



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:29 AM UTC

PDB ID : 7Z4D / pdb_00007z4d
Title : Crystal structure of SpCas9 bound to a 10 nucleotide complementary DNA substrate
Authors : Pacesa, M.; Jinek, M.
Deposited on : 2022-03-03
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
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

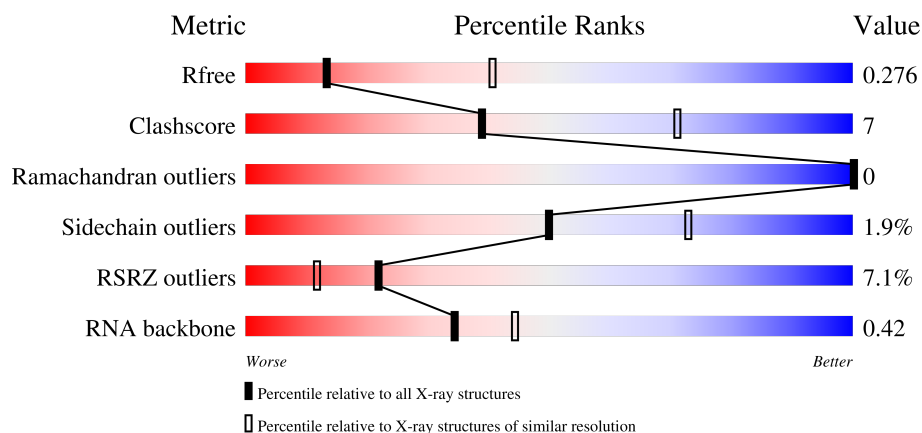
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	84	5% 39% 43% 7% 11%
1	F	84	5% 35% 44% 13% 8%
2	B	1368	6% 78% 13% 8%
2	E	1368	7% 70% 15% 15%

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Mol	Chain	Length	Quality of chain
3	C	30	3% 37% 63%
3	G	30	7% 33% 57% 10%
4	D	30	13% 50% 23% 27%
4	H	30	7% 43% 20% 37%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25082 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 RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	75	Total	C	N	O	P	0	0	0
			1610	723	303	510	74			
1	F	77	Total	C	N	O	P	0	0	0
			1652	742	310	524	76			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1259	Total	C	N	O	S	0	0	0
			10259	6549	1769	1921	20			
2	E	1166	Total	C	N	O	S	0	0	0
			9537	6102	1640	1776	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
E	10	ALA	ASP	engineered mutation	UNP Q99ZW2
E	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called Target strand of 10 nucleotide complementary DNA substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			606	291	105	181	29			
3	G	27	Total	C	N	O	P	0	0	1
			526	252	90	159	25			

- Molecule 4 is a DNA chain called Non-target strand of 10 nucleotide complementary DNA substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	22	Total	C	N	O	P	0	0	1
			429	207	75	127	20			
4	H	19	Total	C	N	O	P	0	0	1
			359	172	64	106	17			

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	K	0	0
			6	6		
5	B	3	Total	K	0	0
			3	3		
5	C	1	Total	K	0	0
			1	1		
5	E	2	Total	K	0	0
			2	2		
5	F	3	Total	K	0	0
			3	3		
5	G	1	Total	K	0	0
			1	1		

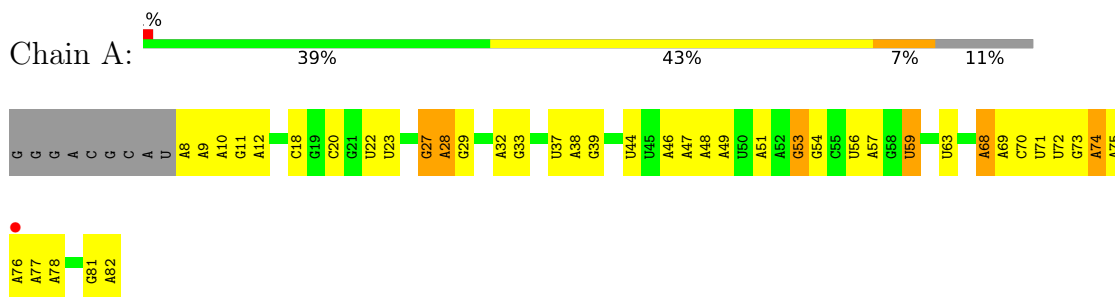
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total	O	0	0
			15	15		
6	B	22	Total	O	0	0
			22	22		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		
6	E	29	Total	O	0	0
			29	29		
6	F	14	Total	O	0	0
			14	14		
6	G	1	Total	O	0	0
			1	1		
6	H	4	Total	O	0	0
			4	4		

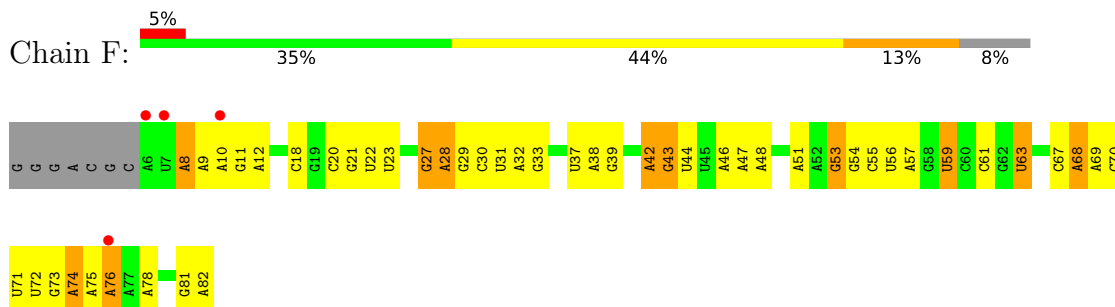
3 Residue-property plots [i](#)

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.

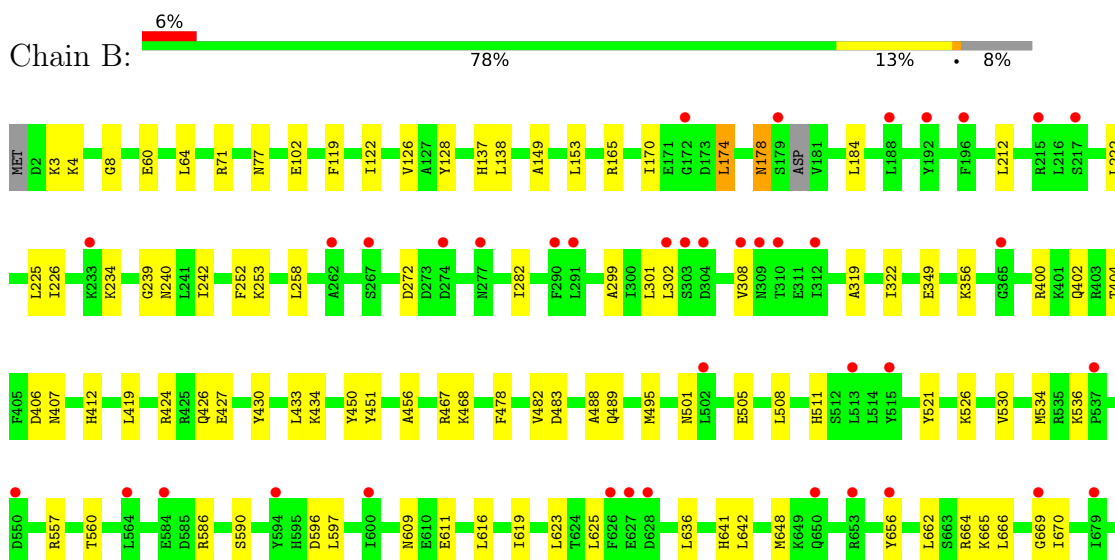
• Molecule 1: sgRNA

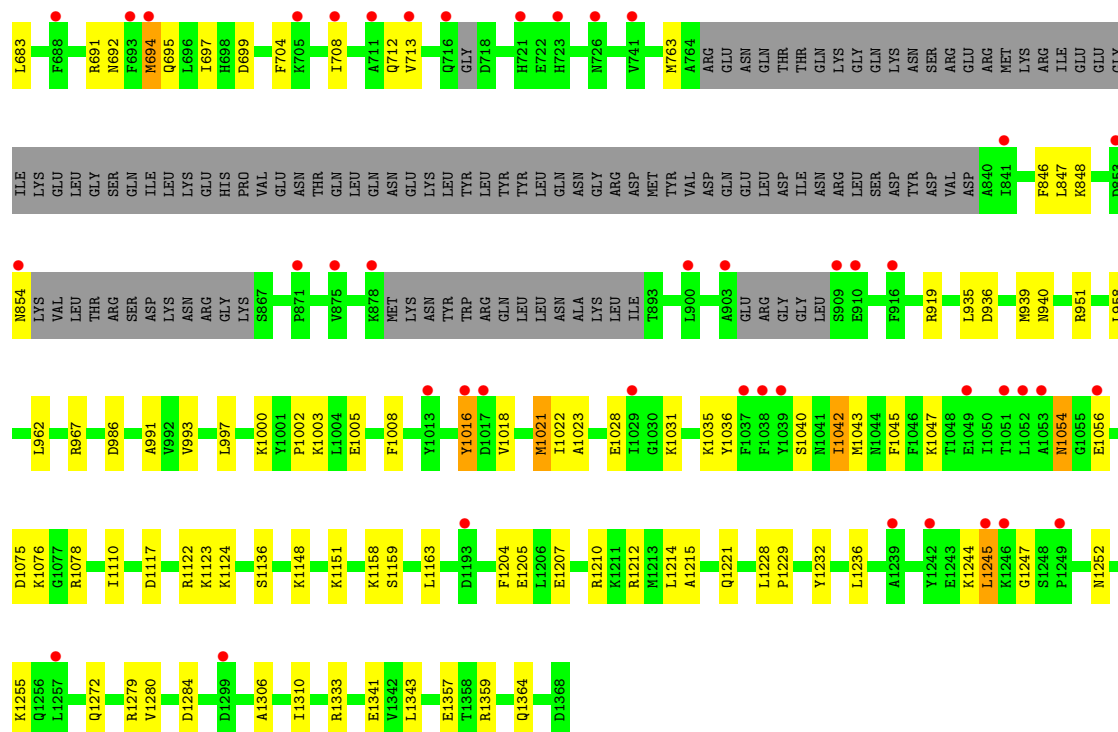


• Molecule 1: sgRNA

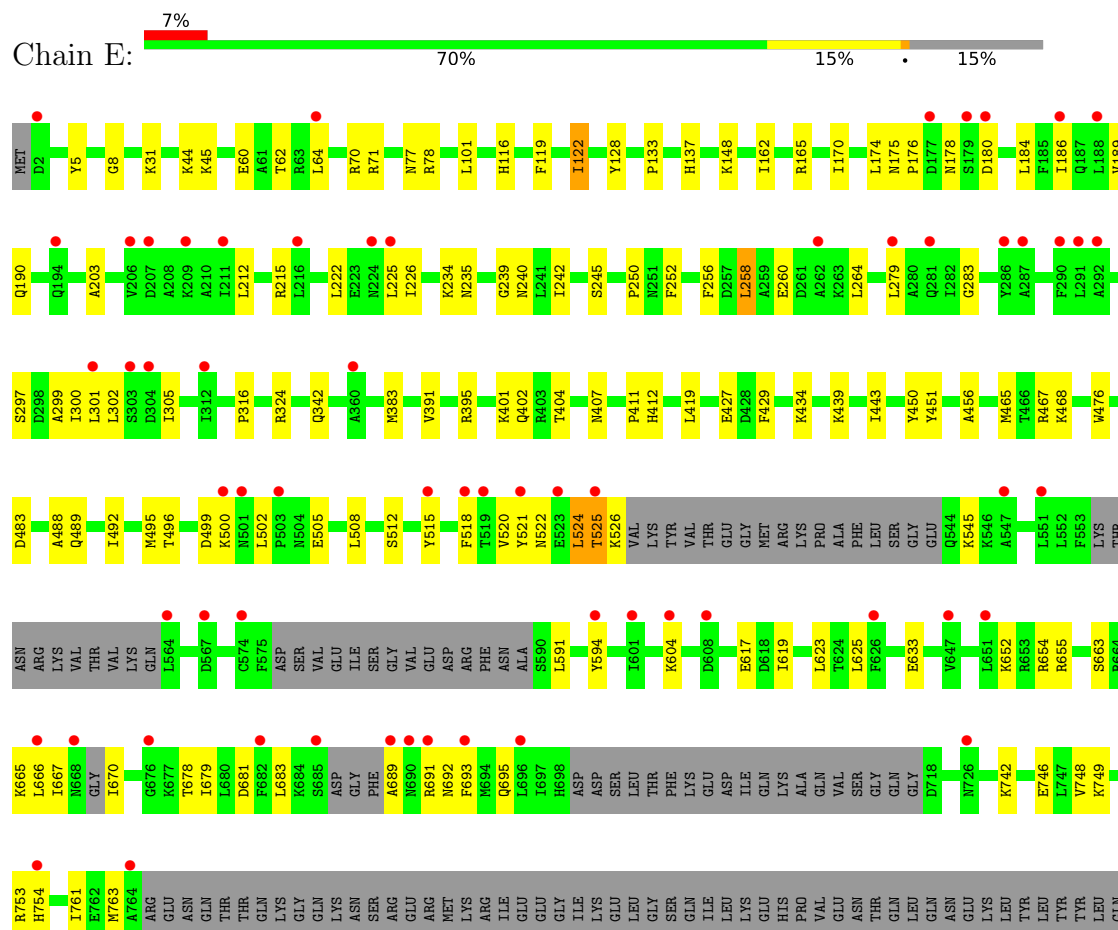


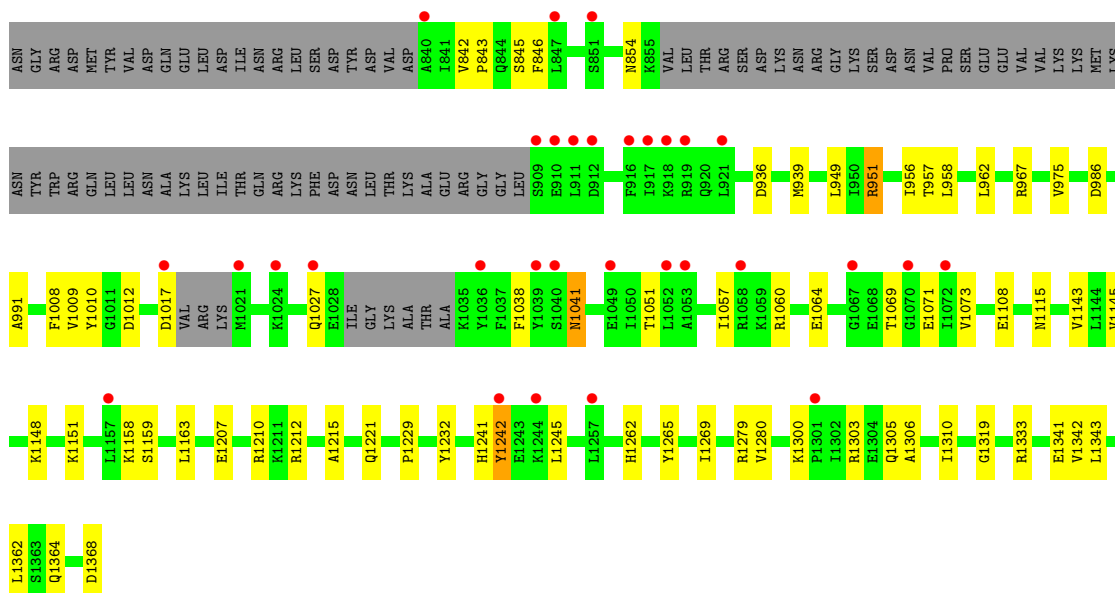
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



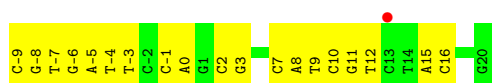


• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1





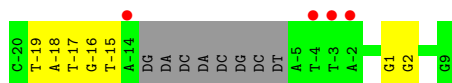
- Molecule 3: Target strand of 10 nucleotide complementary DNA substrate



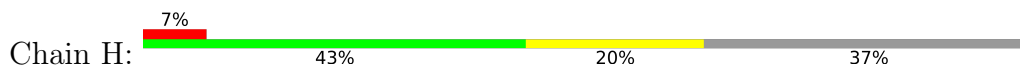
- Molecule 3: Target strand of 10 nucleotide complementary DNA substrate



- Molecule 4: Non-target strand of 10 nucleotide complementary DNA substrate



- Molecule 4: Non-target strand of 10 nucleotide complementary DNA substrate



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	88.64Å 95.51Å 169.80Å 80.83° 78.04° 62.34°	Depositor
Resolution (Å)	66.49 – 3.10 66.49 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.2 (66.49-3.10) 89.2 (66.49-3.10)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.276 0.247 , 0.276	Depositor DCC
R_{free} test set	4132 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	25082	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.13% 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:
K

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	0.14	0/1807	0.34	0/2816
1	F	0.15	0/1854	0.34	0/2889
2	B	0.14	2/10440 (0.0%)	0.30	0/14026
2	E	0.11	0/9706	0.30	0/13036
3	C	0.23	0/677	0.40	0/1042
3	G	0.21	0/586	0.40	0/901
4	D	0.21	0/479	0.42	0/737
4	H	0.21	0/401	0.42	0/616
All	All	0.14	2/25950 (0.0%)	0.32	0/36063

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1021	MET	SD-CE	6.31	1.95	1.79
2	B	1021	MET	CG-SD	5.61	1.94	1.80

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1610	0	809	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1652	0	830	37	0
2	B	10259	0	10425	109	0
2	E	9537	0	9689	127	0
3	C	606	0	341	18	0
3	G	526	0	297	18	0
4	D	429	0	242	5	0
4	H	359	0	201	7	0
5	A	6	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	E	2	0	0	0	0
5	F	3	0	0	0	0
5	G	1	0	0	0	0
6	A	15	0	0	0	0
6	B	22	0	0	1	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	E	29	0	0	1	0
6	F	14	0	0	1	0
6	G	1	0	0	0	0
6	H	4	0	0	0	0
All	All	25082	0	22834	323	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 7.

All (323) 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:A:10:A:H62	3:C:11:DG:H1	1.14	0.92
2:E:1051:THR:HG22	2:E:1057:ILE:HG22	1.65	0.78
2:B:847:LEU:HD21	2:B:919:ARG:HH11	1.49	0.76
3:G:-8:DG:H2''	3:G:-7:DT:H5'	1.68	0.75
2:E:1148:LYS:HG2	2:E:1159:SER:HA	1.66	0.75
2:E:174:LEU:HD21	2:E:302:LEU:HD21	1.71	0.73
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.23	0.72
3:C:10:DC:H2'	3:C:11:DG:C8	2.24	0.71
2:E:967:ARG:NH1	2:E:986:ASP:OD1	2.24	0.71
2:B:1018:VAL:HG12	2:B:1022:ILE:HG12	1.73	0.69
2:B:846:PHE:HA	2:B:1040:SER:HB2	1.74	0.69
2:E:949:LEU:HD23	2:E:951:ARG:HE	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1027:GLN:HE21	2:E:1038:PHE:HD2	1.42	0.68
3:G:12:DT:H2'	3:G:13:DC:C6	2.29	0.68
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.76	0.67
2:E:654:ARG:HE	2:E:655:ARG:H	1.43	0.66
2:E:522:ASN:HA	2:E:683:LEU:HD22	1.76	0.66
1:A:8:A:H2'	1:A:9:A:C8	2.30	0.65
2:E:222:LEU:HD23	2:E:234:LYS:HE3	1.77	0.65
2:E:176:PRO:HG3	2:E:316:PRO:HG3	1.79	0.64
2:B:1042:ILE:HD12	2:B:1043:MET:HG2	1.78	0.64
2:B:1054:ASN:HD22	2:B:1056:GLU:H	1.45	0.64
2:B:1023:ALA:HA	2:B:1035:LYS:HD3	1.79	0.64
3:G:10:DC:H2'	3:G:11:DG:C8	2.33	0.63
3:G:-9:DC:H2'	3:G:-8:DG:C8	2.33	0.63
2:E:936:ASP:OD2	2:E:951:ARG:NH2	2.32	0.62
2:E:499:ASP:HB2	2:E:663:SER:HB3	1.79	0.62
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.32	0.62
2:E:427:GLU:HB2	2:E:434:LYS:HB2	1.82	0.61
3:C:8:DA:H2'	3:C:9:DT:C6	2.35	0.61
2:E:666:LEU:HD21	2:E:693:PHE:HZ	1.65	0.61
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.81	0.61
1:F:10:A:H62	3:G:11:DG:H1	1.49	0.60
2:E:1279:ARG:HG2	2:E:1280:VAL:HG23	1.82	0.60
2:B:258:LEU:HD11	2:B:282:ILE:HD11	1.84	0.60
2:E:189:VAL:HG21	2:E:203:ALA:HB2	1.83	0.60
2:E:691:ARG:HB3	2:E:695:GLN:HB3	1.83	0.59
3:G:-1:DC:H2''	3:G:0:DA:C8	2.38	0.59
4:H:-17:DT:H2'	4:H:-16:DG:C8	2.36	0.59
2:E:522:ASN:OD1	2:E:692:ASN:ND2	2.36	0.59
3:C:9:DT:H2'	3:C:10:DC:C6	2.37	0.59
3:G:8:DA:H2'	3:G:9:DT:C6	2.38	0.59
2:B:505:GLU:HG2	2:B:665:LYS:HB2	1.85	0.59
2:B:1075:ASP:OD2	2:B:1078:ARG:NH2	2.35	0.59
3:C:-1:DC:H2''	3:C:0:DA:C8	2.37	0.59
2:B:427:GLU:HB2	2:B:434:LYS:HB2	1.84	0.58
3:G:9:DT:H2'	3:G:10:DC:C6	2.38	0.58
2:B:222:LEU:HD23	2:B:234:LYS:HE3	1.85	0.58
1:A:46:A:H2'	1:A:47:A:H8	1.67	0.58
2:B:526:LYS:HD3	2:B:692:ASN:HB3	1.85	0.58
1:F:46:A:H2'	1:F:47:A:H8	1.69	0.58
1:F:71:U:H2'	1:F:72:U:C6	2.39	0.58
1:A:22:U:H2'	1:A:23:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.86	0.57
2:E:184:LEU:HD12	2:E:299:ALA:HB2	1.85	0.57
2:E:402:GLN:OE1	1:F:44:U:O2'	2.22	0.57
1:F:46:A:H2'	1:F:47:A:C8	2.40	0.57
2:E:654:ARG:HE	2:E:655:ARG:N	2.02	0.57
1:F:22:U:H2'	1:F:23:U:C6	2.40	0.57
3:C:9:DT:H2'	3:C:10:DC:H6	1.69	0.57
2:E:215:ARG:NH1	2:E:395:ARG:HA	2.19	0.56
2:E:525:THR:HG23	2:E:683:LEU:HA	1.87	0.56
2:E:1151:LYS:HD2	2:E:1158:LYS:HD2	1.86	0.56
1:A:46:A:H2'	1:A:47:A:C8	2.39	0.56
3:C:15:DA:H2'	3:C:16:DC:C6	2.41	0.56
2:E:1163:LEU:HG	2:E:1343:LEU:HD21	1.86	0.56
1:F:10:A:H2'	1:F:11:G:O4'	2.05	0.56
2:B:1279:ARG:HG2	2:B:1280:VAL:HG23	1.88	0.56
2:E:666:LEU:HD21	2:E:693:PHE:CZ	2.40	0.56
2:E:133:PRO:HG2	2:E:137:HIS:CE1	2.41	0.55
1:F:38:A:H2'	1:F:39:G:C8	2.41	0.55
1:F:21:G:N2	6:F:203:HOH:O	2.39	0.55
2:E:305:ILE:HD13	2:E:411:PRO:HD3	1.88	0.55
2:E:324:ARG:NH1	2:E:401:LYS:O	2.40	0.54
1:A:38:A:H2'	1:A:39:G:C8	2.42	0.54
2:B:662:LEU:HD22	2:B:666:LEU:HD23	1.89	0.54
2:B:1245:LEU:HD22	2:B:1255:LYS:HD2	1.89	0.54
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.41	0.54
1:A:53:G:H2'	1:A:54:G:H8	1.72	0.54
1:A:74:A:H3'	1:A:75:A:H8	1.73	0.53
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.37	0.53
1:A:10:A:H2'	1:A:11:G:O4'	2.08	0.53
2:E:489:GLN:HG3	2:E:625:LEU:HD21	1.91	0.53
1:F:8:A:H2'	1:F:9:A:C8	2.42	0.53
2:B:1333:ARG:NH2	4:D:1:DG:O6	2.42	0.53
2:E:1212:ARG:NH2	2:E:1280:VAL:O	2.42	0.53
2:E:499:ASP:HB3	2:E:502:LEU:O	2.08	0.53
2:E:1069:THR:HG23	2:E:1071:GLU:H	1.73	0.53
1:A:70:C:H2'	1:A:71:U:C6	2.44	0.52
2:E:1215:ALA:HB2	2:E:1221:GLN:HG3	1.90	0.52
3:G:-8:DG:H2'	3:G:-7:DT:C6	2.44	0.52
2:B:308:VAL:HG11	2:B:319:ALA:HB3	1.90	0.52
1:F:53:G:H2'	1:F:54:G:H8	1.74	0.52
2:E:215:ARG:HH12	2:E:395:ARG:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:842:VAL:HG22	2:E:846:PHE:HB2	1.92	0.52
1:F:11:G:H2'	1:F:12:A:C8	2.45	0.52
2:E:8:GLY:HA3	2:E:991:ALA:HB2	1.92	0.51
1:A:22:U:H2'	1:A:23:U:H6	1.75	0.51
1:A:44:U:O2'	2:B:402:GLN:OE1	2.28	0.51
2:B:694:MET:HE2	2:B:697:ILE:HD11	1.92	0.51
1:A:71:U:H2'	1:A:72:U:C6	2.45	0.51
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.92	0.51
2:E:526:LYS:HD2	2:E:692:ASN:HB2	1.91	0.51
3:G:-5:DA:H1'	3:G:-4:DT:H5'	1.93	0.51
2:B:691:ARG:NH1	2:B:699:ASP:OD2	2.38	0.51
2:B:1117:ASP:OD1	2:B:1117:ASP:N	2.44	0.51
2:B:636:LEU:HB3	2:B:648:MET:HE1	1.93	0.51
2:E:170:ILE:HD11	2:E:301:LEU:HD13	1.93	0.51
2:E:342:GLN:HB2	2:E:383:MET:HE3	1.93	0.51
1:F:42:A:H2'	1:F:43:G:C8	2.45	0.51
2:E:279:LEU:O	2:E:283:GLY:N	2.44	0.50
2:B:404:THR:H	2:B:407:ASN:ND2	2.09	0.50
2:E:1064:GLU:O	2:E:1073:VAL:HG22	2.11	0.50
1:F:22:U:H2'	1:F:23:U:H6	1.77	0.50
2:B:468:LYS:HG3	2:B:483:ASP:HB2	1.94	0.50
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.94	0.50
2:E:594:TYR:OH	2:E:604:LYS:HG3	2.12	0.50
2:E:500:LYS:HG3	4:H:-17:DT:OP1	2.12	0.50
2:E:1306:ALA:O	2:E:1310:ILE:HG12	2.11	0.49
2:E:951:ARG:NH1	2:E:1010:TYR:O	2.46	0.49
1:A:9:A:H2'	1:A:10:A:N3	2.28	0.49
2:E:521:TYR:O	2:E:683:LEU:HB3	2.13	0.49
2:B:511:HIS:CD2	2:B:656:TYR:HB3	2.47	0.49
2:E:45:LYS:NZ	6:E:1503:HOH:O	2.45	0.49
1:A:74:A:H3'	1:A:75:A:C8	2.48	0.49
2:B:149:ALA:O	2:B:430:TYR:OH	2.23	0.49
1:F:11:G:H2'	1:F:12:A:H8	1.78	0.49
1:F:27:G:H5'	1:F:28:A:O5'	2.12	0.49
2:B:521:TYR:HB3	2:B:683:LEU:HB3	1.95	0.49
2:E:456:ALA:O	2:E:467:ARG:NH1	2.45	0.49
1:F:70:C:H2'	1:F:71:U:C6	2.47	0.49
2:B:1028:GLU:HA	2:B:1031:LYS:HE3	1.95	0.49
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.44	0.49
1:A:27:G:H5'	1:A:28:A:O5'	2.13	0.49
3:C:15:DA:H2'	3:C:16:DC:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:9:DT:H2'	3:G:10:DC:H6	1.79	0.48
2:B:456:ALA:O	2:B:467:ARG:NH1	2.47	0.48
2:B:560:THR:HA	2:B:586:ARG:HA	1.95	0.48
4:H:-17:DT:H2'	4:H:-16:DG:H8	1.79	0.48
4:D:-18:DA:H2'	4:D:-17:DT:C6	2.49	0.48
2:E:78:ARG:NH1	2:E:162:ILE:O	2.45	0.48
2:E:212:LEU:HD13	2:E:300:ILE:HD11	1.95	0.48
2:B:958:LEU:HD22	2:B:962:LEU:HD12	1.96	0.48
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	1.96	0.48
2:E:843:PRO:HD2	2:E:846:PHE:CD2	2.49	0.48
2:E:1108:GLU:HB2	3:G:1:DG:H5''	1.95	0.48
2:B:495:MET:HB3	3:C:9:DT:H1'	1.94	0.47
2:E:391:VAL:HG12	2:E:395:ARG:HD3	1.95	0.47
1:F:68:A:C4	1:F:69:A:C8	3.02	0.47
1:A:18:C:H41	2:B:71:ARG:NH1	2.12	0.47
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.13	0.47
2:E:404:THR:H	2:E:407:ASN:ND2	2.12	0.47
4:D:-19:DT:H2'	4:D:-18:DA:H8	1.78	0.47
2:E:1148:LYS:HG2	2:E:1159:SER:CA	2.40	0.47
2:B:641:HIS:CE1	2:B:642:LEU:HG	2.49	0.47
2:E:975:VAL:HG11	2:E:1310:ILE:HD12	1.96	0.47
2:E:1210:ARG:NH2	2:E:1341:GLU:OE2	2.48	0.47
2:B:3:LYS:HG3	2:B:4:LYS:H	1.80	0.47
3:C:2:DC:H2''	3:C:3:DG:H5''	1.96	0.47
2:E:450:TYR:CE1	3:G:7:DC:H2''	2.50	0.47
2:E:524:LEU:HG	2:E:545:LYS:HD3	1.97	0.47
2:B:619:ILE:O	2:B:623:LEU:HG	2.16	0.46
2:E:71:ARG:NH1	1:F:18:C:H41	2.13	0.46
1:A:48:A:H2'	1:A:49:A:C8	2.50	0.46
2:E:62:THR:HG22	1:F:63:U:O2'	2.16	0.46
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.79	0.46
2:E:495:MET:HB3	3:G:9:DT:H1'	1.97	0.46
1:F:72:U:H2'	1:F:73:G:O4'	2.15	0.46
2:E:842:VAL:HG12	2:E:854:ASN:OD1	2.16	0.46
2:B:665:LYS:O	2:B:669:GLY:N	2.48	0.46
2:B:665:LYS:HG3	2:B:670:ILE:HG23	1.98	0.46
2:E:258:LEU:HD12	2:E:260:GLU:O	2.16	0.46
2:E:526:LYS:HB3	2:E:526:LYS:HE2	1.73	0.46
2:B:178:ASN:OD1	2:B:178:ASN:N	2.48	0.46
2:B:508:LEU:HD21	2:B:664:ARG:HB2	1.98	0.46
2:E:654:ARG:NH1	2:E:655:ARG:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:-16:DG:H2'	4:D:-15:DT:C6	2.50	0.45
2:E:1300:LYS:O	2:E:1305:GLN:NE2	2.49	0.45
2:B:426:GLN:NE2	6:B:1507:HOH:O	2.49	0.45
2:E:225:LEU:HD23	2:E:242:ILE:HG21	1.99	0.45
2:E:619:ILE:O	2:E:623:LEU:HG	2.16	0.45
1:A:68:A:C4	1:A:69:A:C8	3.04	0.45
3:G:-6:DG:H2''	3:G:-5:DA:H8	1.82	0.45
2:E:1143:VAL:HG12	2:E:1145:VAL:HG13	1.98	0.45
2:E:1333:ARG:NH2	4:H:1:DG:O6	2.49	0.45
3:C:8:DA:H2'	3:C:9:DT:H6	1.80	0.45
2:E:165:ARG:O	2:E:412:HIS:HA	2.16	0.45
2:E:518:PHE:HB2	2:E:667:ILE:HG23	1.97	0.45
2:E:956:ILE:HG12	2:E:1009:VAL:HG22	1.98	0.45
1:F:30:C:H2'	1:F:31:U:C6	2.52	0.45
2:E:467:ARG:NH2	1:F:59:U:OP1	2.50	0.45
2:E:845:SER:O	2:E:1041:ASN:HB2	2.16	0.45
2:E:1229:PRO:HD2	2:E:1232:TYR:HD2	1.81	0.45
2:E:5:TYR:OH	2:E:754:HIS:O	2.33	0.44
2:E:77:ASN:ND2	1:F:59:U:H1'	2.32	0.44
2:B:763:MET:HE3	2:B:763:MET:HB2	1.85	0.44
2:E:515:TYR:OH	4:H:-16:DG:OP1	2.26	0.44
2:B:170:ILE:HD11	2:B:301:LEU:HD13	1.98	0.44
2:B:1002:PRO:O	2:B:1005:GLU:HG3	2.18	0.44
2:B:936:ASP:OD1	2:B:940:ASN:ND2	2.50	0.44
3:C:2:DC:H2''	3:C:3:DG:H8	1.82	0.44
2:E:1241:HIS:O	2:E:1245:LEU:HD23	2.17	0.44
2:E:692:ASN:CG	2:E:693:PHE:H	2.25	0.44
3:G:-4:DT:H2''	3:G:-3:DT:H5''	2.00	0.44
2:B:165:ARG:O	2:B:412:HIS:HA	2.17	0.44
2:B:451:TYR:CD1	2:B:488:ALA:HB2	2.53	0.44
1:F:73:G:O2'	1:F:76:A:N6	2.51	0.44
2:B:993:VAL:O	2:B:997:LEU:HB2	2.18	0.44
2:E:101:LEU:HD23	2:E:101:LEU:HA	1.79	0.44
2:E:842:VAL:HG12	2:E:854:ASN:HD21	1.82	0.44
1:A:70:C:H2'	1:A:71:U:H6	1.81	0.43
2:B:119:PHE:HE2	2:B:128:TYR:HB2	1.83	0.43
2:E:240:ASN:HB3	2:E:252:PHE:CE1	2.53	0.43
2:E:956:ILE:HA	2:E:1008:PHE:O	2.18	0.43
3:G:12:DT:H2'	3:G:13:DC:H6	1.82	0.43
2:E:245:SER:HA	2:E:297:SER:HB2	2.00	0.43
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1060:ARG:NH1	2:E:1064:GLU:OE1	2.51	0.43
4:H:4:DA:C8	4:H:5:DT:H72	2.53	0.43
2:B:1245:LEU:HD21	2:B:1252:ASN:HA	2.01	0.43
2:E:119:PHE:HE2	2:E:128:TYR:HB2	1.83	0.43
3:G:-7:DT:H2''	3:G:-6:DG:H5''	2.00	0.43
1:A:32:A:H2'	1:A:33:G:C8	2.54	0.43
3:C:-9:DC:H2'	3:C:-8:DG:C8	2.54	0.43
2:E:678:THR:HG23	2:E:681:ASP:H	1.83	0.43
1:F:54:G:H2'	1:F:55:C:C6	2.54	0.43
2:B:174:LEU:HD23	2:B:302:LEU:HD21	2.00	0.43
2:B:1047:LYS:O	2:B:1076:LYS:NZ	2.41	0.43
2:E:633:GLU:OE1	2:E:652:LYS:NZ	2.52	0.43
2:E:1221:GLN:HB3	2:E:1319:GLY:C	2.44	0.43
1:F:70:C:H2'	1:F:71:U:H6	1.84	0.43
2:E:148:LYS:HD2	2:E:429:PHE:HB3	2.01	0.43
2:E:465:MET:HE3	2:E:465:MET:HB3	1.97	0.43
1:A:49:A:N3	2:B:1122:ARG:NH2	2.67	0.43
2:B:1245:LEU:C	2:B:1247:GLY:H	2.27	0.43
3:C:11:DG:H2''	3:C:12:DT:H5''	2.01	0.43
2:E:508:LEU:HD12	2:E:667:ILE:HD12	1.99	0.43
2:E:746:GLU:HA	2:E:749:LYS:HE3	2.00	0.43
2:E:116:HIS:NE2	2:E:122:ILE:HD12	2.34	0.42
2:E:186:ILE:O	2:E:190:GLN:HG3	2.19	0.42
3:C:-4:DT:H2''	3:C:-3:DT:H5''	2.00	0.42
2:B:1054:ASN:ND2	2:B:1056:GLU:H	2.14	0.42
2:E:78:ARG:HG2	2:E:443:ILE:HG23	2.02	0.42
1:F:74:A:H3'	1:F:75:A:H8	1.83	0.42
2:B:1204:PHE:HE1	2:B:1214:LEU:HD13	1.85	0.42
2:B:400:ARG:NH2	2:B:406:ASP:OD2	2.52	0.42
2:B:1245:LEU:CD2	2:B:1255:LYS:HD2	2.49	0.42
3:C:-6:DG:H2''	3:C:-5:DA:H8	1.85	0.42
1:F:47:A:H2'	1:F:48:A:C8	2.55	0.42
2:B:226:ILE:HD11	2:B:239:GLY:HA2	2.00	0.42
2:B:501:ASN:HB3	2:B:708:ILE:HD12	2.01	0.42
2:B:536:LYS:HB3	2:B:536:LYS:HE2	1.79	0.42
2:E:525:THR:HA	2:E:689:ALA:HA	2.01	0.42
2:E:1342:VAL:O	2:E:1362:LEU:HD12	2.20	0.42
2:B:704:PHE:O	2:B:708:ILE:HG12	2.20	0.42
2:B:935:LEU:O	2:B:939:MET:HG2	2.20	0.42
2:E:512:SER:OG	2:E:617:GLU:OE1	2.34	0.42
2:E:748:VAL:HG21	2:E:939:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1265:TYR:O	2:E:1269:ILE:HG13	2.19	0.42
2:B:609:ASN:O	2:B:611:GLU:N	2.49	0.42
2:B:1021:MET:HE3	2:B:1036:TYR:CD2	2.55	0.42
2:B:557:ARG:O	2:B:590:SER:HB2	2.19	0.42
2:B:1228:LEU:HD12	2:B:1272:GLN:HG2	2.00	0.42
1:A:28:A:OP2	2:B:126:VAL:HG22	2.20	0.42
2:E:60:GLU:O	2:E:64:LEU:HG	2.19	0.42
2:E:189:VAL:HG11	2:E:203:ALA:HB2	2.02	0.42
2:E:492:ILE:O	2:E:496:THR:HG23	2.20	0.42
2:B:349:GLU:HG3	2:B:356:LYS:HG3	2.02	0.41
2:E:958:LEU:HD22	2:E:962:LEU:HD12	2.02	0.41
2:E:1242:TYR:CD2	2:E:1303:ARG:HD2	2.55	0.41
1:F:27:G:H4'	1:F:28:A:OP2	2.20	0.41
2:B:433:LEU:HD23	2:B:433:LEU:HA	1.88	0.41
2:B:1003:LYS:HG3	2:B:1036:TYR:CZ	2.55	0.41
1:A:27:G:H4'	1:A:28:A:OP2	2.21	0.41
2:B:225:LEU:HD23	2:B:242:ILE:HG21	2.01	0.41
2:B:400:ARG:HH22	2:B:406:ASP:CG	2.29	0.41
2:B:597:LEU:HD13	2:B:616:LEU:HD22	2.01	0.41
2:B:1284:ASP:OD1	2:B:1284:ASP:N	2.53	0.41
2:E:520:VAL:HG11	2:E:591:LEU:HD21	2.01	0.41
2:E:742:LYS:NZ	1:F:67:C:OP1	2.30	0.41
2:E:763:MET:HE3	2:E:763:MET:HB2	1.86	0.41
1:A:53:G:H2'	1:A:54:G:C8	2.55	0.41
2:B:1016:TYR:CD1	2:B:1016:TYR:N	2.87	0.41
2:B:1148:LYS:HG2	2:B:1159:SER:HA	2.03	0.41
2:E:256:PHE:HB2	2:E:258:LEU:HD21	2.02	0.41
1:F:32:A:H2'	1:F:33:G:C8	2.55	0.41
2:B:1151:LYS:HD2	2:B:1158:LYS:HD2	2.03	0.41
2:E:31:LYS:HE2	2:E:44:LYS:HB2	2.01	0.41
2:E:761:ILE:HD11	2:E:957:THR:HG22	2.02	0.41
1:F:38:A:H2'	1:F:39:G:H8	1.85	0.41
2:B:60:GLU:O	2:B:64:LEU:HG	2.20	0.41
2:B:240:ASN:HB3	2:B:252:PHE:CE1	2.56	0.41
2:B:450:TYR:CE1	3:C:7:DC:H2''	2.56	0.41
2:B:940:ASN:ND2	2:B:951:ARG:HG3	2.36	0.41
2:B:1000:LYS:HD3	2:B:1045:PHE:CD2	2.56	0.41
2:E:692:ASN:CG	2:E:693:PHE:N	2.79	0.41
4:H:-18:DA:H2'	4:H:-17:DT:C6	2.56	0.41
2:B:137:HIS:HA	2:B:322:ILE:HD11	2.03	0.40
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-7:DT:H2''	3:C:-6:DG:H8	1.86	0.40
2:E:250:PRO:HD2	2:E:264:LEU:O	2.21	0.40
1:A:59:U:H1'	2:B:77:ASN:ND2	2.36	0.40
2:B:212:LEU:HD21	2:B:225:LEU:HD22	2.03	0.40
2:B:997:LEU:HD12	2:B:997:LEU:HA	1.95	0.40
2:E:439:LYS:HG2	2:E:476:TRP:NE1	2.36	0.40
2:E:505:GLU:HG3	2:E:665:LYS:HG3	2.02	0.40
1:A:11:G:H2'	1:A:12:A:C8	2.57	0.40
2:B:138:LEU:HD21	2:B:153:LEU:HB3	2.03	0.40
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.88	0.40
2:B:253:LYS:HE2	2:B:258:LEU:O	2.21	0.40
2:E:70:ARG:NH1	1:F:61:C:OP1	2.51	0.40
2:E:468:LYS:HG3	2:E:483:ASP:HB2	2.03	0.40
2:E:679:ILE:O	2:E:683:LEU:HG	2.20	0.40
1:F:53:G:H2'	1:F:54:G:C8	2.56	0.40
2:E:226:ILE:HD11	2:E:239:GLY:HA2	2.03	0.40
2:E:451:TYR:CD1	2:E:488:ALA:HB2	2.56	0.40
2:B:530:VAL:HA	2:B:534:MET:SD	2.62	0.40
2:B:848:LYS:HE2	2:B:848:LYS:HB2	1.71	0.40
2:B:1136:SER:HA	4:D:2:DG:O3'	2.22	0.40
2:B:1236:LEU:HB3	2:B:1310:ILE:HD11	2.04	0.40
2:E:101:LEU:O	1:F:47:A:O2'	2.38	0.40
2:E:1262:HIS:O	2:E:1265:TYR:HB2	2.22	0.40
1:F:42:A:O2'	1:F:43:G:OP1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	1245/1368 (91%)	1189 (96%)	56 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	1144/1368 (84%)	1102 (96%)	42 (4%)	0	100	100
All	All	2389/2736 (87%)	2291 (96%)	98 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	B	1125/1225 (92%)	1103 (98%)	22 (2%)	48	72
2	E	1045/1225 (85%)	1025 (98%)	20 (2%)	50	73
All	All	2170/2450 (89%)	2128 (98%)	42 (2%)	50	73

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	102	GLU
2	B	122	ILE
2	B	174	LEU
2	B	178	ASN
2	B	272	ASP
2	B	419	LEU
2	B	424	ARG
2	B	694	MET
2	B	695	GLN
2	B	712	GLN
2	B	713	VAL
2	B	854	ASN
2	B	1008	PHE
2	B	1016	TYR
2	B	1042	ILE
2	B	1054	ASN
2	B	1123	LYS
2	B	1124	LYS

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Mol	Chain	Res	Type
2	B	1207	GLU
2	B	1244	LYS
2	B	1245	LEU
2	B	1364	GLN
2	E	122	ILE
2	E	175	ASN
2	E	178	ASN
2	E	180	ASP
2	E	235	ASN
2	E	258	LEU
2	E	419	LEU
2	E	524	LEU
2	E	525	THR
2	E	670	ILE
2	E	753	ARG
2	E	951	ARG
2	E	1012	ASP
2	E	1017	ASP
2	E	1041	ASN
2	E	1115	ASN
2	E	1207	GLU
2	E	1242	TYR
2	E	1364	GLN
2	E	1368	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	281	GLN
2	B	357	ASN
2	B	394	ASN
2	B	407	ASN
2	B	426	GLN
2	B	459	ASN
2	B	501	ASN
2	B	511	HIS
2	B	612	ASN
2	B	641	HIS
2	B	695	GLN
2	B	854	ASN
2	B	869	ASN
2	B	980	ASN

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Mol	Chain	Res	Type
2	B	983	HIS
2	B	1044	ASN
2	B	1054	ASN
2	B	1101	GLN
2	B	1252	ASN
2	B	1349	HIS
2	E	14	ASN
2	E	357	ASN
2	E	394	ASN
2	E	407	ASN
2	E	426	GLN
2	E	522	ASN
2	E	641	HIS
2	E	692	ASN
2	E	980	ASN
2	E	1027	GLN
2	E	1041	ASN
2	E	1044	ASN
2	E	1101	GLN
2	E	1349	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	74/84 (88%)	18 (24%)	2 (2%)
1	F	76/84 (90%)	18 (23%)	3 (3%)
All	All	150/168 (89%)	36 (24%)	5 (3%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	20	C
1	A	28	A
1	A	29	G
1	A	37	U
1	A	51	A
1	A	53	G
1	A	56	U
1	A	57	A
1	A	59	U
1	A	63	U

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Mol	Chain	Res	Type
1	A	68	A
1	A	73	G
1	A	74	A
1	A	76	A
1	A	77	A
1	A	78	A
1	A	81	G
1	A	82	A
1	F	8	A
1	F	20	C
1	F	28	A
1	F	29	G
1	F	37	U
1	F	43	G
1	F	51	A
1	F	53	G
1	F	56	U
1	F	57	A
1	F	59	U
1	F	63	U
1	F	68	A
1	F	74	A
1	F	76	A
1	F	78	A
1	F	81	G
1	F	82	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	27	G
1	A	28	A
1	F	27	G
1	F	28	A
1	F	42	A

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 16 ligands modelled in this entry, 16 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	75/84 (89%)	-0.01	1 (1%) 75 56	22, 43, 142, 151	0
1	F	77/84 (91%)	0.18	4 (5%) 33 17	25, 46, 153, 210	0
2	B	1259/1368 (92%)	0.59	82 (6%) 25 13	18, 67, 118, 149	0
2	E	1166/1368 (85%)	0.68	93 (7%) 18 10	21, 65, 117, 142	0
3	C	30/30 (100%)	0.34	1 (3%) 49 29	36, 61, 129, 140	0
3	G	27/30 (90%)	0.48	2 (7%) 20 11	32, 55, 126, 130	0
4	D	22/30 (73%)	0.59	4 (18%) 3 1	32, 89, 137, 141	0
4	H	19/30 (63%)	0.55	2 (10%) 11 6	33, 83, 122, 141	0
All	All	2675/3024 (88%)	0.59	189 (7%) 22 12	18, 64, 119, 210	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	519	THR	5.3
1	F	6	A	4.7
2	E	1049	GLU	4.7
2	B	903	ALA	4.3
2	E	207	ASP	4.1
2	B	312	ILE	4.0
2	B	726	ASN	4.0
2	E	292	ALA	3.9
2	B	1052	LEU	3.9
2	E	911	LEU	3.9
2	E	290	PHE	3.8
2	E	594	TYR	3.7
2	E	1244	LYS	3.6
2	E	180	ASP	3.5
2	B	679	ILE	3.5
2	E	689	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	192	TYR	3.4
2	E	521	TYR	3.4
2	E	918	LYS	3.4
2	E	1039	TYR	3.4
2	B	290	PHE	3.4
2	E	1017	ASP	3.4
2	B	1249	PRO	3.4
2	E	726	ASN	3.3
1	F	7	U	3.2
2	E	910	GLU	3.2
2	B	1039	TYR	3.2
2	E	291	LEU	3.2
2	B	1017	ASP	3.2
2	E	666	LEU	3.2
2	E	1052	LEU	3.2
2	B	1193	ASP	3.1
2	E	286	TYR	3.1
2	E	304	ASP	3.1
2	E	525	THR	3.1
4	D	-3	DT	3.1
2	B	716	GLN	3.0
2	B	910	GLU	3.0
2	B	537	PRO	3.0
2	E	301	LEU	3.0
2	E	281	GLN	3.0
2	E	224	ASN	3.0
2	E	1257	LEU	2.9
2	E	647	VAL	2.9
2	E	518	PHE	2.9
2	E	551	LEU	2.9
2	E	564	LEU	2.8
2	E	693	PHE	2.8
2	B	179	SER	2.8
2	E	303	SER	2.8
2	E	567	ASP	2.8
2	B	277	ASN	2.8
2	B	1245	LEU	2.8
2	E	1070	GLY	2.8
2	B	721	HIS	2.8
2	E	1024	LYS	2.8
2	B	713	VAL	2.8
2	E	909	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	523	GLU	2.8
2	B	841	ILE	2.8
2	B	1016	TYR	2.7
2	E	1053	ALA	2.7
2	B	217	SER	2.7
2	E	1072	ILE	2.7
4	H	-15	DT	2.7
2	B	196	PHE	2.7
2	E	676	GLY	2.7
2	E	626	PHE	2.7
2	B	1242	TYR	2.7
2	E	287	ALA	2.7
2	E	1058	ARG	2.7
2	B	1299	ASP	2.7
2	B	1056	GLU	2.6
2	E	651	LEU	2.6
2	E	917	ILE	2.6
2	E	503	PRO	2.6
2	E	912	ASP	2.6
2	E	500	LYS	2.6
2	E	1036	TYR	2.6
2	E	1021	MET	2.6
2	B	669	GLY	2.6
2	B	705	LYS	2.6
4	D	-14	DA	2.6
2	E	840	ALA	2.5
2	E	515	TYR	2.5
2	E	225	LEU	2.5
2	B	878	LYS	2.5
2	B	600	ILE	2.5
1	F	10	A	2.5
2	B	1013	TYR	2.5
2	B	291	LEU	2.5
2	E	312	ILE	2.5
2	B	656	TYR	2.5
2	B	1246	LYS	2.5
2	B	1239	ALA	2.5
2	B	653	ARG	2.5
2	B	688	PHE	2.4
4	D	-2	DA	2.4
2	E	209	LYS	2.4
4	D	-4	DT	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	211	ILE	2.4
2	E	696	LEU	2.4
2	E	847	LEU	2.4
2	B	853	ASP	2.4
2	B	215	ARG	2.4
2	E	921	LEU	2.4
2	E	764	ALA	2.3
2	B	627	GLU	2.3
2	B	1049	GLU	2.3
2	B	267	SER	2.3
2	E	601	ILE	2.3
3	G	18	DT	2.3
2	B	309	ASN	2.3
2	E	690	ASN	2.3
1	A	76	A	2.3
2	E	682	PHE	2.3
2	B	1029	ILE	2.3
2	E	188	LEU	2.3
3	G	14	DT	2.3
2	B	626	PHE	2.3
2	B	550	ASP	2.3
2	B	650	GLN	2.3
3	C	13	DC	2.3
2	E	608	ASP	2.3
2	E	262	ALA	2.2
2	B	693	PHE	2.2
2	B	723	HIS	2.2
2	E	604	LYS	2.2
2	E	851	SER	2.2
2	E	1027	GLN	2.2
2	B	871	PRO	2.2
2	B	564	LEU	2.2
2	B	875	VAL	2.2
2	B	274	ASP	2.2
2	B	694	MET	2.2
2	E	216	LEU	2.2
2	B	1038	PHE	2.2
2	E	919	ARG	2.2
2	B	1051	THR	2.2
2	B	308	VAL	2.2
2	B	741	VAL	2.2
2	B	854	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	513	LEU	2.2
2	E	177	ASP	2.2
2	E	691	ARG	2.2
2	E	916	PHE	2.2
2	B	594	TYR	2.2
2	B	303	SER	2.2
2	E	179	SER	2.2
2	E	194	GLN	2.2
2	B	365	GLY	2.2
2	E	574	CYS	2.2
2	E	206	VAL	2.1
2	E	1242	TYR	2.1
2	E	685	SER	2.1
2	E	668	ASN	2.1
1	F	76	A	2.1
2	E	186	ILE	2.1
2	B	233	LYS	2.1
2	B	262	ALA	2.1
2	B	1053	ALA	2.1
2	E	2	ASP	2.1
2	B	302	LEU	2.1
2	B	310	THR	2.1
2	B	584	GLU	2.1
2	B	188	LEU	2.1
2	B	708	ILE	2.1
2	E	754	HIS	2.1
2	E	547	ALA	2.1
2	B	172	GLY	2.1
2	B	916	PHE	2.1
2	E	501	ASN	2.1
2	E	64	LEU	2.1
2	E	1157	LEU	2.1
2	B	711	ALA	2.1
2	E	1067	GLY	2.1
2	E	279	LEU	2.0
4	H	-2	DA	2.0
2	B	304	ASP	2.0
2	B	515	TYR	2.0
2	B	628	ASP	2.0
2	E	360	ALA	2.0
2	B	900	LEU	2.0
2	B	1257	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	909	SER	2.0
2	E	1040	SER	2.0
2	B	1037	PHE	2.0
2	E	1301	PRO	2.0
2	B	502	LEU	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($\text{\AA}^2$)	Q<0.9
5	K	A	106	1/1	0.81	0.21	80,80,80,80	0
5	K	F	101	1/1	0.84	0.12	93,93,93,93	0
5	K	B	1402	1/1	0.88	0.14	60,60,60,60	0
5	K	E	1401	1/1	0.89	0.13	61,61,61,61	0
5	K	C	101	1/1	0.89	0.12	43,43,43,43	0
5	K	F	103	1/1	0.89	0.09	86,86,86,86	0
5	K	A	101	1/1	0.90	0.14	98,98,98,98	0
5	K	A	104	1/1	0.90	0.11	68,68,68,68	0
5	K	B	1401	1/1	0.92	0.20	53,53,53,53	0
5	K	A	103	1/1	0.93	0.09	52,52,52,52	0
5	K	G	101	1/1	0.94	0.12	48,48,48,48	0
5	K	A	105	1/1	0.95	0.08	73,73,73,73	0
5	K	F	102	1/1	0.95	0.08	58,58,58,58	0
5	K	B	1403	1/1	0.97	0.05	56,56,56,56	0
5	K	E	1402	1/1	0.97	0.13	47,47,47,47	0
5	K	A	102	1/1	0.97	0.05	69,69,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.