



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:14 AM UTC

PDB ID : 6K4Q / pdb_00006k4q
Title : Crystal structure of xCas9 in complex with sgRNA and DNA (CGG PAM)
Authors : Chen, W.; Zhang, H.; Zhang, Y.; Wang, Y.; Gan, J.; Ji, Q.
Deposited on : 2019-05-26
Resolution : 2.70 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

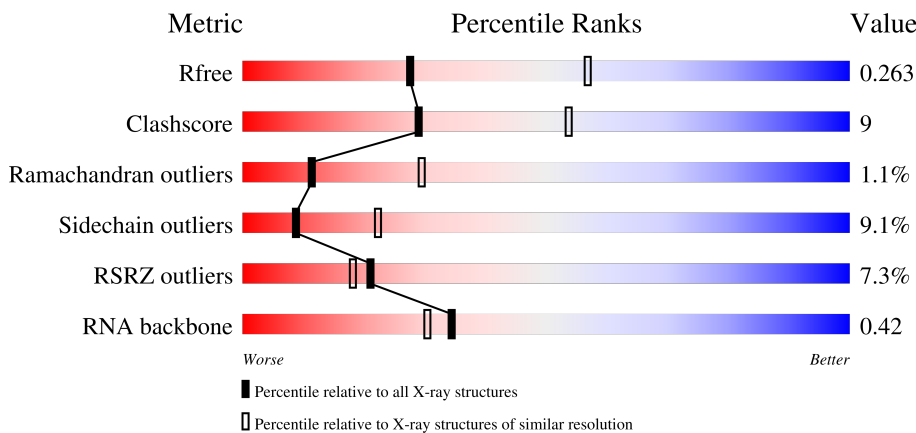
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	83	
2	C	28	
3	D	12	
4	B	1368	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13209 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	81	Total	C	N	O	P	0	0	0
			1732	778	318	555	81			

- 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
			568	276	96	169	27			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*AP*CP*GP*GP*TP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			226	109	44	63	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
			10539	6725	1827	1968	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	574	GLU	CYS	engineered mutation	UNP Q99ZW2
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: O₄P).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total 22	O 22	0	0
6	C	6	Total 6	O 6	0	0
6	D	1	Total 1	O 1	0	0
6	B	70	Total 70	O 70	0	0

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

Chain A: 



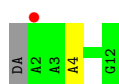
- Molecule 2: DNA (28-MER)

Chain C: 



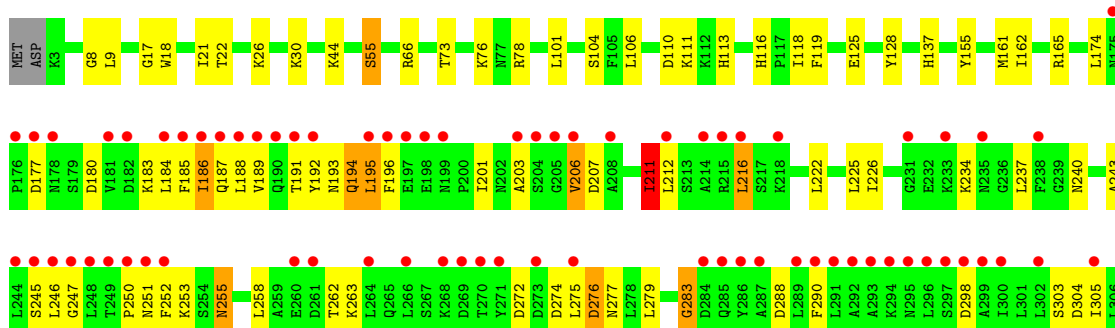
- Molecule 3: DNA (5'-D(*AP*AP*AP*CP*GP*GP*TP*AP*TP*TP*G)-3')

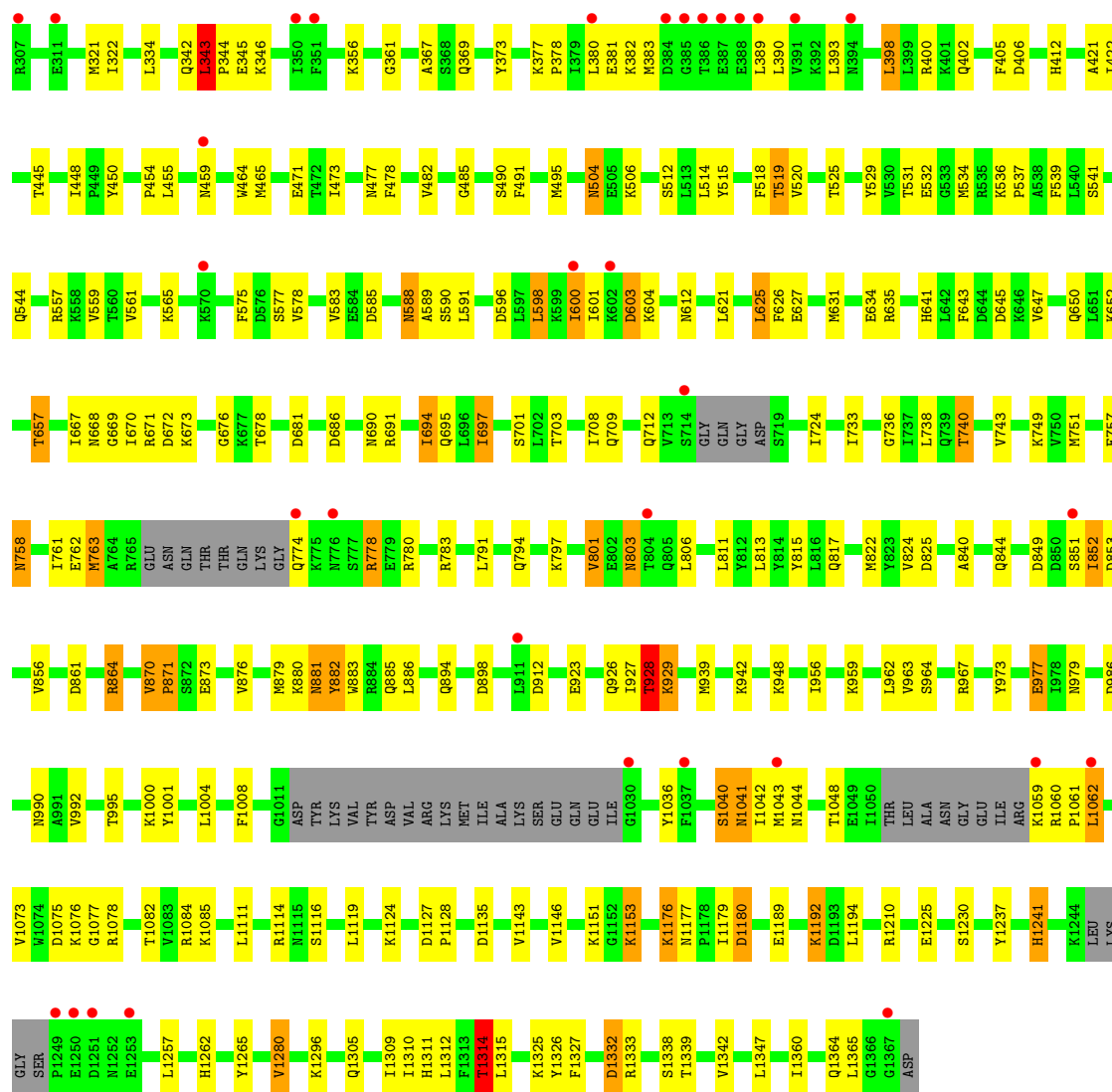
Chain D: 



- Molecule 4: CRISPR-associated endonuclease Cas9/Csn1

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.84Å 69.67Å 189.51Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	49.38 – 2.70 49.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.38-2.70) 94.4 (49.38-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.203 , 0.275 (Not available) , 0.263	Depositor DCC
R_{free} test set	2888 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13209	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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	0.86	9/1942 (0.5%)	1.08	15/3023 (0.5%)
2	C	0.75	2/635 (0.3%)	1.11	4/978 (0.4%)
3	D	0.54	0/254	0.90	0/391
4	B	1.15	6/10727 (0.1%)	1.58	39/14459 (0.3%)
All	All	1.09	17/13558 (0.1%)	1.47	58/18851 (0.3%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	G	O3'-P	-6.99	1.50	1.61
1	A	21	G	O3'-P	-6.52	1.51	1.61
1	A	40	C	O3'-P	-6.10	1.52	1.61
2	C	15	DA	O3'-P	-6.05	1.52	1.61
1	A	24	U	O3'-P	-6.05	1.52	1.61
4	B	421	ALA	C-O	5.90	1.30	1.24
1	A	65	A	O3'-P	-5.86	1.52	1.61
4	B	881	ASN	C-N	-5.82	1.25	1.33
4	B	763	MET	C-O	-5.80	1.17	1.23
1	A	20	A	O3'-P	-5.74	1.52	1.61
4	B	454	PRO	C-O	-5.41	1.17	1.23
2	C	16	DC	O3'-P	-5.29	1.53	1.61
1	A	64	U	O3'-P	-5.28	1.53	1.61
1	A	41	A	O3'-P	-5.27	1.53	1.61
4	B	459	ASN	C-O	-5.21	1.18	1.24
4	B	101	LEU	C-O	-5.07	1.18	1.24
1	A	42	A	O3'-P	-5.05	1.53	1.61

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1314	THR	N-CA-C	-7.71	102.88	111.82
4	B	757	GLU	N-CA-C	-7.66	102.86	111.14
2	C	2	DA	C4'-C3'-O3'	7.48	121.22	110.00
4	B	1153	LYS	CA-C-N	7.12	129.82	120.28
4	B	1153	LYS	C-N-CA	7.12	129.82	120.28
1	A	73	G	C1'-C2'-O2'	7.08	119.01	108.40
4	B	406	ASP	CA-CB-CG	7.06	119.66	112.60
4	B	612	ASN	CA-C-N	7.06	129.74	120.28
4	B	612	ASN	C-N-CA	7.06	129.74	120.28
1	A	18	A	C3'-C2'-O2'	6.59	120.59	110.70
4	B	882	TYR	CA-C-N	-6.58	109.74	120.72
4	B	882	TYR	C-N-CA	-6.58	109.74	120.72
4	B	657	THR	CA-CB-OG1	-6.48	99.87	109.60
4	B	871	PRO	CA-C-N	6.41	130.24	120.82
4	B	871	PRO	C-N-CA	6.41	130.24	120.82
4	B	1332	ASP	CA-CB-CG	-6.29	106.31	112.60
4	B	645	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	10	U	C3'-C2'-O2'	6.11	119.86	110.70
1	A	68	A	C3'-C2'-O2'	6.07	119.81	110.70
4	B	177	ASP	CA-CB-CG	6.01	118.61	112.60
4	B	928	THR	N-CA-C	-5.90	104.92	111.36
1	A	81	G	C2'-C3'-O3'	5.90	118.35	109.50
4	B	55	SER	CA-C-N	5.79	125.48	119.92
4	B	55	SER	C-N-CA	5.79	125.48	119.92
1	A	17	A	C3'-C2'-O2'	5.78	119.36	110.70
1	A	59	U	C1'-C2'-O2'	-5.76	99.76	108.40
4	B	288	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	7	C	C3'-C2'-O2'	5.71	119.27	110.70
2	C	18	DA	C2'-C3'-O3'	-5.71	102.93	111.50
1	A	31	U	C3'-C2'-O2'	5.68	119.21	110.70
1	A	39	G	C1'-C2'-O2'	5.58	116.78	108.40
4	B	603	ASP	CB-CA-C	5.57	118.94	109.80
2	C	10	DT	C2'-C3'-O3'	-5.53	103.21	111.50
2	C	5	DA	C4'-C3'-O3'	-5.52	101.72	110.00
4	B	926	GLN	CB-CA-C	5.52	119.95	110.79
4	B	110	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	19	A	C4'-C3'-O3'	-5.42	104.87	113.00
4	B	881	ASN	N-CA-C	-5.40	105.32	112.34
4	B	588	ASN	N-CA-C	-5.37	105.33	111.07
1	A	38	A	C3'-C2'-O2'	5.36	118.75	110.70
4	B	283	GLY	CA-C-O	-5.32	117.73	121.88
4	B	44	LYS	CA-C-O	-5.31	114.99	121.05
4	B	591	LEU	CA-C-N	5.31	125.99	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	591	LEU	C-N-CA	5.31	125.99	119.99
1	A	24	U	C2'-C3'-O3'	-5.30	105.74	113.70
4	B	276	ASP	CA-CB-CG	5.29	117.89	112.60
4	B	873	GLU	CA-C-N	5.20	127.57	120.54
4	B	873	GLU	C-N-CA	5.20	127.57	120.54
4	B	272	ASP	CA-C-N	5.20	127.67	120.29
4	B	272	ASP	C-N-CA	5.20	127.67	120.29
1	A	71	U	C3'-C2'-O2'	5.13	118.40	110.70
4	B	912	ASP	CA-C-N	5.13	127.15	120.28
4	B	912	ASP	C-N-CA	5.13	127.15	120.28
4	B	22	THR	CA-CB-OG1	-5.10	101.96	109.60
1	A	10	U	C2'-C3'-O3'	5.04	121.27	113.70
4	B	504	ASN	CB-CA-C	5.04	118.42	109.65
4	B	1116	SER	CA-C-N	5.01	128.69	120.63
4	B	1116	SER	C-N-CA	5.01	128.69	120.63

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	1732	0	869	12	0
2	C	568	0	322	9	0
3	D	226	0	126	1	0
4	B	10539	0	10458	200	0
5	A	10	0	0	0	0
5	B	35	0	0	1	0
6	A	22	0	0	0	0
6	B	70	0	0	3	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
All	All	13209	0	11775	216	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 9.

All (216) 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:212:LEU:CD2	4:B:246:LEU:HD21	1.71	1.18
4:B:813:LEU:O	4:B:817:GLN:HG3	1.47	1.13
4:B:212:LEU:HD23	4:B:246:LEU:HD21	1.42	0.98
4:B:211:ILE:HD11	4:B:225:LEU:HD12	1.50	0.93
4:B:212:LEU:HD22	4:B:246:LEU:HD21	1.50	0.92
4:B:116:HIS:HB3	4:B:125:GLU:HG3	1.55	0.88
4:B:211:ILE:HD12	4:B:225:LEU:HA	1.54	0.86
4:B:794:GLN:OE1	4:B:797:LYS:CB	2.25	0.84
4:B:541:SER:H	4:B:544:GLN:HE21	1.29	0.80
4:B:212:LEU:CD2	4:B:246:LEU:CD2	2.61	0.76
4:B:840:ALA:O	4:B:864:ARG:NH2	2.20	0.75
4:B:118:ILE:N	4:B:125:GLU:OE1	2.20	0.75
4:B:194:GLN:NE2	4:B:195:LEU:HD13	2.02	0.74
4:B:183:LYS:O	4:B:184:LEU:C	2.28	0.74
4:B:212:LEU:HD22	4:B:246:LEU:CD2	2.17	0.73
2:C:11:DT:C2'	2:C:12:DT:H5'	2.19	0.72
4:B:187:GLN:O	4:B:191:THR:HG23	1.89	0.71
4:B:1311:HIS:O	4:B:1314:THR:HG23	1.91	0.71
2:C:11:DT:H2''	2:C:12:DT:H5'	1.73	0.71
4:B:870:VAL:HG22	4:B:871:PRO:HD2	1.73	0.70
4:B:189:VAL:HG11	4:B:203:ALA:HB2	1.73	0.70
4:B:1179:ILE:HD11	4:B:1192:LYS:HG3	1.74	0.69
4:B:211:ILE:HD12	4:B:225:LEU:CA	2.22	0.69
4:B:342:GLN:OE1	4:B:383:MET:HB2	1.93	0.68
4:B:967:ARG:NH1	4:B:986:ASP:OD1	2.27	0.68
4:B:1042:ILE:HG23	4:B:1043:MET:HG2	1.75	0.67
4:B:803:ASN:H	4:B:803:ASN:HD22	1.40	0.66
4:B:678:THR:O	4:B:681:ASP:HB2	1.96	0.66
1:A:23:U:O5'	1:A:23:U:H6	1.78	0.66
4:B:1210:ARG:HA	4:B:1280:VAL:HG22	1.76	0.66
4:B:185:PHE:O	4:B:189:VAL:HG23	1.96	0.65
4:B:813:LEU:O	4:B:817:GLN:CG	2.36	0.63
4:B:525:THR:O	4:B:690:ASN:HB3	1.99	0.62
4:B:455:LEU:HA	4:B:465:MET:HE2	1.82	0.62
4:B:211:ILE:CG1	4:B:212:LEU:N	2.62	0.62
4:B:671:ARG:NH1	4:B:676:GLY:O	2.32	0.62
4:B:942:LYS:HB2	6:B:1539:HOH:O	1.98	0.62
4:B:211:ILE:HG13	4:B:212:LEU:N	2.15	0.62
4:B:211:ILE:HD11	4:B:225:LEU:CD1	2.28	0.61
4:B:369:GLN:OE1	4:B:400:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:226:ILE:HD13	4:B:234:LYS:HA	1.83	0.60
4:B:880:LYS:C	4:B:882:TYR:N	2.57	0.60
4:B:250:PRO:O	4:B:263:LYS:HA	2.02	0.59
4:B:557:ARG:NH2	4:B:596:ASP:OD1	2.36	0.59
1:A:76:A:H2'	1:A:77:A:O4'	2.02	0.58
4:B:183:LYS:O	4:B:186:ILE:N	2.36	0.58
4:B:817:GLN:O	4:B:882:TYR:OH	2.22	0.57
4:B:774:GLN:O	4:B:778:ARG:HB2	2.04	0.57
4:B:1237:TYR:O	4:B:1241:HIS:CD2	2.58	0.57
2:C:2:DA:H2'	2:C:3:DA:C8	2.40	0.57
4:B:1111:LEU:HD11	4:B:1135:ASP:HB2	1.87	0.56
4:B:531:THR:HG22	4:B:577:SER:O	2.06	0.56
4:B:923:GLU:HG2	4:B:928:THR:OG1	2.06	0.56
4:B:373:TYR:CE1	4:B:398:LEU:HB3	2.40	0.56
1:A:1:A:H5''	4:B:929:LYS:HE2	1.87	0.55
4:B:207:ASP:O	4:B:211:ILE:HG23	2.06	0.55
4:B:849:ASP:OD1	4:B:851:SER:HB3	2.07	0.55
4:B:673:LYS:HB2	4:B:703:THR:HG21	1.88	0.55
4:B:803:ASN:HD22	4:B:803:ASN:N	2.01	0.55
4:B:240:ASN:ND2	4:B:255:ASN:OD1	2.31	0.55
4:B:1114:ARG:HG2	4:B:1119:LEU:HD11	1.87	0.55
4:B:561:VAL:HG22	4:B:585:ASP:O	2.07	0.54
4:B:180:ASP:OD1	4:B:183:LYS:HD2	2.08	0.54
4:B:274:ASP:HA	4:B:277:ASN:ND2	2.23	0.54
4:B:880:LYS:O	4:B:883:TRP:N	2.40	0.54
4:B:194:GLN:HE21	4:B:195:LEU:HD13	1.73	0.54
4:B:733:ILE:HG12	4:B:763:MET:HE1	1.90	0.54
4:B:118:ILE:HB	4:B:125:GLU:OE1	2.07	0.53
4:B:824:VAL:O	4:B:825:ASP:HB3	2.08	0.53
4:B:211:ILE:CG1	4:B:212:LEU:H	2.22	0.53
4:B:973:TYR:CD1	4:B:1237:TYR:CE2	2.97	0.53
4:B:1194:LEU:HD22	4:B:1365:LEU:HB3	1.91	0.53
4:B:334:LEU:HD23	4:B:389:LEU:HD21	1.90	0.53
4:B:1177:ASN:ND2	4:B:1180:ASP:OD1	2.42	0.53
4:B:345:GLU:HG2	4:B:346:LYS:HG2	1.91	0.52
4:B:801:VAL:HG11	4:B:815:TYR:CE2	2.44	0.52
1:A:45:U:H5'	4:B:402:GLN:HE21	1.74	0.52
4:B:113:HIS:ND1	5:B:1403:PO4:O2	2.42	0.51
4:B:973:TYR:CE1	4:B:1237:TYR:CE2	2.98	0.51
4:B:1312:LEU:HD21	4:B:1326:TYR:CD1	2.46	0.51
4:B:519:THR:HG22	4:B:589:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:686:ASP:OD2	4:B:691:ARG:HB2	2.10	0.51
1:A:6:U:O4'	4:B:588:ASN:HB3	2.11	0.51
4:B:1347:LEU:N	4:B:1360:ILE:O	2.43	0.51
4:B:106:LEU:O	4:B:111:LYS:NZ	2.44	0.50
4:B:626:PHE:CE2	4:B:635:ARG:HD3	2.47	0.50
4:B:672:ASP:HA	4:B:703:THR:OG1	2.11	0.50
4:B:531:THR:HG21	4:B:575:PHE:CG	2.47	0.50
1:A:29:G:H2'	1:A:30:C:O5'	2.11	0.50
4:B:377:LYS:HB3	4:B:378:PRO:HD3	1.94	0.50
4:B:165:ARG:O	4:B:412:HIS:HA	2.12	0.49
4:B:879:MET:O	4:B:882:TYR:N	2.44	0.49
4:B:161:MET:HE1	4:B:422:ILE:HD12	1.94	0.49
4:B:180:ASP:O	4:B:184:LEU:N	2.37	0.49
4:B:758:ASN:ND2	4:B:995:THR:HG22	2.27	0.49
4:B:66:ARG:NH1	6:B:1501:HOH:O	2.37	0.49
4:B:381:GLU:C	4:B:383:MET:H	2.21	0.49
4:B:1305:GLN:O	4:B:1309:ILE:HG12	2.12	0.49
4:B:825:ASP:CG	4:B:825:ASP:O	2.56	0.49
4:B:393:LEU:HD23	4:B:393:LEU:O	2.13	0.48
4:B:861:ASP:O	4:B:864:ARG:HG2	2.13	0.48
4:B:8:GLY:O	4:B:18:TRP:HA	2.13	0.48
4:B:211:ILE:CD1	4:B:225:LEU:HA	2.35	0.48
4:B:226:ILE:HG21	4:B:234:LYS:HA	1.94	0.48
4:B:450:TYR:CD1	4:B:450:TYR:C	2.92	0.48
4:B:116:HIS:HB3	4:B:125:GLU:CG	2.37	0.48
2:C:2:DA:H4'	2:C:3:DA:OP1	2.14	0.48
4:B:536:LYS:HB3	4:B:537:PRO:HD2	1.96	0.47
4:B:600:ILE:HG22	4:B:650:GLN:HB3	1.95	0.47
2:C:16:DC:H2'	2:C:17:DA:C8	2.48	0.47
4:B:736:GLY:O	4:B:740:THR:HG23	2.14	0.47
4:B:879:MET:O	4:B:882:TYR:HB3	2.14	0.47
4:B:667:ILE:HG22	4:B:668:ASN:HB2	1.96	0.47
1:A:15:A:N3	4:B:450:TYR:HB2	2.30	0.47
4:B:600:ILE:CG2	4:B:650:GLN:HB3	2.45	0.46
4:B:697:ILE:HD12	4:B:708:ILE:CD1	2.45	0.46
4:B:880:LYS:C	4:B:882:TYR:H	2.22	0.46
4:B:963:VAL:HG21	4:B:990:ASN:ND2	2.30	0.46
4:B:822:MET:HE1	4:B:886:LEU:HD12	1.97	0.46
4:B:9:LEU:HA	4:B:17:GLY:O	2.15	0.46
4:B:803:ASN:H	4:B:803:ASN:ND2	2.11	0.46
4:B:183:LYS:C	4:B:185:PHE:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:881:ASN:O	4:B:885:GLN:HG3	2.16	0.46
4:B:251:ASN:C	4:B:253:LYS:N	2.74	0.46
4:B:561:VAL:HG12	4:B:583:VAL:HG13	1.96	0.46
4:B:600:ILE:O	4:B:647:VAL:HG23	2.16	0.46
4:B:1314:THR:O	4:B:1315:LEU:C	2.58	0.46
4:B:155:TYR:CD2	4:B:155:TYR:C	2.95	0.45
4:B:448:ILE:HG12	4:B:455:LEU:HD11	1.98	0.45
4:B:211:ILE:HG12	4:B:212:LEU:H	1.81	0.45
4:B:956:ILE:HA	4:B:1008:PHE:O	2.16	0.45
4:B:539:PHE:HB3	4:B:690:ASN:ND2	2.32	0.45
4:B:1041:ASN:O	4:B:1044:ASN:ND2	2.46	0.45
4:B:485:GLY:HA2	4:B:631:MET:CE	2.45	0.45
4:B:1312:LEU:O	4:B:1315:LEU:HB3	2.16	0.45
4:B:119:PHE:HE2	4:B:128:TYR:HB2	1.80	0.45
4:B:275:LEU:HD11	4:B:290:PHE:CD2	2.51	0.45
4:B:529:TYR:O	4:B:537:PRO:HA	2.17	0.45
4:B:1176:LYS:HE3	4:B:1177:ASN:HB2	1.99	0.45
4:B:1339:THR:O	4:B:1342:VAL:HG22	2.15	0.45
4:B:894:GLN:NE2	4:B:898:ASP:OD1	2.47	0.45
4:B:565:LYS:HG2	4:B:578:VAL:HG13	1.98	0.45
4:B:531:THR:HG21	4:B:575:PHE:CB	2.47	0.45
2:C:2:DA:H2''	2:C:3:DA:O5'	2.18	0.44
4:B:192:TYR:CD1	4:B:192:TYR:C	2.95	0.44
4:B:977:GLU:CG	4:B:1310:ILE:HG23	2.47	0.44
4:B:691:ARG:HA	4:B:695:GLN:OE1	2.17	0.44
4:B:979:ASN:HB2	4:B:1225:GLU:OE2	2.16	0.44
4:B:21:ILE:HA	4:B:26:LYS:O	2.16	0.44
4:B:192:TYR:CE1	4:B:201:ILE:HD11	2.53	0.44
4:B:817:GLN:NE2	4:B:822:MET:HB2	2.33	0.44
4:B:1262:HIS:O	4:B:1265:TYR:HB2	2.18	0.44
4:B:196:PHE:CE1	4:B:237:LEU:HD23	2.52	0.43
4:B:343:LEU:N	4:B:344:PRO:CD	2.81	0.43
4:B:514:LEU:HD21	4:B:668:ASN:HD22	1.83	0.43
2:C:3:DA:C2	2:C:4:DT:C2	3.07	0.43
4:B:1210:ARG:HG3	4:B:1280:VAL:HA	2.00	0.43
4:B:222:LEU:C	4:B:222:LEU:HD23	2.43	0.43
4:B:531:THR:HG21	4:B:575:PHE:CD2	2.53	0.43
1:A:74:A:H2'	1:A:75:A:O4'	2.18	0.43
2:C:8:DG:C6	3:D:4:DA:N6	2.87	0.43
4:B:450:TYR:OH	4:B:627:GLU:HG3	2.17	0.43
4:B:780:ARG:NH1	4:B:806:LEU:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:852:ILE:HD13	4:B:852:ILE:HA	1.88	0.43
4:B:601:ILE:O	4:B:601:ILE:HG13	2.18	0.43
4:B:192:TYR:CD1	4:B:201:ILE:HD12	2.54	0.43
4:B:1060:ARG:HB2	4:B:1061:PRO:CD	2.48	0.43
4:B:137:HIS:HA	4:B:322:ILE:HD11	2.00	0.43
1:A:25:U:H1'	4:B:104:SER:O	2.18	0.42
4:B:491:PHE:O	4:B:495:MET:HE2	2.19	0.42
4:B:844:GLN:OE1	4:B:844:GLN:HA	2.19	0.42
4:B:465:MET:HE1	4:B:473:ILE:HD11	2.01	0.42
4:B:192:TYR:CE1	4:B:201:ILE:CD1	3.02	0.42
4:B:405:PHE:N	6:B:1510:HOH:O	2.51	0.42
4:B:1036:TYR:O	4:B:1040:SER:OG	2.33	0.42
4:B:557:ARG:O	4:B:590:SER:HB2	2.20	0.42
4:B:1036:TYR:CD1	4:B:1036:TYR:C	2.97	0.42
4:B:361:GLY:C	4:B:367:ALA:HB3	2.45	0.42
4:B:939:MET:HA	4:B:939:MET:HE3	2.02	0.42
4:B:708:ILE:O	4:B:712:GLN:HG2	2.20	0.42
4:B:30:LYS:HE3	4:B:751:MET:HE1	2.01	0.42
4:B:736:GLY:O	4:B:740:THR:CG2	2.67	0.42
1:A:63:U:H4'	1:A:64:U:OP2	2.20	0.42
1:A:29:G:C2'	1:A:30:C:O5'	2.67	0.41
4:B:817:GLN:HE22	4:B:822:MET:HB2	1.85	0.41
4:B:1075:ASP:O	4:B:1077:GLY:N	2.53	0.41
4:B:849:ASP:OD1	4:B:851:SER:CB	2.68	0.41
4:B:1127:ASP:HA	4:B:1128:PRO:HD3	1.89	0.41
4:B:1176:LYS:CE	4:B:1177:ASN:HB2	2.51	0.41
4:B:203:ALA:O	4:B:206:VAL:HB	2.20	0.41
4:B:598:LEU:O	4:B:601:ILE:O	2.39	0.41
4:B:78:ARG:NH1	4:B:162:ILE:O	2.47	0.41
4:B:243:ALA:O	4:B:246:LEU:HB2	2.21	0.41
4:B:477:ASN:C	4:B:477:ASN:OD1	2.64	0.41
4:B:478:PHE:CE1	4:B:482:VAL:HG21	2.55	0.41
4:B:724:ILE:CD1	4:B:738:LEU:HA	2.49	0.41
4:B:1000:LYS:HG3	4:B:1001:TYR:CE1	2.55	0.41
1:A:40:C:H2'	1:A:41:A:O4'	2.21	0.41
4:B:189:VAL:O	4:B:193:ASN:HB2	2.21	0.41
4:B:643:PHE:HB3	4:B:647:VAL:CG1	2.51	0.41
4:B:343:LEU:HB2	4:B:383:MET:HE1	2.03	0.41
4:B:515:TYR:O	4:B:518:PHE:HB3	2.21	0.41
4:B:724:ILE:HD13	4:B:738:LEU:HA	2.02	0.41
4:B:876:VAL:HA	4:B:883:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:927:ILE:HG23	4:B:928:THR:N	2.35	0.41
4:B:464:TRP:CZ2	4:B:491:PHE:HD1	2.39	0.41
4:B:531:THR:HG21	4:B:575:PHE:HB3	2.03	0.41
4:B:621:LEU:O	4:B:625:LEU:HB2	2.21	0.41
4:B:694:ILE:HG12	4:B:694:ILE:O	2.21	0.41
4:B:380:LEU:HD21	4:B:389:LEU:HB3	2.03	0.40
4:B:724:ILE:HD12	4:B:738:LEU:HD13	2.02	0.40
4:B:1004:LEU:CD1	4:B:1042:ILE:HD11	2.51	0.40
2:C:6:DC:H2''	2:C:7:DC:O5'	2.21	0.40
4:B:191:THR:O	4:B:194:GLN:CG	2.69	0.40
4:B:251:ASN:C	4:B:253:LYS:H	2.27	0.40
4:B:279:LEU:O	4:B:283:GLY:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	B	1311/1368 (96%)	1193 (91%)	104 (8%)	14 (1%)	11 29

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	252	PHE
4	B	471	GLU
4	B	652	LYS
4	B	1076	LYS
4	B	298	ASP
4	B	382	LYS
4	B	532	GLU
4	B	1062	LEU
4	B	1327	PHE

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Mol	Chain	Res	Type
4	B	216	LEU
4	B	343	LEU
4	B	247	GLY
4	B	669	GLY
4	B	211	ILE

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	1114/1226 (91%)	1013 (91%)	101 (9%)	9 22

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	55	SER
4	B	73	THR
4	B	76	LYS
4	B	174	LEU
4	B	186	ILE
4	B	188	LEU
4	B	194	GLN
4	B	195	LEU
4	B	206	VAL
4	B	211	ILE
4	B	216	LEU
4	B	245	SER
4	B	255	ASN
4	B	258	LEU
4	B	262	THR
4	B	276	ASP
4	B	303	SER
4	B	304	ASP
4	B	305	ILE
4	B	321	MET
4	B	343	LEU

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Mol	Chain	Res	Type
4	B	356	LYS
4	B	390	LEU
4	B	398	LEU
4	B	445	THR
4	B	490	SER
4	B	504	ASN
4	B	506	LYS
4	B	512	SER
4	B	519	THR
4	B	520	VAL
4	B	534	MET
4	B	559	VAL
4	B	598	LEU
4	B	600	ILE
4	B	603	ASP
4	B	604	LYS
4	B	625	LEU
4	B	634	GLU
4	B	641	HIS
4	B	657	THR
4	B	670	ILE
4	B	694	ILE
4	B	697	ILE
4	B	701	SER
4	B	709	GLN
4	B	740	THR
4	B	743	VAL
4	B	749	LYS
4	B	758	ASN
4	B	761	ILE
4	B	762	GLU
4	B	778	ARG
4	B	783	ARG
4	B	791	LEU
4	B	801	VAL
4	B	803	ASN
4	B	811	LEU
4	B	852	ILE
4	B	853	ASP
4	B	856	VAL
4	B	864	ARG
4	B	870	VAL

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Mol	Chain	Res	Type
4	B	928	THR
4	B	929	LYS
4	B	948	LYS
4	B	959	LYS
4	B	962	LEU
4	B	964	SER
4	B	977	GLU
4	B	992	VAL
4	B	1040	SER
4	B	1041	ASN
4	B	1048	THR
4	B	1059	LYS
4	B	1062	LEU
4	B	1073	VAL
4	B	1078	ARG
4	B	1082	THR
4	B	1084	ARG
4	B	1085	LYS
4	B	1124	LYS
4	B	1143	VAL
4	B	1146	VAL
4	B	1151	LYS
4	B	1153	LYS
4	B	1176	LYS
4	B	1180	ASP
4	B	1189	GLU
4	B	1192	LYS
4	B	1230	SER
4	B	1241	HIS
4	B	1257	LEU
4	B	1280	VAL
4	B	1296	LYS
4	B	1314	THR
4	B	1325	LYS
4	B	1332	ASP
4	B	1333	ARG
4	B	1338	SER
4	B	1364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	14	ASN
4	B	83	GLN
4	B	194	GLN
4	B	265	GLN
4	B	354	GLN
4	B	402	GLN
4	B	436	ASN
4	B	501	ASN
4	B	544	GLN
4	B	758	ASN
4	B	803	ASN
4	B	805	GLN
4	B	807	GLN
4	B	990	ASN
4	B	1115	ASN
4	B	1252	ASN
4	B	1272	GLN
4	B	1286	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/83 (96%)	14 (17%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	28	A
1	A	29	G
1	A	30	C
1	A	32	A
1	A	35	A
1	A	36	A
1	A	51	A
1	A	52	A
1	A	59	U
1	A	63	U
1	A	68	A
1	A	77	A
1	A	81	G

There are no RNA pucker outliers to report.

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](#)

9 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	A	102	-	4,4,4	0.51	0	6,6,6	0.55	0
5	PO4	B	1405	-	4,4,4	0.61	0	6,6,6	0.52	0
5	PO4	A	101	-	4,4,4	0.67	0	6,6,6	0.55	0
5	PO4	B	1406	-	4,4,4	0.51	0	6,6,6	0.57	0
5	PO4	B	1402	-	4,4,4	0.55	0	6,6,6	0.70	0
5	PO4	B	1403	-	4,4,4	0.84	0	6,6,6	0.50	0
5	PO4	B	1404	-	4,4,4	0.84	0	6,6,6	0.45	0
5	PO4	B	1407	-	4,4,4	0.69	0	6,6,6	0.42	0
5	PO4	B	1401	-	4,4,4	0.69	0	6,6,6	0.51	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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1403	PO4	1	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

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	81/83 (97%)	-0.57	0	100 100	22, 39, 93, 105	0
2	C	28/28 (100%)	-0.40	0	100 100	27, 45, 70, 75	0
3	D	11/12 (91%)	0.25	1 (9%)	15 12	35, 52, 113, 140	0
4	B	1323/1368 (96%)	0.35	104 (7%)	18 16	20, 49, 94, 115	0
All	All	1443/1491 (96%)	0.28	105 (7%)	21 18	20, 48, 95, 140	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	385	GLY	6.4
4	B	291	LEU	5.4
4	B	287	ALA	5.2
4	B	286	TYR	4.9
4	B	215	ARG	4.8
4	B	774	GLN	4.8
4	B	196	PHE	4.7
4	B	384	ASP	4.4
4	B	295	ASN	4.4
4	B	776	ASN	4.3
4	B	198	GLU	4.2
4	B	181	VAL	4.2
4	B	206	VAL	4.2
4	B	203	ALA	4.2
4	B	1249	PRO	4.0
4	B	296	LEU	4.0
4	B	292	ALA	3.9
4	B	289	LEU	3.9
3	D	2	DA	3.7
4	B	190	GLN	3.6
4	B	176	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
4	B	251	ASN	3.6
4	B	266	LEU	3.6
4	B	212	LEU	3.5
4	B	271	TYR	3.4
4	B	247	GLY	3.4
4	B	1037	PHE	3.4
4	B	249	THR	3.3
4	B	851	SER	3.3
4	B	300	ILE	3.2
4	B	285	GLN	3.2
4	B	388	GLU	3.1
4	B	299	ALA	3.0
4	B	185	PHE	3.0
4	B	284	ASP	3.0
4	B	252	PHE	3.0
4	B	208	ALA	2.9
4	B	177	ASP	2.9
4	B	238	PHE	2.9
4	B	184	LEU	2.9
4	B	305	ILE	2.9
4	B	246	LEU	2.9
4	B	216	LEU	2.8
4	B	297	SER	2.8
4	B	387	GLU	2.8
4	B	307	ARG	2.8
4	B	1251	ASP	2.8
4	B	199	ASN	2.8
4	B	1059	LYS	2.7
4	B	273	ASP	2.7
4	B	391	VAL	2.7
4	B	205	GLY	2.7
4	B	182	ASP	2.6
4	B	195	LEU	2.6
4	B	1367	GLY	2.6
4	B	191	THR	2.6
4	B	270	THR	2.6
4	B	1250	GLU	2.6
4	B	186	ILE	2.5
4	B	248	LEU	2.5
4	B	264	LEU	2.5
4	B	293	ALA	2.5
4	B	245	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	B	261	ASP	2.5
4	B	275	LEU	2.5
4	B	1253	GLU	2.5
4	B	294	LYS	2.5
4	B	394	ASN	2.5
4	B	189	VAL	2.5
4	B	459	ASN	2.4
4	B	188	LEU	2.4
4	B	218	LYS	2.4
4	B	298	ASP	2.4
4	B	1043	MET	2.4
4	B	244	LEU	2.4
4	B	268	LYS	2.4
4	B	570	LYS	2.4
4	B	250	PRO	2.4
4	B	192	TYR	2.3
4	B	1062	LEU	2.3
4	B	389	LEU	2.3
4	B	602	LYS	2.3
4	B	235	ASN	2.3
4	B	386	THR	2.3
4	B	214	ALA	2.2
4	B	600	ILE	2.2
4	B	290	PHE	2.2
4	B	260	GLU	2.2
4	B	187	GLN	2.2
4	B	233	LYS	2.2
4	B	350	ILE	2.2
4	B	311	GLU	2.2
4	B	178	ASN	2.2
4	B	302	LEU	2.2
4	B	204	SER	2.2
4	B	911	LEU	2.1
4	B	1030	GLY	2.1
4	B	269	ASP	2.1
4	B	351	PHE	2.1
4	B	231	GLY	2.1
4	B	714	SER	2.1
4	B	175	ASN	2.1
4	B	197	GLU	2.0
4	B	804	THR	2.0
4	B	380	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	PO4	B	1401	5/5	0.70	0.10	108,116,120,121	0
5	PO4	B	1406	5/5	0.73	0.14	87,89,94,95	0
5	PO4	B	1405	5/5	0.80	0.15	93,98,101,102	0
5	PO4	B	1404	5/5	0.82	0.14	51,54,67,70	0
5	PO4	B	1407	5/5	0.86	0.10	62,64,75,78	0
5	PO4	A	101	5/5	0.88	0.25	70,70,75,83	0
5	PO4	B	1403	5/5	0.90	0.10	60,70,74,75	0
5	PO4	A	102	5/5	0.93	0.17	70,75,81,82	0
5	PO4	B	1402	5/5	0.94	0.11	36,37,41,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.