LEU	2.0
5	H	341	SER	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, 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
8	MN	A	802	1/1	0.99	0.12	66,66,66,66	0
7	ZN	A	801	1/1	1.00	0.09	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.