



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:14 PM BST

PDB ID : 3R1C
Title : Crystal structure of GCGGCGGC duplex
Authors : Kiliszek, A.; Kierzek, R.; Krzyzosiak, W.J.; Rypniewski, W.
Deposited on : 2011-03-10
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

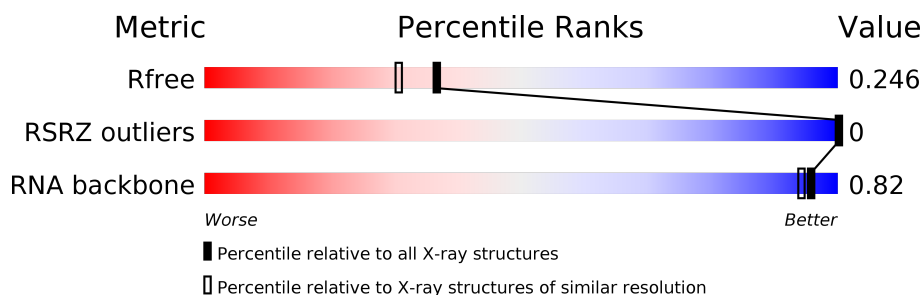
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

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


















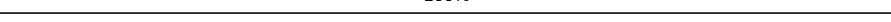
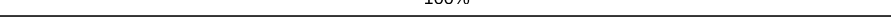
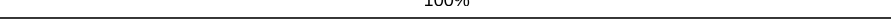
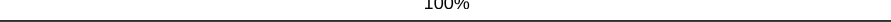
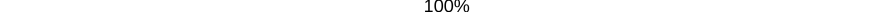
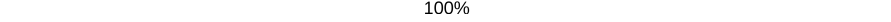
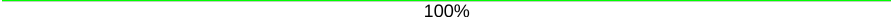
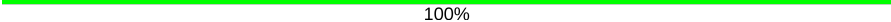

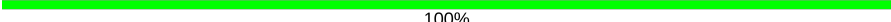
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)
RNA backbone	3102	1015 (2.52-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	8	
1	B	8	
1	C	8	
1	D	8	
1	E	8	
1	F	8	
1	G	8	
1	H	8	




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Mol	Chain	Length	Quality of chain
1	I	8	 100%
1	J	8	 100%
1	K	8	 88% 13%
1	L	8	 100%
1	M	8	 100%
1	N	8	 100%
1	O	8	 100%
1	P	8	 100%
1	Q	8	 88% 13%
1	R	8	 100%
1	S	8	 100%
1	T	8	 100%
1	U	8	 100%
1	V	8	 100%
1	W	8	 100%
1	X	8	 100%
1	Y	8	 100%
1	Z	8	 100%
1	a	8	 100%
1	b	8	 100%
1	c	8	 100%
1	d	8	 100%
1	e	8	 100%
1	f	8	 100%
1	g	8	 100%

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Mol	Chain	Length	Quality of chain
1	h	8	 88%13%
1	i	8	 100%
1	j	8	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6865 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 RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	B	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	C	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	D	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	E	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	F	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	G	8	Total	C	N	O	P	0	1	0
			195	87	39	61	8			
1	H	8	Total	C	N	O	P	0	1	0
			195	87	39	61	8			
1	I	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	J	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	K	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	L	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	M	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	N	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	O	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			
1	P	8	Total	C	N	O	P	0	0	0
			172	77	34	54	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	R	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	S	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	Y	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	T	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	U	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	W	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	X	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	V	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	Z	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	a	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	b	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	c	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	d	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	e	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	f	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	g	8	Total 215	C 96	N 42	O 68	P 9	0	2	0
1	h	8	Total 195	C 87	N 39	O 61	P 8	0	1	0
1	i	8	Total 172	C 77	N 34	O 54	P 7	0	0	0
1	j	8	Total 172	C 77	N 34	O 54	P 7	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	S	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	1
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	b	1	Total	O	S	0	1
			5	4	1		
2	c	1	Total	O	S	0	1
			5	4	1		
2	d	1	Total	O	S	0	0
			5	4	1		
2	e	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	19	Total	O	0	0
			19	19		
3	C	19	Total	O	0	0
			19	19		
3	D	13	Total	O	0	0
			13	13		
3	E	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	13	Total O 13 13	0	0
3	G	18	Total O 18 18	0	0
3	H	10	Total O 10 10	0	1
3	I	29	Total O 29 29	0	0
3	J	28	Total O 28 28	0	0
3	K	29	Total O 29 29	0	0
3	L	26	Total O 26 26	0	0
3	M	17	Total O 17 17	0	0
3	N	6	Total O 6 6	0	0
3	O	12	Total O 12 12	0	0
3	P	12	Total O 12 12	0	0
3	Q	23	Total O 23 23	0	0
3	R	15	Total O 15 15	0	0
3	S	2	Total O 2 2	0	0
3	Y	3	Total O 3 3	0	0
3	T	10	Total O 10 10	0	0
3	U	19	Total O 19 19	0	0
3	W	11	Total O 11 11	0	0
3	X	18	Total O 19 19	0	1
3	V	4	Total O 4 4	0	0
3	Z	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	a	3	Total 3	O 3	0	0
3	b	4	Total 4	O 4	0	0
3	c	13	Total 13	O 13	0	0
3	d	14	Total 14	O 14	0	0
3	e	22	Total 22	O 22	0	0
3	f	17	Total 17	O 17	0	0
3	g	9	Total 9	O 9	0	0
3	h	10	Total 10	O 10	0	0
3	i	17	Total 18	O 18	0	1
3	j	10	Total 10	O 10	0	0

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: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain B:  100%


There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain D:  88% 13%



- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain I:  100%


There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain K:  88% 13%



- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain O:  100%


There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain Q:  88% 13%



- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain f:  100%


There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain h:  88% 13%



- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(*GP*CP*GP*GP*CP*GP*GP*C)-3')

Chain j:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.70 Å 76.89 Å 85.40 Å 89.98° 88.61° 77.29°	Depositor
Resolution (Å)	19.36 – 2.05 19.83 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.36-2.05) 98.1 (19.83-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.06 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.216 , 0.257 0.204 , 0.246	Depositor DCC
R_{free} test set	3052 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,h-k,-l 0.000 for -h,-k,l 0.000 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6865	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7299e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4

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	0.60	0/192	1.14	0/299
1	B	0.61	0/192	1.17	0/299
1	C	0.51	0/192	1.07	0/299
1	D	0.60	0/192	1.14	1/299 (0.3%)
1	E	0.61	0/192	1.13	0/299
1	F	0.62	0/192	1.25	0/299
1	G	0.58	0/218	1.18	0/340
1	H	0.46	0/218	1.04	0/340
1	I	0.66	0/192	1.18	0/299
1	J	0.64	0/192	1.08	0/299
1	K	0.70	0/192	1.26	1/299 (0.3%)
1	L	0.63	0/192	1.06	0/299
1	M	0.57	0/192	1.22	0/299
1	N	0.55	0/192	1.13	0/299
1	O	0.57	0/192	1.07	0/299
1	P	0.60	0/192	1.19	0/299
1	Q	0.61	0/192	1.18	1/299 (0.3%)
1	R	0.62	0/192	1.06	0/299
1	S	0.49	0/192	0.96	0/299
1	T	0.51	0/192	1.12	0/299
1	U	0.57	0/192	1.20	0/299
1	V	0.49	0/192	1.04	0/299
1	W	0.55	0/192	1.15	0/299
1	X	0.57	0/192	1.12	0/299
1	Y	0.49	0/192	1.05	0/299
1	Z	0.49	0/192	1.07	0/299
1	a	0.45	0/192	1.09	0/299
1	b	0.47	0/192	0.95	0/299
1	c	0.50	0/192	1.12	0/299
1	d	0.60	0/192	1.14	0/299
1	e	0.59	0/192	1.17	0/299
1	f	0.56	0/192	1.07	0/299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.56	0/240	1.04	0/374
1	h	0.60	0/218	1.12	1/340 (0.3%)
1	i	0.64	0/192	1.08	0/299
1	j	0.56	0/192	1.02	0/299
All	All	0.57	0/7038	1.11	4/10962 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	3	G	O4'-C1'-N9	6.59	113.47	108.20
1	Q	6	G	O4'-C1'-N9	5.62	112.70	108.20
1	D	6	G	O4'-C1'-N9	5.32	112.45	108.20
1	h	6	G	O4'-C1'-N9	5.04	112.23	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	7/8 (87%)	0	0
1	B	7/8 (87%)	0	0
1	C	7/8 (87%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	7/8 (87%)	0	0
1	E	7/8 (87%)	0	0
1	F	7/8 (87%)	0	0
1	G	6/8 (75%)	0	0
1	H	6/8 (75%)	0	0
1	I	7/8 (87%)	0	0
1	J	7/8 (87%)	0	0
1	K	7/8 (87%)	0	0
1	L	7/8 (87%)	0	0
1	M	7/8 (87%)	0	0
1	N	7/8 (87%)	0	0
1	O	7/8 (87%)	0	0
1	P	7/8 (87%)	0	0
1	Q	7/8 (87%)	0	0
1	R	7/8 (87%)	0	0
1	S	7/8 (87%)	0	0
1	T	7/8 (87%)	0	0
1	U	7/8 (87%)	0	0
1	V	7/8 (87%)	0	0
1	W	7/8 (87%)	0	0
1	X	7/8 (87%)	0	0
1	Y	7/8 (87%)	0	0
1	Z	7/8 (87%)	0	0
1	a	7/8 (87%)	0	0
1	b	7/8 (87%)	0	0
1	c	7/8 (87%)	0	0
1	d	7/8 (87%)	0	0
1	e	7/8 (87%)	0	0
1	f	7/8 (87%)	0	0
1	g	5/8 (62%)	0	0
1	h	6/8 (75%)	0	0
1	i	7/8 (87%)	0	0
1	j	7/8 (87%)	0	0
All	All	247/288 (85%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
2	SO4	d	9	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	e	9	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	b	9[A]	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	X	9	-	4,4,4	0.12	0	6,6,6	0.07	0
2	SO4	W	9[A]	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	S	9	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	c	9[A]	-	4,4,4	0.14	0	6,6,6	0.13	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.

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	8/8 (100%)	-0.61	0 100 100	17, 19, 22, 24	0
1	B	8/8 (100%)	-0.71	0 100 100	17, 21, 23, 27	0
1	C	8/8 (100%)	-0.38	0 100 100	20, 22, 41, 43	0
1	D	8/8 (100%)	-0.40	0 100 100	26, 27, 27, 30	0
1	E	8/8 (100%)	-0.67	0 100 100	17, 19, 24, 25	0
1	F	8/8 (100%)	-0.61	0 100 100	17, 21, 25, 27	0
1	G	8/8 (100%)	-0.38	0 100 100	23, 26, 27, 29	0
1	H	8/8 (100%)	-0.44	0 100 100	26, 27, 33, 34	0
1	I	8/8 (100%)	-0.77	0 100 100	13, 14, 19, 19	0
1	J	8/8 (100%)	-0.80	0 100 100	13, 15, 18, 18	0
1	K	8/8 (100%)	-0.83	0 100 100	13, 14, 17, 19	0
1	L	8/8 (100%)	-0.79	0 100 100	13, 15, 17, 17	0
1	M	8/8 (100%)	-0.77	0 100 100	17, 18, 32, 34	0
1	N	8/8 (100%)	-0.70	0 100 100	18, 31, 35, 41	0
1	O	8/8 (100%)	-0.65	0 100 100	22, 25, 30, 35	0
1	P	8/8 (100%)	-0.59	0 100 100	21, 24, 38, 40	0
1	Q	8/8 (100%)	-0.84	0 100 100	17, 18, 25, 26	0
1	R	8/8 (100%)	-0.84	0 100 100	18, 24, 26, 31	0
1	S	8/8 (100%)	-0.20	0 100 100	29, 43, 51, 52	0
1	T	8/8 (100%)	-0.73	0 100 100	19, 26, 32, 33	0
1	U	8/8 (100%)	-0.77	0 100 100	20, 22, 27, 30	0
1	V	8/8 (100%)	-0.23	0 100 100	32, 36, 38, 40	0
1	W	8/8 (100%)	-0.76	0 100 100	22, 25, 25, 27	0
1	X	8/8 (100%)	-0.89	0 100 100	22, 25, 30, 30	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9		
1	Y	8/8 (100%)	0.01	0	100	100	27, 46, 53, 53	0
1	Z	8/8 (100%)	-0.63	0	100	100	29, 30, 32, 35	0
1	a	8/8 (100%)	-0.16	0	100	100	25, 44, 47, 49	0
1	b	8/8 (100%)	-0.48	0	100	100	26, 37, 44, 45	0
1	c	8/8 (100%)	-0.75	0	100	100	21, 23, 26, 27	0
1	d	8/8 (100%)	-0.82	0	100	100	20, 22, 28, 29	0
1	e	8/8 (100%)	-0.70	0	100	100	24, 27, 28, 28	0
1	f	8/8 (100%)	-0.80	0	100	100	24, 26, 32, 32	0
1	g	8/8 (100%)	-0.48	0	100	100	22, 24, 30, 36	0
1	h	8/8 (100%)	-0.50	0	100	100	21, 25, 37, 40	0
1	i	8/8 (100%)	-0.58	0	100	100	22, 23, 27, 32	0
1	j	8/8 (100%)	-0.60	0	100	100	23, 28, 30, 34	0
All	All	288/288 (100%)	-0.61	0	100	100	13, 25, 44, 53	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	W	9[A]	5/5	0.75	0.29	37,40,60,61	5
2	SO4	X	9	5/5	0.81	0.27	33,38,45,47	5
2	SO4	e	9	5/5	0.83	0.26	31,46,57,62	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	d	9	5/5	0.85	0.33	42,46,59,65	5
2	SO4	S	9	5/5	0.87	0.31	39,41,46,48	5
2	SO4	c	9[A]	5/5	0.87	0.26	32,38,46,52	5
2	SO4	b	9[A]	5/5	0.90	0.50	39,42,48,51	5

6.5 Other polymers [i](#)

There are no such residues in this entry.