



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:16 AM UTC

PDB ID : 6K4P / pdb_00006k4p
Title : Crystal structure of xCas9 in complex with sgRNA and DNA (TGG PAM)
Authors : Chen, W.; Zhang, H.; Zhang, Y.; Wang, Y.; Gan, J.; Ji, Q.
Deposited on : 2019-05-25
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 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

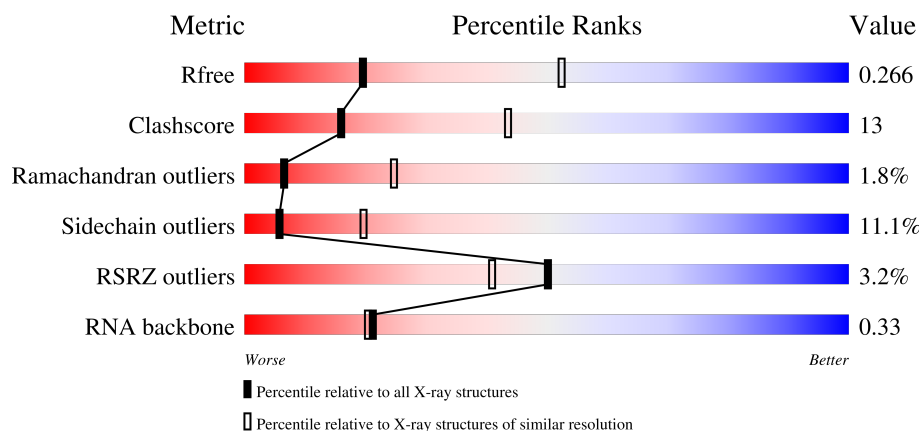
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	
2	C	28	
3	D	12	
4	B	1368	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	B	1404	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13124 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	82	Total	C	N	O	P	0	0	0
			1737	779	318	558	82			

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	28	Total	C	N	O	P	0	0	0
			567	276	96	168	27			

- Molecule 3 is a DNA chain called non-targeted DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			227	110	43	64	10			

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1323	Total	C	N	O	S	0	0	0
			10546	6730	1827	1970	19			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	80	LEU	CYS	engineered mutation	UNP Q99ZW2
B	262	THR	ALA	engineered mutation	UNP Q99ZW2
B	324	LEU	ARG	engineered mutation	UNP Q99ZW2
B	409	ILE	SER	engineered mutation	UNP Q99ZW2
B	480	LYS	GLU	engineered mutation	UNP Q99ZW2
B	543	ASP	GLU	engineered mutation	UNP Q99ZW2
B	574	GLU	CYS	engineered mutation	UNP Q99ZW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	694	ILE	MET	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1219	VAL	GLU	engineered mutation	UNP Q99ZW2

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	C	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		

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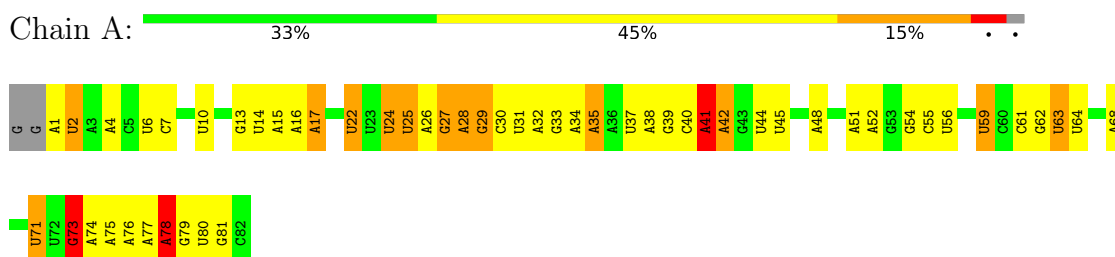
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	15	Total	O	0	0
			15	15		

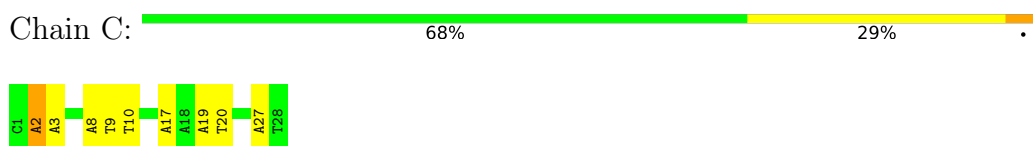
3 Residue-property plots

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.

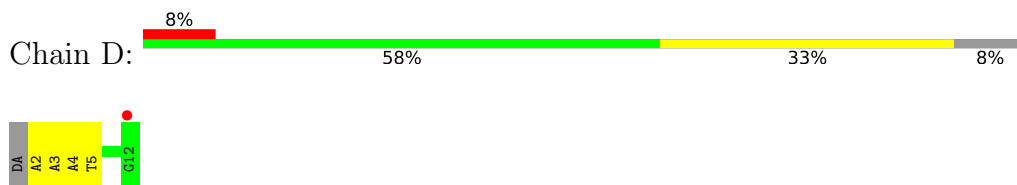
- Molecule 1: sgRNA



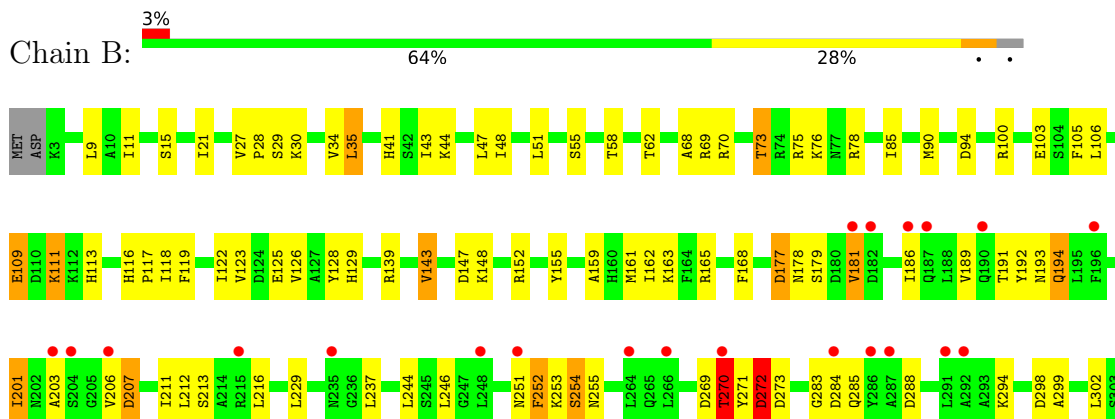
- Molecule 2: DNA (28-MER)

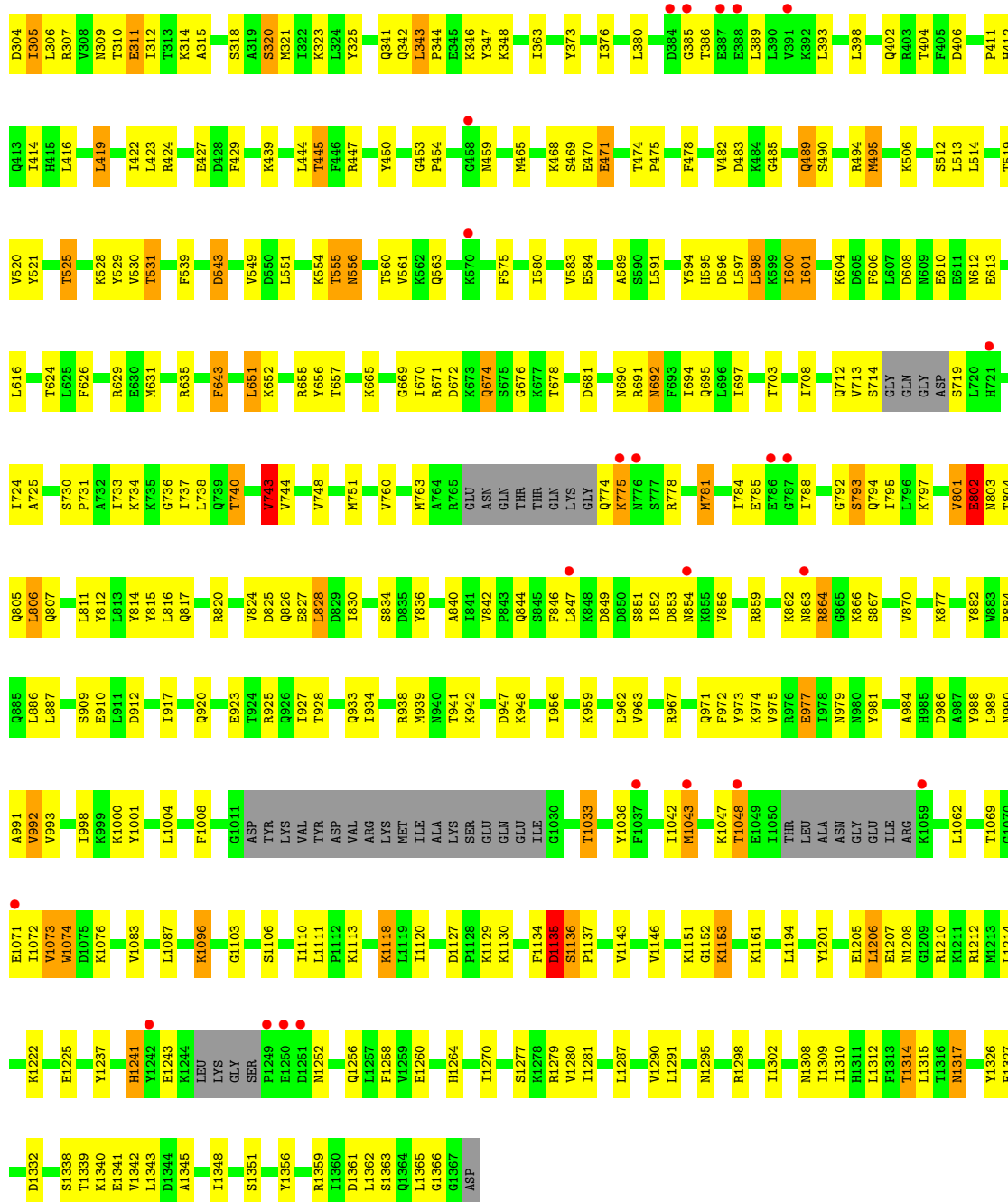


- Molecule 3: non-targeted DNA



- Molecule 4: CRISPR-associated endonuclease Cas9/Csn1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.78Å 69.67Å 189.02Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	46.77 – 2.90 46.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.4 (46.77-2.90) 91.8 (46.77-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.203 , 0.269 0.207 , 0.266	Depositor DCC
R_{free} test set	2285 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 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	0.93	EDS
Total number of atoms	13124	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: PO4

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	0.75	4/1947 (0.2%)	1.13	21/3031 (0.7%)
2	C	0.57	0/634	0.96	2/976 (0.2%)
3	D	0.80	1/255 (0.4%)	0.95	0/393
4	B	1.08	2/10734 (0.0%)	1.56	35/14468 (0.2%)
All	All	1.02	7/13570 (0.1%)	1.46	58/18868 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	DT	O3'-P	-7.41	1.50	1.61
1	A	26	A	O3'-P	-7.32	1.50	1.61
1	A	24	U	O3'-P	-6.72	1.51	1.61
4	B	1103	GLY	C-O	6.54	1.28	1.24
1	A	25	U	O3'-P	-5.46	1.52	1.61
4	B	1106	SER	C-O	-5.02	1.18	1.24
1	A	7	C	O3'-P	-5.01	1.53	1.61

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	G	C4'-C3'-O3'	-8.69	99.97	113.00
1	A	73	G	C4'-C3'-O3'	-8.57	100.14	113.00
1	A	48	A	C3'-C2'-O2'	7.29	121.64	110.70
4	B	445	THR	CA-CB-OG1	-7.28	98.68	109.60
1	A	79	G	C1'-C2'-O2'	7.22	119.23	108.40
1	A	22	U	C3'-C2'-O2'	7.14	121.42	110.70
4	B	177	ASP	CA-CB-CG	7.09	119.69	112.60
4	B	406	ASP	CA-CB-CG	6.72	119.32	112.60
4	B	1135	ASP	CA-CB-CG	6.47	119.07	112.60
4	B	866	LYS	CA-C-N	6.46	129.23	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	866	LYS	C-N-CA	6.46	129.23	120.38
1	A	71	U	C3'-C2'-O2'	6.45	120.38	110.70
1	A	42	A	C4'-C3'-O3'	-6.06	103.91	113.00
1	A	24	U	C2'-C3'-O3'	-6.02	104.67	113.70
1	A	59	U	C3'-C2'-O2'	5.98	119.66	110.70
1	A	13	G	C3'-C2'-O2'	5.93	119.60	110.70
4	B	123	VAL	CA-C-N	5.92	128.81	120.28
4	B	123	VAL	C-N-CA	5.92	128.81	120.28
4	B	123	VAL	O-C-N	5.92	128.04	121.94
4	B	743	VAL	N-CA-C	-5.85	104.81	110.72
4	B	1153	LYS	CA-C-N	5.85	128.11	120.28
4	B	1153	LYS	C-N-CA	5.85	128.11	120.28
4	B	1314	THR	N-CA-C	-5.77	105.07	111.36
4	B	1129	LYS	N-CA-C	-5.68	105.61	112.54
4	B	1152	GLY	CA-C-N	5.63	128.10	120.38
4	B	1152	GLY	C-N-CA	5.63	128.10	120.38
2	C	2	DA	C4'-C3'-O3'	5.62	118.44	110.00
4	B	273	ASP	CA-C-N	5.62	127.80	120.28
4	B	273	ASP	C-N-CA	5.62	127.80	120.28
4	B	294	LYS	CA-C-N	5.59	128.03	120.38
4	B	294	LYS	C-N-CA	5.59	128.03	120.38
1	A	16	A	C2'-C3'-O3'	-5.43	105.55	113.70
1	A	17	A	C3'-C2'-O2'	5.37	118.76	110.70
1	A	41	A	C3'-C2'-O2'	5.37	118.75	110.70
4	B	1048	THR	CA-CB-OG1	-5.35	101.58	109.60
4	B	591	LEU	CA-C-N	5.30	125.96	120.03
4	B	591	LEU	C-N-CA	5.30	125.96	120.03
1	A	29	G	C2'-C3'-O3'	-5.29	105.76	113.70
4	B	643	PHE	CA-C-N	5.25	129.14	121.31
4	B	643	PHE	C-N-CA	5.25	129.14	121.31
2	C	10	DT	C4'-C3'-O3'	5.25	117.87	110.00
1	A	78	A	C1'-C2'-O2'	5.22	116.23	108.40
1	A	6	U	C1'-C2'-O2'	5.20	116.20	108.40
1	A	78	A	C3'-C2'-O2'	5.19	118.48	110.70
4	B	1302	ILE	CA-C-N	5.14	127.13	120.44
4	B	1302	ILE	C-N-CA	5.14	127.13	120.44
4	B	555	THR	N-CA-C	-5.12	108.78	114.62
4	B	270	THR	CB-CA-C	5.12	120.60	110.42
1	A	33	G	C3'-C2'-O2'	5.11	118.37	110.70
4	B	43	ILE	CA-C-N	5.10	128.71	121.42
4	B	43	ILE	C-N-CA	5.10	128.71	121.42
1	A	38	A	C4'-C3'-O3'	-5.08	105.38	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	669	GLY	CA-C-N	5.07	127.29	120.50
4	B	669	GLY	C-N-CA	5.07	127.29	120.50
1	A	35	A	C1'-C2'-O2'	5.07	116.00	108.40
4	B	68	ALA	CA-C-N	5.04	127.34	120.54
4	B	68	ALA	C-N-CA	5.04	127.34	120.54
1	A	14	U	C3'-C2'-O2'	5.04	118.25	110.70

There are no chirality outliers.

There are no planarity outliers.

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	1737	0	868	34	0
2	C	567	0	322	14	0
3	D	227	0	127	7	0
4	B	10546	0	10471	303	0
5	B	25	0	0	2	0
6	A	5	0	0	0	0
6	B	15	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	13124	0	11788	327	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 13.

All (327) 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)
4:B:781:MET:HG3	4:B:803:ASN:HB3	1.15	1.09
4:B:781:MET:HG3	4:B:803:ASN:CB	1.82	1.09
4:B:106:LEU:O	4:B:111:LYS:HE3	1.55	1.06
4:B:963:VAL:HG21	4:B:990:ASN:ND2	1.88	0.88
4:B:781:MET:HG2	4:B:806:LEU:HD12	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:561:VAL:HG13	4:B:580:ILE:HD11	1.59	0.83
4:B:781:MET:CG	4:B:803:ASN:HB3	2.04	0.82
4:B:1135:ASP:O	4:B:1136:SER:OG	1.97	0.82
4:B:192:TYR:CE2	4:B:201:ILE:HD12	2.16	0.81
4:B:1135:ASP:O	4:B:1136:SER:CB	2.25	0.80
2:C:8:DA:H4'	2:C:9:DT:OP2	1.81	0.79
4:B:116:HIS:HB3	4:B:125:GLU:HG3	1.64	0.78
4:B:1222:LYS:HE2	4:B:1317:ASN:O	1.84	0.76
4:B:560:THR:HG22	4:B:563:GLN:NE2	2.03	0.73
4:B:161:MET:HE1	4:B:419:LEU:HA	1.71	0.72
4:B:191:THR:HG21	4:B:288:ASP:O	1.89	0.72
4:B:78:ARG:NH1	4:B:162:ILE:O	2.22	0.72
4:B:1207:GLU:OE1	4:B:1210:ARG:NH1	2.23	0.71
4:B:106:LEU:O	4:B:111:LYS:CE	2.36	0.71
2:C:2:DA:H2''	2:C:3:DA:O5'	1.91	0.69
4:B:556:ASN:ND2	4:B:563:GLN:OE1	2.26	0.69
2:C:2:DA:H2'	2:C:3:DA:C8	2.28	0.69
4:B:1111:LEU:HD11	4:B:1135:ASP:OD1	1.92	0.69
4:B:963:VAL:CG2	4:B:990:ASN:ND2	2.58	0.67
1:A:27:G:H5'	1:A:28:A:H5''	1.76	0.67
4:B:910:GLU:OE2	4:B:1033:THR:HG23	1.96	0.66
4:B:181:VAL:HG13	4:B:299:ALA:HB1	1.77	0.66
4:B:21:ILE:HG22	4:B:27:VAL:HG12	1.78	0.65
4:B:555:THR:C	4:B:595:HIS:HE1	2.05	0.65
4:B:736:GLY:O	4:B:740:THR:HG23	1.98	0.63
4:B:596:ASP:O	4:B:600:ILE:HG23	1.99	0.63
4:B:601:ILE:HG13	4:B:643:PHE:CE1	2.33	0.63
4:B:411:PRO:HD2	4:B:414:ILE:HG13	1.80	0.63
4:B:784:ILE:HD12	4:B:815:TYR:HB3	1.81	0.62
4:B:531:THR:HG21	4:B:575:PHE:HB3	1.81	0.62
4:B:708:ILE:O	4:B:712:GLN:HG2	1.99	0.62
4:B:161:MET:HE3	4:B:419:LEU:HD12	1.82	0.61
4:B:979:ASN:HB2	4:B:1225:GLU:OE2	2.01	0.60
4:B:100:ARG:HA	4:B:103:GLU:HG2	1.82	0.60
4:B:939:MET:HA	4:B:939:MET:HE3	1.84	0.60
4:B:189:VAL:HG11	4:B:203:ALA:CB	2.31	0.60
4:B:967:ARG:NH1	4:B:986:ASP:OD1	2.35	0.60
4:B:178:ASN:OD1	4:B:310:THR:HG23	2.02	0.59
4:B:380:LEU:HG	4:B:386:THR:CB	2.32	0.59
4:B:556:ASN:N	4:B:556:ASN:OD1	2.36	0.58
4:B:555:THR:HG22	4:B:556:ASN:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:817:GLN:O	4:B:882:TYR:OH	2.22	0.58
4:B:489:GLN:HE21	4:B:635:ARG:HH12	1.51	0.58
1:A:25:U:O2'	4:B:111:LYS:NZ	2.36	0.58
4:B:802:GLU:CG	4:B:803:ASN:N	2.67	0.58
4:B:812:TYR:CZ	4:B:816:LEU:HD11	2.39	0.58
4:B:977:GLU:HG3	4:B:1310:ILE:HG23	1.86	0.58
4:B:1161:LYS:HE2	4:B:1366:GLY:HA3	1.86	0.57
4:B:963:VAL:HG21	4:B:990:ASN:HD22	1.67	0.57
1:A:61:C:OP2	4:B:70:ARG:HD3	2.04	0.57
4:B:781:MET:HG3	4:B:803:ASN:CA	2.35	0.57
1:A:74:A:H2'	1:A:75:A:O4'	2.05	0.57
4:B:601:ILE:HG13	4:B:643:PHE:HE1	1.68	0.56
4:B:189:VAL:HG11	4:B:203:ALA:HB2	1.86	0.56
1:A:81:G:C2	4:B:35:LEU:HD22	2.39	0.56
2:C:17:DA:O4'	4:B:495:MET:HE3	2.05	0.56
4:B:15:SER:HA	4:B:51:LEU:O	2.06	0.56
4:B:514:LEU:HD11	4:B:613:GLU:OE2	2.05	0.56
4:B:1004:LEU:CD1	4:B:1042:ILE:HD11	2.35	0.56
4:B:283:GLY:C	4:B:285:GLN:H	2.12	0.56
2:C:8:DA:C4'	2:C:9:DT:OP2	2.54	0.56
4:B:560:THR:HG22	4:B:563:GLN:HE21	1.69	0.55
4:B:521:TYR:CZ	4:B:549:VAL:HG21	2.41	0.55
4:B:161:MET:CE	4:B:419:LEU:HA	2.35	0.55
4:B:844:GLN:OE1	4:B:844:GLN:HA	2.04	0.55
4:B:923:GLU:OE2	4:B:925:ARG:HG3	2.06	0.55
4:B:836:TYR:CE1	4:B:859:ARG:HG3	2.42	0.55
4:B:201:ILE:HG23	4:B:229:LEU:HD22	1.88	0.55
4:B:626:PHE:CE2	4:B:635:ARG:HD3	2.41	0.55
4:B:531:THR:HG21	4:B:575:PHE:CG	2.42	0.55
4:B:600:ILE:HD11	4:B:651:LEU:HG	1.89	0.54
4:B:849:ASP:OD1	4:B:851:SER:OG	2.21	0.54
4:B:525:THR:HG23	4:B:690:ASN:HB3	1.89	0.54
4:B:604:LYS:HE3	4:B:608:ASP:OD2	2.08	0.54
4:B:69:ARG:NH2	6:B:1501:HOH:O	2.37	0.54
4:B:11:ILE:HG12	4:B:740:THR:HG21	1.90	0.54
4:B:9:LEU:HD11	4:B:744:VAL:CG2	2.38	0.54
4:B:529:TYR:CB	4:B:580:ILE:HG22	2.37	0.54
1:A:45:U:H5'	4:B:402:GLN:NE2	2.23	0.54
4:B:343:LEU:N	4:B:344:PRO:CD	2.71	0.54
1:A:34:A:H2'	1:A:35:A:O4'	2.08	0.53
4:B:113:HIS:HD2	5:B:1404:PO4:O2	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:988:TYR:O	4:B:991:ALA:N	2.41	0.53
1:A:76:A:H2'	1:A:77:A:O4'	2.08	0.53
4:B:1290:VAL:HG21	4:B:1312:LEU:HD13	1.91	0.53
4:B:725:ALA:O	4:B:734:LYS:NZ	2.42	0.53
4:B:1222:LYS:CE	4:B:1317:ASN:O	2.55	0.53
4:B:118:ILE:N	4:B:125:GLU:OE1	2.40	0.52
4:B:119:PHE:HE2	4:B:128:TYR:HB2	1.73	0.52
4:B:271:TYR:O	4:B:272:ASP:C	2.52	0.52
4:B:763:MET:HE2	4:B:925:ARG:NH2	2.25	0.52
4:B:1161:LYS:CE	4:B:1366:GLY:HA3	2.40	0.52
4:B:1252:ASN:O	4:B:1256:GLN:CB	2.57	0.52
4:B:192:TYR:CE2	4:B:201:ILE:CD1	2.92	0.52
4:B:192:TYR:CD2	4:B:201:ILE:HD12	2.45	0.52
4:B:597:LEU:O	4:B:601:ILE:HG22	2.09	0.52
4:B:691:ARG:HA	4:B:695:GLN:OE1	2.10	0.52
4:B:781:MET:HE2	4:B:785:GLU:OE2	2.09	0.52
4:B:802:GLU:CD	4:B:805:GLN:HG2	2.34	0.52
4:B:376:ILE:C	4:B:376:ILE:HD12	2.35	0.51
1:A:44:U:O2'	4:B:402:GLN:NE2	2.37	0.51
4:B:724:ILE:CD1	4:B:738:LEU:HA	2.40	0.51
4:B:148:LYS:HD2	4:B:429:PHE:HB3	1.92	0.51
4:B:788:ILE:HG23	4:B:793:SER:HB3	1.92	0.51
4:B:191:THR:CG2	4:B:288:ASP:O	2.58	0.51
2:C:19:DA:C8	2:C:20:DT:H71	2.45	0.51
4:B:763:MET:HE2	4:B:925:ARG:HH21	1.76	0.51
4:B:788:ILE:HD13	4:B:795:ILE:CG2	2.41	0.51
1:A:22:U:O2'	4:B:1110:ILE:O	2.26	0.50
4:B:113:HIS:CD2	5:B:1404:PO4:O2	2.63	0.50
4:B:1314:THR:O	4:B:1315:LEU:C	2.52	0.50
1:A:81:G:N2	4:B:35:LEU:HD22	2.27	0.50
4:B:393:LEU:C	4:B:393:LEU:HD23	2.37	0.50
4:B:760:VAL:HG11	4:B:990:ASN:O	2.12	0.50
4:B:974:LYS:NZ	4:B:986:ASP:OD2	2.44	0.50
4:B:1161:LYS:HE2	4:B:1366:GLY:CA	2.41	0.50
4:B:554:LYS:HE2	4:B:594:TYR:CZ	2.46	0.50
1:A:27:G:O2'	4:B:129:HIS:CG	2.64	0.50
4:B:251:ASN:O	4:B:253:LYS:N	2.45	0.50
4:B:781:MET:HG2	4:B:806:LEU:CD1	2.35	0.49
1:A:63:U:H2'	4:B:62:THR:HG23	1.93	0.49
4:B:597:LEU:C	4:B:601:ILE:HG22	2.37	0.49
4:B:555:THR:C	4:B:556:ASN:OD1	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1042:ILE:HG23	4:B:1043:MET:N	2.27	0.49
4:B:1194:LEU:CD2	4:B:1365:LEU:HD13	2.43	0.49
2:C:2:DA:C2	2:C:3:DA:C4	3.01	0.49
4:B:992:VAL:CG2	4:B:993:VAL:N	2.76	0.49
1:A:77:A:C2	1:A:78:A:C5	3.01	0.49
4:B:1212:ARG:NH2	4:B:1280:VAL:O	2.43	0.49
4:B:802:GLU:OE1	4:B:805:GLN:HG2	2.13	0.49
4:B:1120:ILE:N	4:B:1134:PHE:O	2.46	0.49
1:A:54:G:C6	1:A:55:C:N4	2.81	0.48
4:B:1136:SER:H	4:B:1137:PRO:HD3	1.78	0.48
4:B:1206:LEU:CD1	4:B:1345:ALA:HB2	2.43	0.48
4:B:470:GLU:O	4:B:471:GLU:HB3	2.12	0.48
4:B:598:LEU:HD12	4:B:598:LEU:O	2.12	0.48
4:B:478:PHE:CE2	4:B:482:VAL:HG21	2.49	0.48
4:B:740:THR:HA	4:B:743:VAL:HG13	1.96	0.48
4:B:763:MET:SD	4:B:928:THR:HG22	2.52	0.48
4:B:963:VAL:CG2	4:B:990:ASN:HD22	2.24	0.48
4:B:528:LYS:HG2	4:B:539:PHE:HA	1.95	0.48
4:B:626:PHE:HE2	4:B:635:ARG:HD3	1.77	0.48
1:A:15:A:O2'	4:B:453:GLY:HA2	2.14	0.48
1:A:62:G:C5	4:B:69:ARG:HD3	2.48	0.48
4:B:310:THR:O	4:B:311:GLU:C	2.57	0.48
4:B:713:VAL:CG1	4:B:714:SER:N	2.75	0.48
1:A:44:U:H5'	4:B:363:ILE:HD12	1.95	0.48
4:B:165:ARG:O	4:B:412:HIS:HA	2.13	0.48
4:B:802:GLU:HG2	4:B:803:ASN:N	2.27	0.48
1:A:44:U:C2	4:B:325:TYR:CD1	3.02	0.48
4:B:450:TYR:CD1	4:B:450:TYR:C	2.91	0.48
4:B:554:LYS:HE3	4:B:594:TYR:CE1	2.50	0.47
4:B:1208:ASN:O	4:B:1279:ARG:NH1	2.47	0.47
4:B:1135:ASP:O	4:B:1136:SER:HB2	2.10	0.47
4:B:882:TYR:CZ	4:B:886:LEU:HD11	2.50	0.47
4:B:600:ILE:HG12	4:B:601:ILE:N	2.29	0.47
4:B:760:VAL:HA	4:B:956:ILE:O	2.15	0.47
4:B:310:THR:O	4:B:312:ILE:N	2.48	0.47
4:B:318:SER:O	4:B:321:MET:HB2	2.14	0.47
3:D:2:DA:C5'	4:B:774:GLN:CB	2.93	0.47
4:B:159:ALA:O	4:B:163:LYS:N	2.48	0.47
4:B:346:LYS:O	4:B:347:TYR:C	2.58	0.47
4:B:34:VAL:CG1	4:B:1359:ARG:HD2	2.45	0.46
4:B:555:THR:C	4:B:595:HIS:CE1	2.91	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:979:ASN:OD1	4:B:981:TYR:HB2	2.16	0.46
1:A:61:C:P	4:B:70:ARG:HH11	2.38	0.46
4:B:724:ILE:HD13	4:B:737:ILE:HG22	1.97	0.46
4:B:733:ILE:HD12	4:B:733:ILE:HA	1.87	0.46
4:B:781:MET:CA	4:B:781:MET:HE3	2.46	0.46
4:B:972:PHE:CE2	4:B:1083:VAL:HG11	2.50	0.46
4:B:560:THR:HG23	4:B:563:GLN:H	1.80	0.46
4:B:1270:ILE:HD11	4:B:1309:ILE:HD12	1.97	0.46
3:D:3:DA:C2'	3:D:4:DA:C8	2.98	0.46
4:B:805:GLN:C	4:B:807:GLN:H	2.23	0.46
4:B:1096:LYS:HD2	4:B:1201:TYR:CD1	2.51	0.46
4:B:1264:HIS:C	4:B:1264:HIS:CD2	2.94	0.46
4:B:103:GLU:O	4:B:103:GLU:HG3	2.16	0.46
4:B:794:GLN:OE1	4:B:797:LYS:CB	2.63	0.46
4:B:802:GLU:OE1	4:B:805:GLN:CD	2.58	0.46
4:B:1194:LEU:HD22	4:B:1365:LEU:HB3	1.98	0.46
1:A:27:G:O2'	4:B:129:HIS:CB	2.64	0.46
4:B:100:ARG:NH1	4:B:117:PRO:O	2.49	0.46
4:B:341:GLN:HG2	4:B:342:GLN:HG3	1.98	0.46
4:B:824:VAL:O	4:B:825:ASP:HB3	2.15	0.46
4:B:1194:LEU:HD21	4:B:1365:LEU:HD22	1.98	0.46
4:B:177:ASP:O	4:B:299:ALA:HB2	2.16	0.45
4:B:1073:VAL:O	4:B:1074:TRP:HB2	2.16	0.45
3:D:2:DA:H5'	4:B:774:GLN:CB	2.46	0.45
4:B:519:THR:HG22	4:B:589:ALA:CB	2.46	0.45
4:B:531:THR:HG21	4:B:575:PHE:CB	2.45	0.45
1:A:40:C:H2'	1:A:41:A:O4'	2.15	0.45
1:A:45:U:H5'	4:B:402:GLN:HE21	1.81	0.45
4:B:713:VAL:HG12	4:B:714:SER:N	2.32	0.45
4:B:842:VAL:HB	4:B:854:ASN:HD21	1.80	0.45
4:B:1237:TYR:O	4:B:1241:HIS:CD2	2.69	0.45
4:B:598:LEU:HD12	4:B:598:LEU:C	2.41	0.45
4:B:191:THR:O	4:B:194:GLN:HG3	2.16	0.45
4:B:320:SER:O	4:B:323:LYS:N	2.50	0.45
4:B:826:GLN:HG3	4:B:827:GLU:O	2.17	0.45
2:C:17:DA:O4'	4:B:495:MET:CE	2.65	0.45
4:B:1339:THR:O	4:B:1342:VAL:HG22	2.17	0.45
4:B:803:ASN:N	4:B:803:ASN:OD1	2.49	0.45
2:C:17:DA:C1'	4:B:495:MET:HE3	2.47	0.45
4:B:1277:SER:HA	4:B:1281:ILE:CG1	2.47	0.45
4:B:846:PHE:O	4:B:920:GLN:NE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:343:LEU:N	4:B:344:PRO:HD3	2.31	0.44
4:B:513:LEU:HD12	4:B:616:LEU:HB3	1.99	0.44
4:B:1317:ASN:HD22	4:B:1317:ASN:HA	1.68	0.44
4:B:781:MET:HG3	4:B:803:ASN:HA	1.98	0.44
4:B:393:LEU:HD23	4:B:393:LEU:O	2.17	0.44
4:B:554:LYS:NZ	4:B:608:ASP:OD1	2.46	0.44
4:B:801:VAL:C	4:B:802:GLU:O	2.59	0.44
4:B:109:GLU:OE2	4:B:1130:LYS:HE2	2.17	0.44
4:B:763:MET:HB2	4:B:925:ARG:HH22	1.82	0.44
4:B:191:THR:O	4:B:194:GLN:CG	2.66	0.44
4:B:485:GLY:HA2	4:B:631:MET:HE1	1.99	0.44
4:B:814:TYR:HE2	4:B:828:LEU:O	2.01	0.44
4:B:1207:GLU:O	4:B:1210:ARG:HB3	2.18	0.44
4:B:283:GLY:C	4:B:285:GLN:N	2.76	0.44
4:B:672:ASP:HA	4:B:703:THR:OG1	2.18	0.44
4:B:784:ILE:HD11	4:B:816:LEU:HG	2.00	0.44
4:B:927:ILE:HG23	4:B:928:THR:N	2.32	0.44
4:B:30:LYS:HD2	4:B:751:MET:HE1	2.00	0.43
1:A:24:U:O2	4:B:105:PHE:CD1	2.71	0.43
4:B:373:TYR:CE1	4:B:398:LEU:HB3	2.52	0.43
4:B:801:VAL:O	4:B:802:GLU:O	2.36	0.43
1:A:61:C:OP1	4:B:70:ARG:NH1	2.52	0.43
4:B:820:ARG:NH1	4:B:825:ASP:OD1	2.51	0.43
4:B:975:VAL:HG12	4:B:977:GLU:HG2	2.00	0.43
4:B:1287:LEU:HA	4:B:1290:VAL:HG12	1.99	0.43
2:C:2:DA:C2	2:C:3:DA:C5	3.06	0.43
4:B:48:ILE:HG12	4:B:984:ALA:HB1	2.01	0.43
4:B:474:THR:O	4:B:475:PRO:C	2.60	0.43
4:B:155:TYR:CD2	4:B:155:TYR:C	2.97	0.43
4:B:69:ARG:O	4:B:73:THR:HG23	2.18	0.43
4:B:75:ARG:HD2	4:B:163:LYS:HG3	2.00	0.43
4:B:781:MET:HE3	4:B:781:MET:O	2.19	0.43
4:B:788:ILE:O	4:B:792:GLY:N	2.52	0.43
2:C:27:DA:O4'	4:B:692:ASN:ND2	2.51	0.43
3:D:3:DA:H2''	3:D:4:DA:C8	2.54	0.43
4:B:122:ILE:O	4:B:126:VAL:HG23	2.19	0.43
4:B:189:VAL:HG11	4:B:203:ALA:HB3	2.01	0.43
4:B:737:ILE:O	4:B:738:LEU:C	2.61	0.43
4:B:1161:LYS:NZ	4:B:1343:LEU:O	2.52	0.43
4:B:956:ILE:HA	4:B:1008:PHE:O	2.19	0.42
4:B:1000:LYS:HG3	4:B:1001:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:28:PRO:HG2	4:B:47:LEU:HD12	2.02	0.42
4:B:674:GLN:HA	4:B:674:GLN:NE2	2.34	0.42
4:B:678:THR:O	4:B:681:ASP:HB2	2.19	0.42
4:B:1308:ASN:ND2	4:B:1327:PHE:H	2.16	0.42
1:A:63:U:H4'	1:A:64:U:OP2	2.19	0.42
4:B:389:LEU:HD23	4:B:389:LEU:HA	1.84	0.42
4:B:1351:SER:HB3	4:B:1356:TYR:HB2	2.02	0.42
4:B:1361:ASP:CG	4:B:1363:SER:OG	2.63	0.42
4:B:94:ASP:OD2	4:B:100:ARG:NH2	2.48	0.42
4:B:988:TYR:CD2	4:B:989:LEU:HD23	2.54	0.42
4:B:1312:LEU:HD21	4:B:1326:TYR:CD1	2.54	0.42
4:B:1206:LEU:HD13	4:B:1345:ALA:CB	2.50	0.42
4:B:1214:LEU:HD12	4:B:1214:LEU:HA	1.79	0.42
2:C:27:DA:H1'	4:B:694:ILE:HG21	2.00	0.42
4:B:811:LEU:O	4:B:814:TYR:HB3	2.20	0.42
1:A:1:A:H2'	1:A:2:U:O5'	2.20	0.42
3:D:3:DA:H2'	3:D:4:DA:C8	2.55	0.42
4:B:1127:ASP:OD1	4:B:1127:ASP:C	2.60	0.42
4:B:468:LYS:HG2	4:B:483:ASP:HB2	2.02	0.42
1:A:73:G:O2'	1:A:75:A:N7	2.31	0.42
4:B:763:MET:HG3	4:B:928:THR:HG22	2.01	0.42
4:B:781:MET:HE3	4:B:781:MET:HA	2.02	0.42
4:B:909:SER:O	4:B:912:ASP:N	2.53	0.42
1:A:56:U:H1'	4:B:459:ASN:HD21	1.84	0.42
4:B:143:VAL:HG12	4:B:422:ILE:HG13	2.02	0.42
4:B:189:VAL:O	4:B:193:ASN:HB2	2.20	0.42
4:B:423:LEU:O	4:B:427:GLU:HG2	2.20	0.42
4:B:85:ILE:HD11	4:B:439:LYS:HE2	2.02	0.41
4:B:543:ASP:OD1	4:B:543:ASP:N	2.50	0.41
4:B:1277:SER:HA	4:B:1281:ILE:HG12	2.02	0.41
4:B:90:MET:HE1	4:B:152:ARG:HA	2.02	0.41
4:B:237:LEU:HA	4:B:255:ASN:ND2	2.35	0.41
4:B:763:MET:CG	4:B:928:THR:HG22	2.50	0.41
4:B:775:LYS:HA	4:B:778:ARG:NH2	2.35	0.41
4:B:934:ILE:O	4:B:938:ARG:HB2	2.20	0.41
4:B:490:SER:O	4:B:494:ARG:HG2	2.20	0.41
4:B:189:VAL:HG12	4:B:193:ASN:ND2	2.35	0.41
4:B:626:PHE:N	4:B:626:PHE:CD1	2.89	0.41
4:B:1136:SER:H	4:B:1137:PRO:CD	2.33	0.41
1:A:56:U:O2	4:B:459:ASN:ND2	2.53	0.41
4:B:801:VAL:HG21	4:B:815:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1210:ARG:HD2	4:B:1280:VAL:HA	2.03	0.41
2:C:8:DA:C5	3:D:4:DA:N6	2.89	0.41
4:B:75:ARG:O	4:B:78:ARG:N	2.52	0.41
4:B:148:LYS:HD2	4:B:429:PHE:CB	2.51	0.41
4:B:812:TYR:CE1	4:B:816:LEU:HD11	2.55	0.41
1:A:31:U:O2'	1:A:32:A:H5'	2.19	0.41
4:B:103:GLU:OE1	4:B:111:LYS:HG2	2.20	0.41
4:B:781:MET:HE2	4:B:781:MET:HB3	1.71	0.41
1:A:15:A:O3'	4:B:454:PRO:HD3	2.21	0.41
4:B:168:PHE:CE1	4:B:412:HIS:CE1	3.09	0.41
4:B:212:LEU:HD22	4:B:246:LEU:HD21	2.03	0.41
4:B:306:LEU:N	4:B:306:LEU:HD23	2.36	0.41
4:B:730:SER:O	4:B:731:PRO:C	2.63	0.41
4:B:814:TYR:CE1	4:B:830:ILE:HD12	2.56	0.41
4:B:971:GLN:HG2	4:B:973:TYR:OH	2.20	0.41
4:B:1036:TYR:CD1	4:B:1036:TYR:C	2.99	0.41
4:B:1118:LYS:HE3	4:B:1118:LYS:CA	2.51	0.41
4:B:1206:LEU:HD13	4:B:1345:ALA:HB2	2.01	0.41
4:B:1295:ASN:HA	4:B:1298:ARG:NE	2.36	0.41
4:B:1340:LYS:O	4:B:1341:GLU:C	2.64	0.41
4:B:143:VAL:HG21	4:B:315:ALA:HB2	2.03	0.40
4:B:424:ARG:HD3	4:B:424:ARG:HA	1.86	0.40
4:B:840:ALA:O	4:B:864:ARG:NH2	2.54	0.40
1:A:15:A:OP1	4:B:70:ARG:NH2	2.50	0.40
2:C:8:DA:C6	3:D:4:DA:N6	2.90	0.40
4:B:805:GLN:C	4:B:807:GLN:N	2.79	0.40
4:B:416:LEU:HB2	4:B:444:LEU:HD22	2.03	0.40
4:B:606:PHE:CE2	4:B:612:ASN:ND2	2.89	0.40
4:B:624:THR:HA	4:B:656:TYR:O	2.21	0.40
4:B:1205:GLU:HB2	4:B:1348:ILE:HD11	2.03	0.40
4:B:671:ARG:NH1	4:B:676:GLY:O	2.55	0.40
4:B:1342:VAL:O	4:B:1362:LEU:HD12	2.22	0.40
1:A:27:G:H5'	1:A:28:A:C5'	2.48	0.40
4:B:139:ARG:CZ	4:B:161:MET:HG2	2.51	0.40
4:B:763:MET:HE3	4:B:763:MET:HB3	1.87	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	
4	B	1311/1368 (96%)	1147 (88%)	140 (11%)	24 (2%)	6	25

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	1136	SER
4	B	252	PHE
4	B	284	ASP
4	B	311	GLU
4	B	471	GLU
4	B	802	GLU
4	B	1074	TRP
4	B	207	ASP
4	B	272	ASP
4	B	385	GLY
4	B	947	ASP
4	B	1062	LEU
4	B	1071	GLU
4	B	1243	GLU
4	B	270	THR
4	B	298	ASP
4	B	629	ARG
4	B	674	GLN
4	B	775	LYS
4	B	254	SER
4	B	305	ILE
4	B	692	ASN
4	B	1258	PHE
4	B	806	LEU

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
4	B	1116/1226 (91%)	992 (89%)	124 (11%)	6 20

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	29	SER
4	B	35	LEU
4	B	41	HIS
4	B	44	LYS
4	B	55	SER
4	B	58	THR
4	B	73	THR
4	B	76	LYS
4	B	109	GLU
4	B	111	LYS
4	B	143	VAL
4	B	147	ASP
4	B	179	SER
4	B	181	VAL
4	B	186	ILE
4	B	194	GLN
4	B	201	ILE
4	B	206	VAL
4	B	207	ASP
4	B	211	ILE
4	B	213	SER
4	B	216	LEU
4	B	244	LEU
4	B	252	PHE
4	B	254	SER
4	B	269	ASP
4	B	270	THR
4	B	272	ASP
4	B	302	LEU
4	B	304	ASP

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Mol	Chain	Res	Type
4	B	305	ILE
4	B	307	ARG
4	B	309	ASN
4	B	314	LYS
4	B	320	SER
4	B	343	LEU
4	B	348	LYS
4	B	404	THR
4	B	419	LEU
4	B	445	THR
4	B	447	ARG
4	B	465	MET
4	B	469	SER
4	B	489	GLN
4	B	495	MET
4	B	506	LYS
4	B	512	SER
4	B	520	VAL
4	B	525	THR
4	B	530	VAL
4	B	531	THR
4	B	543	ASP
4	B	551	LEU
4	B	556	ASN
4	B	583	VAL
4	B	584	GLU
4	B	598	LEU
4	B	600	ILE
4	B	601	ILE
4	B	610	GLU
4	B	651	LEU
4	B	652	LYS
4	B	655	ARG
4	B	657	THR
4	B	665	LYS
4	B	670	ILE
4	B	697	ILE
4	B	719	SER
4	B	740	THR
4	B	743	VAL
4	B	748	VAL
4	B	781	MET

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Mol	Chain	Res	Type
4	B	793	SER
4	B	801	VAL
4	B	802	GLU
4	B	804	THR
4	B	828	LEU
4	B	834	SER
4	B	847	LEU
4	B	852	ILE
4	B	853	ASP
4	B	856	VAL
4	B	862	LYS
4	B	863	ASN
4	B	864	ARG
4	B	867	SER
4	B	870	VAL
4	B	877	LYS
4	B	884	ARG
4	B	887	LEU
4	B	917	ILE
4	B	933	GLN
4	B	941	THR
4	B	942	LYS
4	B	948	LYS
4	B	959	LYS
4	B	962	LEU
4	B	977	GLU
4	B	992	VAL
4	B	998	ILE
4	B	1033	THR
4	B	1043	MET
4	B	1047	LYS
4	B	1048	THR
4	B	1069	THR
4	B	1072	ILE
4	B	1073	VAL
4	B	1076	LYS
4	B	1087	LEU
4	B	1096	LYS
4	B	1113	LYS
4	B	1118	LYS
4	B	1135	ASP
4	B	1143	VAL

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Mol	Chain	Res	Type
4	B	1146	VAL
4	B	1151	LYS
4	B	1153	LYS
4	B	1206	LEU
4	B	1241	HIS
4	B	1260	GLU
4	B	1291	LEU
4	B	1317	ASN
4	B	1332	ASP
4	B	1338	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	77	ASN
4	B	113	HIS
4	B	121	ASN
4	B	224	ASN
4	B	402	GLN
4	B	459	ASN
4	B	489	GLN
4	B	595	HIS
4	B	612	ASN
4	B	668	ASN
4	B	674	GLN
4	B	807	GLN
4	B	885	GLN
4	B	983	HIS
4	B	990	ASN
4	B	1044	ASN
4	B	1221	GLN
4	B	1261	GLN
4	B	1305	GLN
4	B	1308	ASN
4	B	1317	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/84 (95%)	20 (25%)	2 (2%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	10	U
1	A	17	A
1	A	28	A
1	A	29	G
1	A	30	C
1	A	37	U
1	A	39	G
1	A	41	A
1	A	42	A
1	A	51	A
1	A	52	A
1	A	59	U
1	A	63	U
1	A	68	A
1	A	71	U
1	A	73	G
1	A	78	A
1	A	80	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	28	A
1	A	29	G

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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	B	1404	-	4,4,4	0.59	0	6,6,6	0.58	0
5	PO4	B	1403	-	4,4,4	0.78	0	6,6,6	0.43	0
5	PO4	B	1402	-	4,4,4	0.78	0	6,6,6	0.48	0
5	PO4	B	1405	-	4,4,4	0.66	0	6,6,6	0.50	0
5	PO4	B	1401	-	4,4,4	0.67	0	6,6,6	0.56	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1404	PO4	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	82/84 (97%)	-0.68	0 100 100	28, 49, 86, 93	0
2	C	28/28 (100%)	-0.50	0 100 100	39, 54, 71, 76	0
3	D	11/12 (91%)	-0.04	1 (9%) 15 12	36, 54, 121, 148	0
4	B	1323/1368 (96%)	0.10	45 (3%) 48 39	30, 62, 109, 137	0
All	All	1444/1492 (96%)	0.04	46 (3%) 50 41	28, 61, 108, 148	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	384	ASP	4.7
4	B	385	GLY	4.5
4	B	266	LEU	4.3
4	B	1249	PRO	3.8
4	B	292	ALA	3.6
4	B	1242	TYR	3.1
4	B	776	ASN	3.1
4	B	786	GLU	3.0
4	B	287	ALA	3.0
4	B	291	LEU	2.9
4	B	286	TYR	2.9
4	B	1059	LYS	2.8
4	B	187	GLN	2.7
4	B	1250	GLU	2.7
4	B	215	ARG	2.6
4	B	181	VAL	2.6
4	B	284	ASP	2.6
4	B	387	GLU	2.6
4	B	1048	THR	2.6
4	B	264	LEU	2.5
4	B	1037	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	12	DG	2.5
4	B	235	ASN	2.5
4	B	196	PHE	2.4
4	B	1043	MET	2.4
4	B	206	VAL	2.3
4	B	863	ASN	2.3
4	B	1071	GLU	2.3
4	B	190	GLN	2.3
4	B	248	LEU	2.3
4	B	570	LYS	2.2
4	B	721	HIS	2.2
4	B	270	THR	2.2
4	B	1251	ASP	2.2
4	B	787	GLY	2.2
4	B	775	LYS	2.2
4	B	203	ALA	2.2
4	B	458	GLY	2.2
4	B	204	SER	2.2
4	B	391	VAL	2.1
4	B	388	GLU	2.1
4	B	186	ILE	2.1
4	B	854	ASN	2.1
4	B	847	LEU	2.1
4	B	251	ASN	2.0
4	B	182	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	PO4	B	1405	5/5	0.63	0.13	107,112,117,122	0
5	PO4	B	1402	5/5	0.84	0.13	71,86,92,94	0
5	PO4	B	1403	5/5	0.86	0.11	78,81,85,86	0
5	PO4	B	1404	5/5	0.88	0.12	64,69,74,82	0
5	PO4	B	1401	5/5	0.91	0.12	52,58,61,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.