



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:20 AM GMT

PDB ID : 3TAB
Title : 5-hydroxycytosine paired with dGMP in RB69 gp43
Authors : Zahn, K.E.
Deposited on : 2011-08-03
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

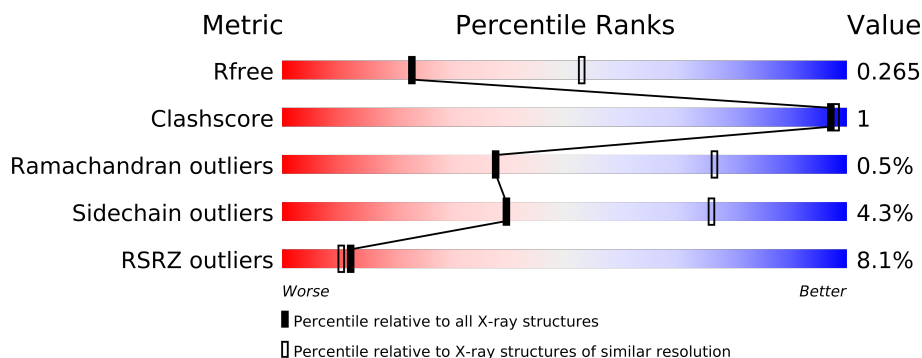
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	906	
1	B	906	
1	C	906	
1	D	906	
2	E	18	
2	G	18	
2	I	18	
2	K	18	
3	F	15	
3	H	15	
3	J	15	
3	L	15	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32383 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	904	Total	C	N	O	S	0	0	0
			7384	4743	1229	1379	33			
1	B	904	Total	C	N	O	S	0	0	0
			7384	4743	1229	1379	33			
1	C	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			
1	D	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	904	HIS	-	EXPRESSION TAG	UNP Q38087
A	905	HIS	-	EXPRESSION TAG	UNP Q38087
A	906	HIS	-	EXPRESSION TAG	UNP Q38087
B	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	904	HIS	-	EXPRESSION TAG	UNP Q38087
B	905	HIS	-	EXPRESSION TAG	UNP Q38087
B	906	HIS	-	EXPRESSION TAG	UNP Q38087
C	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	904	HIS	-	EXPRESSION TAG	UNP Q38087
C	905	HIS	-	EXPRESSION TAG	UNP Q38087
C	906	HIS	-	EXPRESSION TAG	UNP Q38087
D	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	904	HIS	-	EXPRESSION TAG	UNP Q38087
D	905	HIS	-	EXPRESSION TAG	UNP Q38087
D	906	HIS	-	EXPRESSION TAG	UNP Q38087

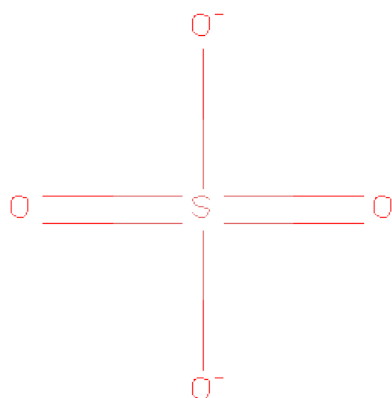
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			
2	G	18	Total	C	N	O	P	0	0	0
			370	173	70	109	18			
2	I	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			
2	K	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			
3	H	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			
3	J	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			
3	L	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

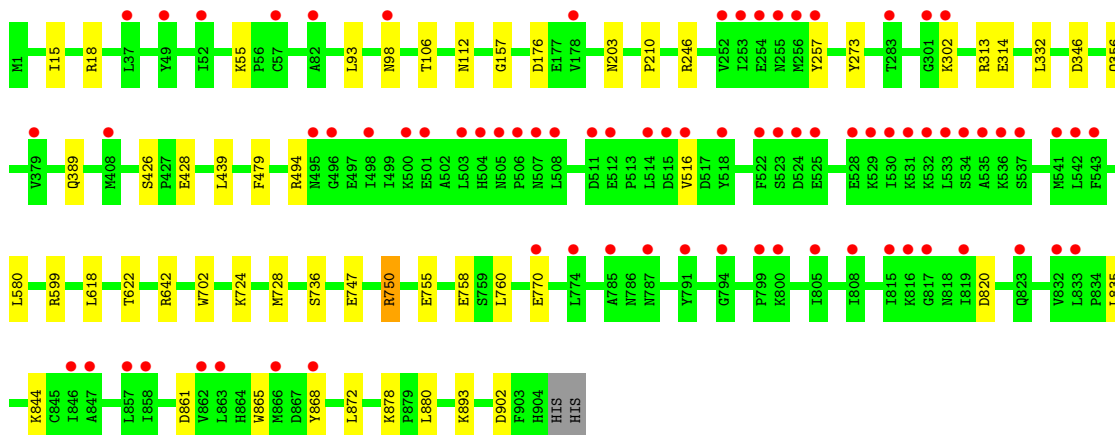
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	E	1	Total O 1 1	0	0
5	B	71	Total O 71 71	0	0
5	G	6	Total O 6 6	0	0
5	H	6	Total O 6 6	0	0
5	C	39	Total O 39 39	0	0
5	I	4	Total O 4 4	0	0
5	D	10	Total O 10 10	0	0
5	K	1	Total O 1 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

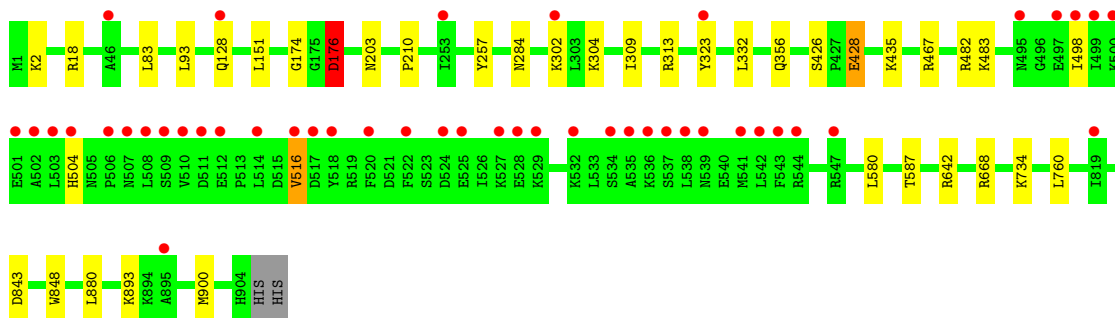
- Molecule 1: DNA polymerase

Chain A: 



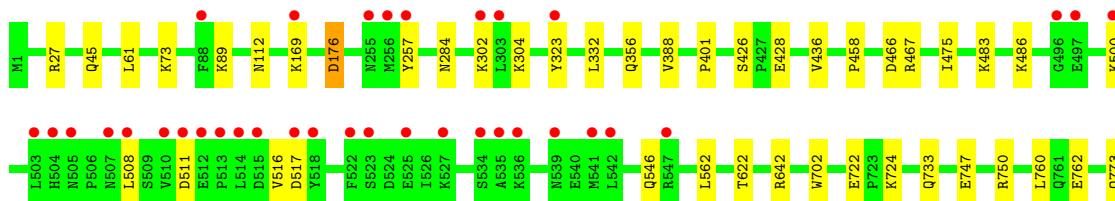
- Molecule 1: DNA polymerase

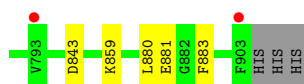
Chain B: 



- Molecule 1: DNA polymerase

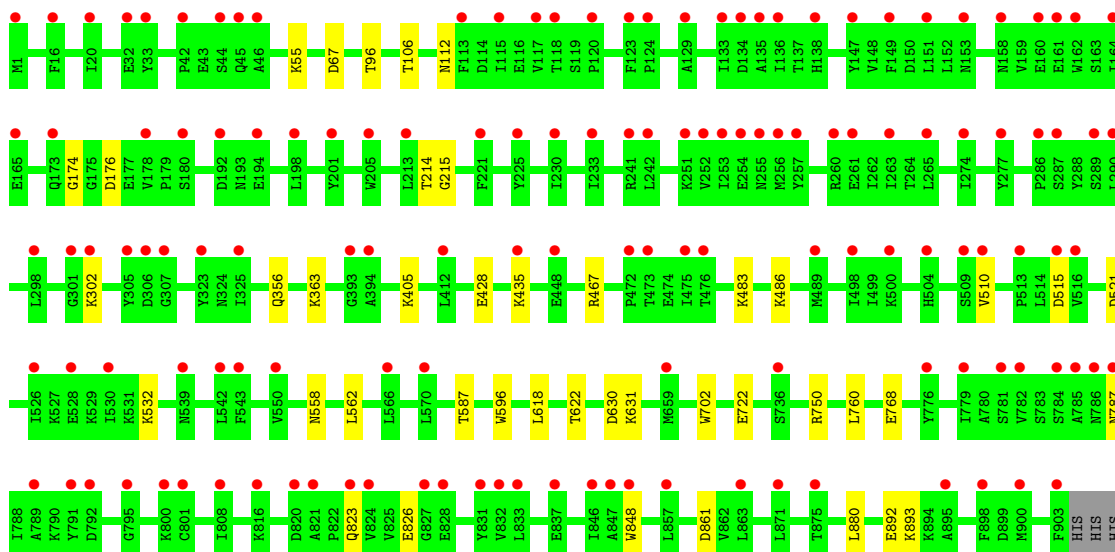
Chain C: 





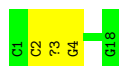
- Molecule 1: DNA polymerase

Chain D:



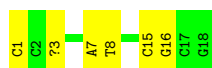
- Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain E:



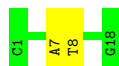
- Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:



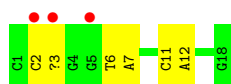
- Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:



- Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:



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

Chain F:



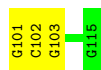
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain H:



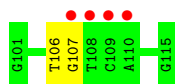
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain J:



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

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.76Å 121.93Å 168.91Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 49.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.80) 100.0 (49.48-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.232 , 0.281 0.221 , 0.265	Depositor DCC
R_{free} test set	12706 reflections (10.67%)	DCC
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 131746 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32383	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5OC, 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	0.41	2/7566 (0.0%)	0.48	0/10224
1	B	0.41	1/7566 (0.0%)	0.50	0/10224
1	C	0.41	1/7555 (0.0%)	0.49	0/10209
1	D	0.41	3/7555 (0.0%)	0.46	0/10209
2	E	0.22	0/387	0.75	0/593
2	G	0.54	1/391 (0.3%)	0.77	0/597
2	I	0.23	0/387	0.78	0/593
2	K	0.21	0/387	0.78	0/593
3	F	0.21	0/340	0.77	0/523
3	H	0.24	0/340	0.83	1/523 (0.2%)
3	J	0.28	0/340	0.82	1/523 (0.2%)
3	L	0.20	0/340	0.83	0/523
All	All	0.40	8/33154 (0.0%)	0.52	2/45334 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	DC	OP3-P	-9.49	1.49	1.61
1	C	702	TRP	CD2-CE2	5.15	1.47	1.41
1	B	848	TRP	CD2-CE2	5.07	1.47	1.41
1	A	702	TRP	CD2-CE2	5.07	1.47	1.41
1	D	596	TRP	CD2-CE2	5.04	1.47	1.41
1	D	702	TRP	CD2-CE2	5.03	1.47	1.41
1	A	865	TRP	CD2-CE2	5.01	1.47	1.41
1	D	848	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	101	DG	P-O3'-C3'	5.70	126.54	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	101	DG	P-O3'-C3'	5.23	125.97	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7384	0	6	7	0
1	B	7384	0	6	6	0
1	C	7374	0	0	2	0
1	D	7374	0	0	1	0
2	E	366	0	201	3	0
2	G	370	0	200	4	0
2	I	366	0	201	1	0
2	K	366	0	201	3	0
3	F	304	0	170	2	0
3	H	304	0	170	2	0
3	J	304	0	170	1	0
3	L	304	0	170	1	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
4	K	5	0	0	0	0
5	A	25	0	0	2	0
5	B	71	0	0	1	0
5	C	39	0	0	0	0
5	D	10	0	0	0	0
5	E	1	0	0	0	0
5	G	6	0	0	0	0
5	H	6	0	0	0	0
5	I	4	0	0	0	0
5	K	1	0	0	0	0
All	All	32383	0	1495	30	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:734:LYS:NZ	5:B:976:HOH:O	2.29	0.65
2:G:15:DC:H2'	2:G:16:DG:C8	2.44	0.53
3:J:102:DC:H2''	3:J:103:DG:C8	2.45	0.51
1:D:214:THR:OG1	1:D:215:GLY:N	2.45	0.50
2:I:7:DA:H2'	2:I:8:DT:H71	1.93	0.50
1:A:868:TYR:O	1:A:872:LEU:N	2.46	0.48
1:A:157:GLY:O	1:A:313:ARG:NH2	2.46	0.48
3:H:101:DG:H2''	3:H:102:DC:OP2	2.13	0.47
1:B:18:ARG:NH2	1:B:210:PRO:O	2.47	0.47
2:K:11:DC:H2''	2:K:12:DA:C8	2.51	0.45
3:L:106:DT:H2''	3:L:107:DG:C8	2.51	0.45
2:G:7:DA:H2''	2:G:8:DT:H5'	1.99	0.45
2:E:3:5OC:O2	3:F:115:DG:N2	2.41	0.45
1:C:304:LYS:O	1:C:323:TYR:OH	2.34	0.45
1:B:304:LYS:O	1:B:323:TYR:OH	2.34	0.44
1:C:747:GLU:OE2	1:C:750:ARG:NH1	2.51	0.44
1:B:426:SER:OG	1:B:428:GLU:OE2	2.36	0.44
2:K:2:DC:H2'	2:K:3:5OC:H6	2.00	0.43
1:A:736:SER:OG	3:F:112:DA:H5''	2.19	0.43
2:E:2:DC:H2'	2:E:3:5OC:H6	2.01	0.42
1:B:151:LEU:O	1:B:313:ARG:NH1	2.52	0.42
1:B:176:ASP:OD1	1:B:176:ASP:N	2.52	0.42
1:A:747:GLU:OE2	1:A:750:ARG:NH1	2.53	0.42
2:K:6:DT:H2''	2:K:7:DA:H8	1.84	0.41
2:G:7:DA:H2'	2:G:8:DT:C6	2.55	0.41
1:A:18:ARG:NH2	1:A:210:PRO:O	2.54	0.41
1:A:246:ARG:NE	5:A:917:HOH:O	2.54	0.41
2:E:3:5OC:H2'	2:E:4:DG:C8	2.56	0.41
2:G:3:5OC:O2	3:H:115:DG:N2	2.45	0.40
1:A:112:ASN:ND2	5:A:919:HOH:O	2.55	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	
1	A	902/906 (100%)	858 (95%)	41 (4%)	3 (0%)	50	84
1	B	902/906 (100%)	859 (95%)	39 (4%)	4 (0%)	43	80
1	C	901/906 (99%)	864 (96%)	32 (4%)	5 (1%)	33	72
1	D	901/906 (99%)	855 (95%)	41 (5%)	5 (1%)	33	72
All	All	3606/3624 (100%)	3436 (95%)	153 (4%)	17 (0%)	38	76

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	893	LYS
1	B	176	ASP
1	C	622	THR
1	D	622	THR
1	B	893	LYS
1	C	176	ASP
1	D	892	GLU
1	A	176	ASP
1	C	466	ASP
1	A	622	THR
1	A	893	LYS
1	B	174	GLY
1	C	401	PRO
1	D	176	ASP
1	B	516	VAL
1	D	174	GLY
1	C	458	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	801/803 (100%)	763 (95%)	38 (5%)	36	73
1	B	801/803 (100%)	773 (96%)	28 (4%)	48	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	800/803 (100%)	760 (95%)	40 (5%)	34	70
1	D	800/803 (100%)	767 (96%)	33 (4%)	41	77
All	All	3202/3212 (100%)	3063 (96%)	139 (4%)	40	76

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	55	LYS
1	A	93	LEU
1	A	98	ASN
1	A	106	THR
1	A	203	ASN
1	A	257	TYR
1	A	273	TYR
1	A	302	LYS
1	A	314	GLU
1	A	332	LEU
1	A	346	ASP
1	A	356	GLN
1	A	389	GLN
1	A	426	SER
1	A	428	GLU
1	A	439	LEU
1	A	479	PHE
1	A	494	ARG
1	A	516	VAL
1	A	580	LEU
1	A	599	ARG
1	A	618	LEU
1	A	642	ARG
1	A	724	LYS
1	A	728	MET
1	A	750	ARG
1	A	755	GLU
1	A	758	GLU
1	A	760	LEU
1	A	770	GLU
1	A	820	ASP
1	A	835	LEU
1	A	844	LYS

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Mol	Chain	Res	Type
1	A	861	ASP
1	A	878	LYS
1	A	880	LEU
1	A	902	ASP
1	B	2	LYS
1	B	83	LEU
1	B	93	LEU
1	B	128	GLN
1	B	176	ASP
1	B	203	ASN
1	B	257	TYR
1	B	284	ASN
1	B	302	LYS
1	B	309	ILE
1	B	332	LEU
1	B	356	GLN
1	B	428	GLU
1	B	435	LYS
1	B	467	ARG
1	B	482	ARG
1	B	483	LYS
1	B	498	ILE
1	B	504	HIS
1	B	516	VAL
1	B	580	LEU
1	B	587	THR
1	B	642	ARG
1	B	668	ARG
1	B	760	LEU
1	B	843	ASP
1	B	880	LEU
1	B	900	MET
1	C	27	ARG
1	C	45	GLN
1	C	61	LEU
1	C	73	LYS
1	C	89	LYS
1	C	112	ASN
1	C	169	LYS
1	C	176	ASP
1	C	257	TYR
1	C	284	ASN

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Mol	Chain	Res	Type
1	C	302	LYS
1	C	332	LEU
1	C	356	GLN
1	C	388	VAL
1	C	426	SER
1	C	428	GLU
1	C	436	VAL
1	C	467	ARG
1	C	475	ILE
1	C	483	LYS
1	C	486	LYS
1	C	500	LYS
1	C	508	LEU
1	C	511	ASP
1	C	516	VAL
1	C	517	ASP
1	C	546	GLN
1	C	562	LEU
1	C	642	ARG
1	C	722	GLU
1	C	724	LYS
1	C	733	GLN
1	C	760	LEU
1	C	762	GLU
1	C	773	GLN
1	C	843	ASP
1	C	859	LYS
1	C	880	LEU
1	C	881	GLU
1	C	883	PHE
1	D	55	LYS
1	D	67	ASP
1	D	96	THR
1	D	106	THR
1	D	112	ASN
1	D	302	LYS
1	D	356	GLN
1	D	363	LYS
1	D	405	LYS
1	D	428	GLU
1	D	435	LYS
1	D	467	ARG

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Mol	Chain	Res	Type
1	D	483	LYS
1	D	486	LYS
1	D	510	VAL
1	D	515	ASP
1	D	521	ASP
1	D	532	LYS
1	D	558	ASN
1	D	562	LEU
1	D	587	THR
1	D	618	LEU
1	D	630	ASP
1	D	631	LYS
1	D	722	GLU
1	D	750	ARG
1	D	760	LEU
1	D	768	GLU
1	D	787	ASN
1	D	823	GLN
1	D	826	GLU
1	D	861	ASP
1	D	880	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues 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	5OC	E	3	2	21,21,22	0.80	0	26,30,33	1.54	3 (11%)
2	5OC	G	3	2	21,21,22	0.81	0	26,30,33	1.57	4 (15%)
2	5OC	I	3	2	21,21,22	0.81	0	26,30,33	1.53	3 (11%)
2	5OC	K	3	2	21,21,22	0.81	0	26,30,33	1.52	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5OC	E	3	2	-	0/6/21/22	0/2/2/2
2	5OC	G	3	2	-	0/6/21/22	0/2/2/2
2	5OC	I	3	2	-	0/6/21/22	0/2/2/2
2	5OC	K	3	2	-	0/6/21/22	0/2/2/2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	5OC	C2-N3-C4	5.07	120.00	115.41
2	E	3	5OC	C2-N3-C4	5.04	119.98	115.41
2	K	3	5OC	C2-N3-C4	5.04	119.97	115.41
2	I	3	5OC	C2-N3-C4	5.02	119.95	115.41
2	K	3	5OC	O5-C5-C4	3.75	122.57	115.99
2	G	3	5OC	O5-C5-C4	3.74	122.55	115.99
2	I	3	5OC	O5-C5-C4	3.72	122.51	115.99
2	E	3	5OC	O5-C5-C4	3.71	122.50	115.99
2	E	3	5OC	C6-N1-C2	3.43	120.31	118.62
2	I	3	5OC	C6-N1-C2	3.40	120.29	118.62
2	G	3	5OC	C6-N1-C2	3.32	120.25	118.62
2	K	3	5OC	C6-N1-C2	3.31	120.25	118.62
2	G	3	5OC	OP1-P-O5'	-2.34	106.01	113.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
4	SO4	E	19	-	4,4,4	0.45	0	6,6,6	0.11	0
4	SO4	G	19	-	4,4,4	0.47	0	6,6,6	0.10	0
4	SO4	I	19	-	4,4,4	0.46	0	6,6,6	0.08	0
4	SO4	K	19	-	4,4,4	0.42	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	E	19	-	-	0/0/0/0	0/0/0/0
4	SO4	G	19	-	-	0/0/0/0	0/0/0/0
4	SO4	I	19	-	-	0/0/0/0	0/0/0/0
4	SO4	K	19	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	904/906 (99%)	0.55	77 (8%) 11 9	48, 84, 166, 266	0
1	B	904/906 (99%)	0.34	46 (5%) 27 27	35, 63, 156, 343	0
1	C	903/906 (99%)	0.30	37 (4%) 35 36	38, 68, 137, 233	0
1	D	903/906 (99%)	0.92	138 (15%) 3 2	69, 115, 201, 249	0
2	E	18/18 (100%)	-0.16	0 100 100	69, 88, 133, 141	0
2	G	18/18 (100%)	-0.53	0 100 100	37, 52, 71, 72	0
2	I	18/18 (100%)	-0.47	0 100 100	50, 60, 78, 81	0
2	K	18/18 (100%)	1.08	3 (16%) 2 2	87, 123, 145, 148	0
3	F	15/15 (100%)	-0.09	0 100 100	65, 97, 160, 162	0
3	H	15/15 (100%)	-0.54	0 100 100	40, 53, 77, 82	0
3	J	15/15 (100%)	-0.50	0 100 100	45, 66, 99, 100	0
3	L	15/15 (100%)	1.33	4 (26%) 1 1	104, 145, 162, 163	0
All	All	3746/3756 (99%)	0.51	305 (8%) 12 10	35, 82, 181, 343	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	ALA	14.0
1	D	256	MET	11.5
1	D	847	ALA	10.5
1	B	510	VAL	9.7
1	D	789	ALA	8.8
1	B	499	ILE	7.8
1	A	770	GLU	7.6
1	B	302	LYS	7.6
1	A	256	MET	7.5
1	B	508	LEU	6.9
1	C	511	ASP	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	507	ASN	6.8
1	C	500	LYS	6.8
1	B	516	VAL	6.6
1	D	900	MET	6.3
1	C	512	GLU	6.3
1	D	253	ILE	6.2
1	B	502	ALA	6.1
1	C	503	LEU	6.1
1	A	257	TYR	6.1
1	A	799	PRO	5.9
1	A	532	LYS	5.9
1	B	895	ALA	5.9
1	A	508	LEU	5.8
1	D	257	TYR	5.8
1	A	858	ILE	5.7
1	D	823	GLN	5.7
1	D	115	ILE	5.6
1	A	528	GLU	5.6
1	D	787	ASN	5.5
1	D	306	ASP	5.4
1	C	508	LEU	5.4
1	D	779	ILE	5.4
1	B	509	SER	5.3
1	D	117	VAL	5.3
1	A	862	VAL	5.3
1	A	504	HIS	5.3
1	D	786	ASN	5.2
1	D	277	TYR	5.2
1	A	514	LEU	5.1
1	D	165	GLU	5.1
1	D	831	TYR	5.0
1	A	500	LYS	5.0
1	C	303	LEU	5.0
1	D	543	PHE	5.0
1	D	515	ASP	4.9
3	L	108	DT	4.9
1	A	543	PHE	4.9
1	D	801	CYS	4.8
1	B	498	ILE	4.8
1	C	522	PHE	4.7
1	D	828	GLU	4.7
1	D	164	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	302	LYS	4.7
1	B	497	GLU	4.6
1	A	823	GLN	4.6
1	B	534	SER	4.6
1	D	254	GLU	4.5
1	A	533	LEU	4.5
1	B	535	ALA	4.5
1	A	847	ALA	4.5
1	D	800	LYS	4.4
1	B	504	HIS	4.4
1	A	523	SER	4.3
1	A	253	ILE	4.3
1	B	522	PHE	4.3
1	D	178	VAL	4.3
1	C	525	GLU	4.2
1	B	517	ASP	4.2
1	D	192	ASP	4.2
1	D	848	TRP	4.2
1	C	523	SER	4.2
1	A	863	LEU	4.2
1	A	805	ILE	4.2
1	D	393	GLY	4.2
1	A	37	LEU	4.2
1	A	542	LEU	4.1
1	B	503	LEU	4.1
1	D	138	HIS	4.1
1	D	113	PHE	4.1
1	D	134	ASP	4.1
1	D	162	TRP	4.1
1	D	305	TYR	4.0
1	D	513	PRO	4.0
1	A	800	LYS	4.0
1	C	514	LEU	3.9
1	A	537	SER	3.9
1	A	512	GLU	3.9
1	D	160	GLU	3.8
1	A	531	LYS	3.7
1	B	511	ASP	3.7
1	D	530	ILE	3.7
1	D	824	VAL	3.7
1	C	515	ASP	3.7
1	C	504	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	513	PRO	3.7
1	A	530	ILE	3.7
1	D	301	GLY	3.6
1	B	500	LYS	3.6
1	B	529	LYS	3.6
1	D	500	LYS	3.6
1	D	261	GLU	3.6
1	D	118	THR	3.6
1	D	194	GLU	3.6
1	D	857	LEU	3.6
1	C	535	ALA	3.5
1	A	252	VAL	3.5
1	D	158	ASN	3.5
1	D	136	ILE	3.5
1	D	832	VAL	3.5
1	D	509	SER	3.5
1	C	518	TYR	3.5
1	A	535	ALA	3.5
1	D	286	PRO	3.5
1	B	536	LYS	3.4
1	B	527	LYS	3.4
1	A	511	ASP	3.4
1	A	787	ASN	3.4
1	A	501	GLU	3.3
1	B	495	ASN	3.3
1	D	846	ILE	3.3
1	B	518	TYR	3.3
1	B	506	PRO	3.3
1	D	129	ALA	3.3
1	D	833	LEU	3.3
1	D	133	ILE	3.3
1	A	301	GLY	3.3
1	B	538	LEU	3.2
1	C	256	MET	3.2
1	D	550	VAL	3.2
1	D	225	TYR	3.2
1	C	541	MET	3.2
1	D	42	PRO	3.2
1	C	903	PHE	3.1
1	A	819	ILE	3.1
1	A	52	ILE	3.1
1	D	120	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	506	PRO	3.1
1	D	785	ALA	3.1
1	D	821	ALA	3.1
1	D	895	ALA	3.1
1	C	505	ASN	3.1
1	C	169	LYS	3.1
1	A	254	GLU	3.1
1	D	795	GLY	3.1
1	C	527	LYS	3.1
1	D	539	ASN	3.1
1	D	173	GLN	3.0
1	D	45	GLN	3.0
1	C	793	VAL	3.0
1	D	898	PHE	3.0
1	A	541	MET	3.0
1	A	302	LYS	3.0
1	B	537	SER	2.9
1	D	776	TYR	2.9
1	C	536	LYS	2.9
1	A	57	CYS	2.9
1	D	820	ASP	2.9
1	D	542	LEU	2.9
1	D	784	SER	2.9
1	D	123	PHE	2.8
1	D	566	LEU	2.8
1	D	233	ILE	2.8
1	A	857	LEU	2.8
1	D	32	GLU	2.8
1	D	298	LEU	2.8
1	B	520	PHE	2.8
3	L	109	DC	2.8
1	D	302	LYS	2.8
1	A	516	VAL	2.8
1	D	473	THR	2.8
1	A	774	LEU	2.8
1	C	257	TYR	2.8
1	D	504	HIS	2.8
1	A	518	TYR	2.8
1	D	394	ALA	2.8
1	D	1	MET	2.7
1	A	82	ALA	2.7
1	D	153	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	241	ARG	2.7
1	A	498	ILE	2.7
1	B	512	GLU	2.7
1	B	528	GLU	2.7
1	D	516	VAL	2.7
1	D	498	ILE	2.7
1	C	547	ARG	2.7
1	A	255	ASN	2.7
3	L	110	DA	2.7
1	D	526	ILE	2.7
1	C	496	GLY	2.6
1	B	547	ARG	2.6
1	A	846	ILE	2.6
1	A	515	ASP	2.6
1	A	524	ASP	2.6
1	D	659	MET	2.6
1	A	525	GLU	2.6
1	D	528	GLU	2.6
2	K	2	DC	2.6
1	D	255	ASN	2.6
1	D	221	PHE	2.6
1	B	525	GLU	2.6
1	A	785	ALA	2.5
1	B	532	LYS	2.5
1	A	868	TYR	2.5
1	D	16	PHE	2.5
1	D	149	PHE	2.5
1	D	827	GLY	2.5
1	C	510	VAL	2.5
1	A	496	GLY	2.5
1	A	529	LYS	2.5
1	A	536	LYS	2.5
1	C	542	LEU	2.5
1	D	570	LEU	2.5
1	D	124	PRO	2.4
1	B	46	ALA	2.4
1	D	20	ILE	2.4
1	D	475	ILE	2.4
1	A	832	VAL	2.4
1	D	242	LEU	2.4
1	A	49	TYR	2.4
1	D	435	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	5	DG	2.4
1	B	524	ASP	2.4
1	D	33	TYR	2.4
1	D	44	SER	2.4
1	A	815	ILE	2.4
1	D	213	LEU	2.4
1	D	903	PHE	2.4
1	B	544	ARG	2.4
1	D	46	ALA	2.4
1	D	448	GLU	2.4
1	B	543	PHE	2.3
1	D	260	ARG	2.3
1	B	514	LEU	2.3
1	C	323	TYR	2.3
1	D	307	GLY	2.3
1	D	736	SER	2.3
1	D	808	ILE	2.3
1	A	503	LEU	2.3
1	D	274	ILE	2.3
1	A	178	VAL	2.3
1	A	808	ILE	2.3
1	D	489	MET	2.3
1	D	147	TYR	2.3
1	D	791	TYR	2.3
1	C	534	SER	2.3
1	D	252	VAL	2.3
1	D	230	ILE	2.2
1	D	323	TYR	2.2
1	D	863	LEU	2.2
1	D	837	GLU	2.2
2	K	3	5OC	2.2
1	A	794	GLY	2.2
1	B	541	MET	2.2
1	A	379	VAL	2.2
1	D	151	LEU	2.2
1	D	412	LEU	2.2
1	D	875	THR	2.2
1	D	325	ILE	2.2
1	D	180	SER	2.2
1	C	255	ASN	2.2
1	C	497	GLU	2.2
1	A	833	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	819	ILE	2.2
1	D	251	LYS	2.2
1	B	507	ASN	2.2
1	D	792	ASP	2.2
1	D	205	TRP	2.2
1	D	265	LEU	2.2
1	A	505	ASN	2.2
1	D	263	ILE	2.2
1	B	542	LEU	2.1
1	A	495	ASN	2.1
1	A	534	SER	2.1
1	A	866	MET	2.1
3	L	107	DG	2.1
1	A	98	ASN	2.1
1	C	88	PHE	2.1
1	D	289	SER	2.1
1	D	290	LEU	2.1
1	A	817	GLY	2.1
1	D	201	TYR	2.1
1	A	522	PHE	2.1
1	D	476	THR	2.1
1	A	408	MET	2.1
1	A	283	THR	2.1
1	B	323	TYR	2.1
1	C	539	ASN	2.1
1	D	287	SER	2.1
1	B	501	GLU	2.1
1	D	510	VAL	2.1
1	D	782	VAL	2.1
1	B	128	GLN	2.1
1	A	816	LYS	2.1
1	D	816	LYS	2.0
1	B	253	ILE	2.0
1	A	791	TYR	2.0
1	B	539	ASN	2.0
1	D	781	SER	2.0
1	D	161	GLU	2.0
1	D	198	LEU	2.0
1	C	517	ASP	2.0
1	D	472	PRO	2.0
1	C	507	ASN	2.0
1	D	871	LEU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	5OC	K	3	20/21	0.46	3.31	112,114,118,119	0
2	5OC	G	3	20/21	0.17	-0.83	38,40,43,44	0
2	5OC	E	3	20/21	0.14	-1.08	69,76,81,82	0
2	5OC	I	3	20/21	0.14	-1.14	56,60,62,64	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	E	19	5/5	0.21	2.00	99,101,101,104	0
4	SO4	G	19	5/5	0.16	-0.34	77,78,81,85	0
4	SO4	K	19	5/5	0.16	-1.15	126,126,126,128	0
4	SO4	I	19	5/5	0.12	-2.68	84,86,87,90	0

6.5 Other polymers ⓘ

There are no such residues in this entry.