



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:22 am BST

PDB ID : 3TAE  
Title : 5-hydroxycytosine paired with dAMP in RB69 gp43  
Authors : Zahn, K.E.  
Deposited on : 2011-08-04  
Resolution : 2.71 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](mailto: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.

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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 : 2.11  
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) : 2.11

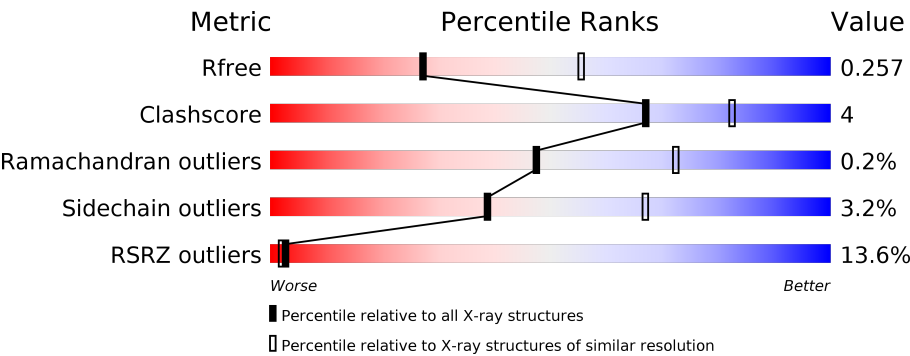
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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.








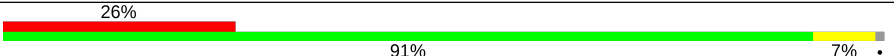
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	E	18	<div><div>11%</div><div>56%</div><div>44%</div></div>
1	G	18	<div><div>33%</div><div>44%</div><div>44%</div><div>6%</div><div>6%</div></div>
1	I	18	<div><div>72%</div><div>22%</div><div>6%</div></div>
1	K	18	<div><div>50%</div><div>72%</div><div>11%</div><div>17%</div></div>
2	F	15	<div><div>7%</div><div>60%</div><div>33%</div><div>7%</div></div>
2	H	15	<div><div>40%</div><div>73%</div><div>13%</div><div>13%</div></div>

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Mol	Chain	Length	Quality of chain
2	J	15	
2	L	15	
3	A	906	
3	B	906	
3	C	906	
3	D	906	

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
1	5OC	I	3	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32066 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 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
1	E	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			
1	I	17	Total	C	N	O	P	0	0	0
			350	164	67	102	17			
1	G	17	Total	C	N	O	P	0	0	1
			313	145	59	93	16			
1	K	15	Total	C	N	O	P	0	0	1
			271	125	52	80	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			286	135	51	86	14			
2	J	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
2	H	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	L	11	Total	C	N	O	P	0	0	0
			223	107	40	66	10			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			
3	B	901	Total	C	N	O	S	0	0	0
			7355	4724	1224	1374	33			
3	C	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	898	Total	C	N	O	S	0	0	0
			7328	4706	1221	1369	32			

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 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	3	Total	O	0	0
			3	3		
5	F	2	Total	O	0	0
			2	2		
5	I	6	Total	O	0	0
			6	6		
5	J	4	Total	O	0	0
			4	4		
5	G	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		
5	A	101	Total	O	0	0
			101	101		
5	B	47	Total	O	0	0
			47	47		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	71	Total 71	O 71	0	0
5	D	4	Total 4	O 4	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

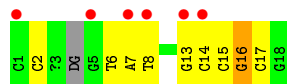
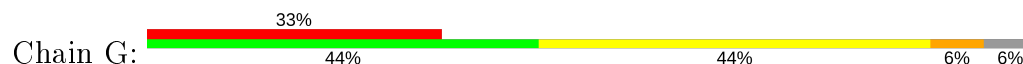
- Molecule 1: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')



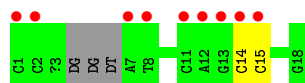
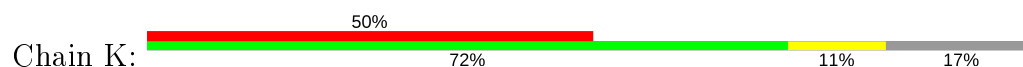
- Molecule 1: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')



- Molecule 1: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')



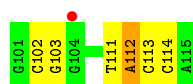
- Molecule 1: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')



- Molecule 2: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*AP\*CP\*CP\*A)-3')



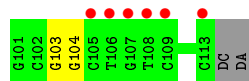
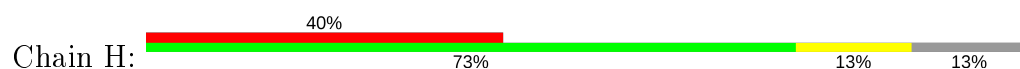




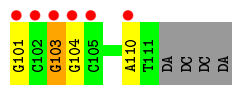
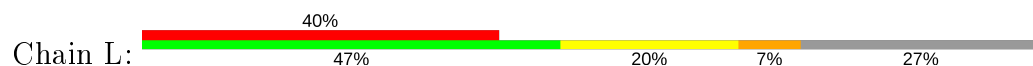
- Molecule 2: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*AP\*CP\*CP\*A)-3')



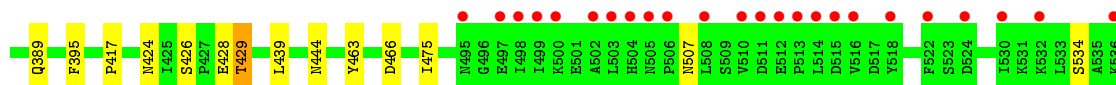
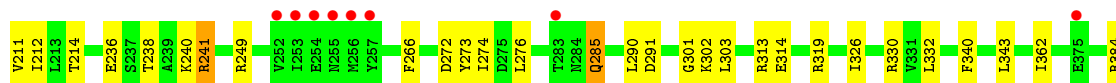
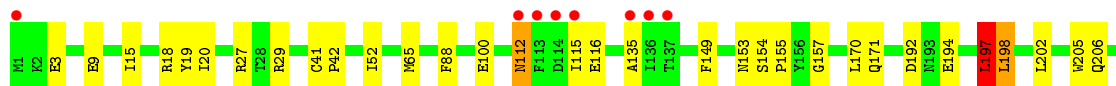
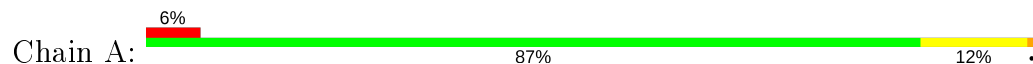
- Molecule 2: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*AP\*CP\*CP\*A)-3')



- Molecule 2: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*AP\*CP\*CP\*A)-3')



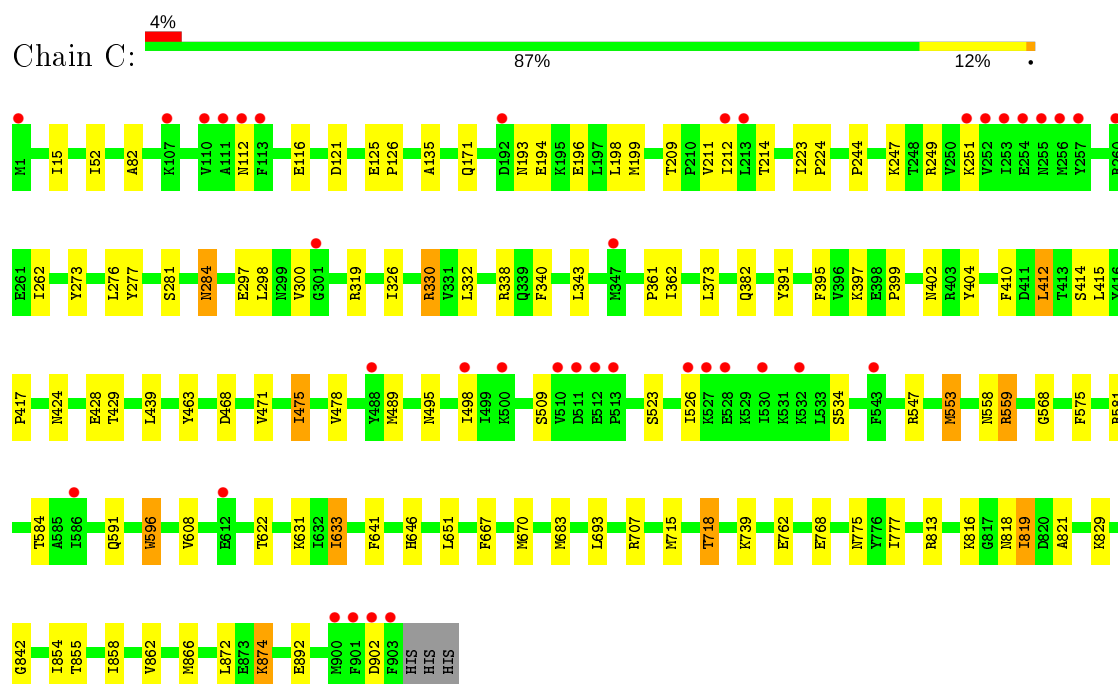
- Molecule 3: DNA polymerase



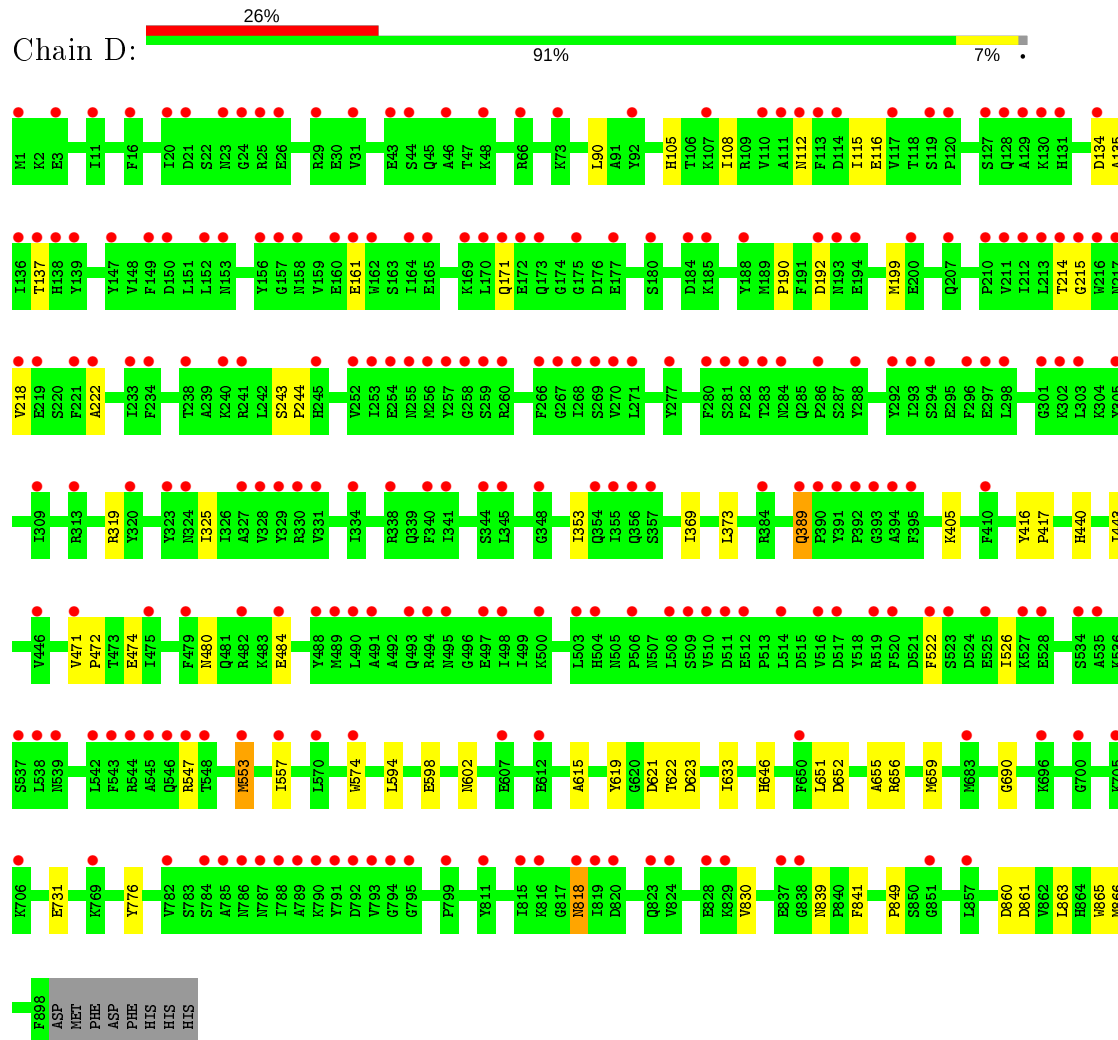
- Molecule 3: DNA polymerase



- Molecule 3: DNA polymerase



● Molecule 3: DNA polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.27Å 123.71Å 165.90Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	30.00 – 2.71 30.31 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.71) 98.1 (30.31-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0116, CNS	Depositor
R, $R_{free}$	0.224 , 0.268 0.216 , 0.257	Depositor DCC
$R_{free}$ test set	13797 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 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	E	0.23	0/387	0.84	0/593
1	G	0.24	0/345	0.80	1/529 (0.2%)
1	I	0.29	0/369	0.78	0/565
1	K	0.21	0/298	0.74	0/456
2	F	0.23	0/319	0.89	1/491 (0.2%)
2	H	0.23	0/294	0.81	0/452
2	J	0.27	0/339	0.83	0/521
2	L	0.23	0/249	0.97	3/383 (0.8%)
3	A	0.43	4/7555 (0.1%)	0.53	1/10209 (0.0%)
3	B	0.42	3/7535 (0.0%)	0.49	0/10182
3	C	0.42	1/7555 (0.0%)	0.51	0/10209
3	D	0.41	2/7507 (0.0%)	0.46	0/10145
All	All	0.41	10/32752 (0.0%)	0.54	6/44735 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	TRP	CD2-CE2	5.30	1.47	1.41
3	A	713	TRP	CD2-CE2	5.13	1.47	1.41
3	D	574	TRP	CD2-CE2	5.12	1.47	1.41
3	A	205	TRP	CD2-CE2	5.12	1.47	1.41
3	C	596	TRP	CD2-CE2	5.12	1.47	1.41
3	A	865	TRP	CD2-CE2	5.10	1.47	1.41
3	B	848	TRP	CD2-CE2	5.09	1.47	1.41
3	B	596	TRP	CD2-CE2	5.08	1.47	1.41
3	D	865	TRP	CD2-CE2	5.07	1.47	1.41
3	A	848	TRP	CD2-CE2	5.02	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	103	DG	P-O3'-C3'	7.96	129.25	119.70
2	L	101	DG	P-O3'-C3'	6.89	127.97	119.70
1	G	16	DG	P-O3'-C3'	6.77	127.83	119.70
2	L	110	DA	P-O3'-C3'	6.12	127.05	119.70
2	F	112	DA	P-O3'-C3'	6.00	126.89	119.70
3	A	197	LEU	CA-CB-CG	5.59	128.16	115.30

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	E	366	0	201	5	0
1	G	313	0	168	7	0
1	I	350	0	189	11	0
1	K	271	0	145	2	0
2	F	286	0	158	6	0
2	H	263	0	148	1	0
2	J	303	0	170	7	0
2	L	223	0	126	1	0
3	A	7374	0	7267	64	0
3	B	7355	0	7254	54	0
3	C	7374	0	7267	61	0
3	D	7328	0	7232	31	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
5	A	101	0	0	3	0
5	B	47	0	0	0	0
5	C	71	0	0	0	0
5	D	4	0	0	0	0
5	E	3	0	0	0	0
5	F	2	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	6	0	0	0	0
5	J	4	0	0	0	0
All	All	32066	0	30325	239	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 4.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:DC:H4'	1:I:3:5OC:H5'A	1.23	1.21
1:I:3:5OC:O2	3:C:568:GLY:HA3	1.47	1.13
1:I:2:DC:H4'	1:I:3:5OC:C5'	1.91	0.99
2:F:112:DA:H2''	2:F:113:DC:H5''	1.49	0.94
1:G:2:DC:O2	1:G:2:DC:H2'	1.73	0.87
3:A:424:ASN:O	3:A:429:THR:HG21	1.74	0.86
3:D:112:ASN:HB3	3:D:214:THR:HG23	1.59	0.82
3:B:65:MET:HE2	3:B:88:PHE:HB2	1.62	0.81
3:A:65:MET:HE3	3:A:88:PHE:HB2	1.61	0.80
3:C:112:ASN:HB3	3:C:214:THR:HG23	1.63	0.80
2:F:112:DA:C2'	2:F:113:DC:H5''	2.12	0.79
3:A:897:LEU:HD23	3:A:897:LEU:H	1.48	0.78
3:A:813:ARG:HH21	3:A:842:GLY:HA3	1.49	0.77
1:E:6:DT:H2''	1:E:7:DA:H5''	1.69	0.75
3:A:65:MET:CE	3:A:88:PHE:HB2	2.19	0.71
1:I:2:DC:C4'	1:I:3:5OC:H5'A	2.14	0.71
2:J:112:DA:H2'	2:J:113:DC:H5''	1.72	0.71
2:J:115:DA:H5'	3:C:622:THR:HG21	1.73	0.71
2:F:111:DT:H2''	2:F:112:DA:H5''	1.73	0.70
3:A:417:PRO:HB3	3:A:475:ILE:HD11	1.75	0.69
3:A:65:MET:HE3	3:A:88:PHE:CB	2.22	0.69
2:J:112:DA:C2'	2:J:113:DC:H5''	2.24	0.67
1:I:3:5OC:O2	3:C:568:GLY:CA	2.33	0.67
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.77	0.67
3:A:211:VAL:HG12	3:A:212:ILE:HD12	1.77	0.67
3:A:739:LYS:HA	3:A:739:LYS:HE3	1.78	0.65
1:G:15:DC:H2''	1:G:16:DG:C8	2.32	0.65
3:A:444:ASN:HD22	3:A:599:ARG:HD2	1.62	0.65
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.78	0.65
3:A:19:TYR:CE1	3:A:29:ARG:HG3	2.33	0.64
3:B:65:MET:CE	3:B:88:PHE:HB2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:641:PHE:HD1	3:C:646:HIS:HD2	1.47	0.62
3:C:424:ASN:O	3:C:429:THR:HG21	2.00	0.62
3:B:211:VAL:HG12	3:B:212:ILE:HD12	1.80	0.62
1:G:13:DG:H2''	1:G:14:DC:H5''	1.81	0.62
3:C:489:MET:SD	3:C:553:MET:HG2	2.40	0.61
3:B:439:LEU:HD13	3:B:443:ILE:HD11	1.83	0.61
1:E:8:DT:H4'	3:A:707:ARG:HD2	1.83	0.60
3:A:285:GLN:HE21	3:A:285:GLN:HA	1.66	0.60
3:A:112:ASN:HB3	3:A:214:THR:HG23	1.85	0.59
1:I:2:DC:O4'	1:I:2:DC:O2	2.19	0.59
2:J:101:DG:H2'	2:J:102:DC:C6	2.37	0.59
1:I:11:DC:OP1	3:C:874:LYS:HE2	2.02	0.59
3:A:202:LEU:O	3:A:206:GLN:HG2	2.03	0.58
3:A:475:ILE:HD12	3:A:566:LEU:HD23	1.85	0.57
3:C:818:ASN:HD22	3:C:821:ALA:HB2	1.69	0.57
3:A:417:PRO:HB3	3:A:475:ILE:CD1	2.35	0.57
3:B:224:PRO:HA	3:B:263:ILE:HD12	1.87	0.57
3:C:343:LEU:HD12	3:C:558:ASN:HD21	1.70	0.57
3:B:236:GLU:HG2	3:B:240:LYS:HE2	1.86	0.57
3:B:209:THR:HG21	3:B:244:PRO:HG3	1.86	0.56
3:B:424:ASN:O	3:B:429:THR:HG21	2.05	0.56
3:D:830:VAL:HG12	3:D:849:PRO:HA	1.88	0.56
3:A:641:PHE:HD1	3:A:646:HIS:HD2	1.52	0.55
3:A:236:GLU:O	3:A:240:LYS:HG2	2.07	0.55
3:B:373:LEU:HD23	3:B:380:ILE:HG22	1.88	0.55
3:D:137:THR:HG21	3:D:325:ILE:HA	1.88	0.55
2:F:102:DC:H2''	2:F:103:DG:C8	2.42	0.55
2:J:114:DC:H2''	2:J:115:DA:OP2	2.07	0.54
3:A:313:ARG:HD2	5:A:917:HOH:O	2.07	0.54
3:B:738:PRO:O	3:B:742:GLN:HB2	2.07	0.54
3:C:862:VAL:O	3:C:866:MET:HG3	2.07	0.54
3:D:171:GLN:HE21	3:D:319:ARG:HH22	1.56	0.54
1:G:16:DG:H2'	1:G:17:DC:O4'	2.07	0.54
2:L:103:DG:H2''	2:L:104:DG:C8	2.42	0.54
3:B:9:GLU:HG2	3:B:266:PHE:HD2	1.73	0.53
1:E:15:DC:H2''	1:E:16:DG:C8	2.44	0.53
1:G:2:DC:C2'	1:G:2:DC:O2	2.47	0.53
3:A:314:GLU:HG3	5:A:923:HOH:O	2.09	0.53
3:C:171:GLN:HE21	3:C:319:ARG:HH22	1.57	0.53
3:A:757:GLU:HB2	3:A:889:LEU:HD22	1.91	0.53
3:A:27:ARG:NH2	3:B:190:PRO:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:897:LEU:CD2	3:A:897:LEU:H	2.20	0.52
3:A:9:GLU:HG2	3:A:266:PHE:HD2	1.75	0.52
3:B:555:ALA:O	3:B:559:ARG:HG2	2.09	0.52
3:C:395:PHE:HB2	3:C:591:GLN:HG2	1.90	0.52
3:C:343:LEU:HD12	3:C:558:ASN:ND2	2.24	0.52
3:B:202:LEU:O	3:B:206:GLN:HG2	2.10	0.52
3:A:854:ILE:HD12	3:A:859:LYS:HA	1.92	0.51
3:C:391:TYR:HB2	3:C:584:THR:HG22	1.91	0.51
3:D:652:ASP:CG	3:D:656:ARG:HH12	2.14	0.51
3:C:523:SER:H	3:C:526:ILE:HD12	1.76	0.51
3:B:788:ILE:HD12	3:B:826:GLU:HG2	1.93	0.51
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.93	0.50
3:D:480:ASN:O	3:D:484:GLU:HB2	2.10	0.50
3:A:596:TRP:HB3	3:A:670:MET:HE2	1.92	0.50
3:C:414:SER:HB3	3:C:417:PRO:HG2	1.93	0.50
3:C:209:THR:HG21	3:C:244:PRO:HG3	1.94	0.50
3:C:641:PHE:HD1	3:C:646:HIS:CD2	2.29	0.50
1:I:3:5OC:OP2	3:C:361:PRO:HD2	2.11	0.50
3:C:818:ASN:O	3:C:819:ILE:C	2.50	0.49
3:B:458:PRO:HG3	3:B:592:MET:SD	2.53	0.49
3:B:655:ALA:HA	3:B:659:MET:HB2	1.93	0.49
1:G:8:DT:H4'	3:B:707:ARG:HD2	1.94	0.49
3:B:116:GLU:HB2	3:B:135:ALA:HB3	1.94	0.49
3:C:715:MET:O	3:C:718:THR:HG23	2.12	0.49
3:D:416:TYR:HB2	3:D:417:PRO:HD3	1.95	0.49
3:B:633:ILE:HD11	3:B:651:LEU:HD11	1.95	0.49
3:B:65:MET:CE	3:B:88:PHE:CB	2.90	0.49
3:B:875:THR:O	3:B:879:PRO:HG2	2.12	0.49
3:C:193:ASN:ND2	3:C:196:GLU:H	2.11	0.49
3:D:440:HIS:HA	3:D:443:ILE:HD12	1.94	0.49
1:G:6:DT:H2''	1:G:7:DA:H5''	1.94	0.49
3:B:410:PHE:HB3	3:B:683:MET:HG2	1.95	0.49
3:B:785:ALA:HB1	3:B:788:ILE:HD11	1.95	0.48
1:I:8:DT:H4'	3:C:707:ARG:HD2	1.96	0.48
3:D:776:TYR:HB3	3:D:863:LEU:HD21	1.95	0.48
3:A:429:THR:HG23	3:A:463:TYR:HD1	1.78	0.48
1:K:14:DC:H2'	1:K:15:DC:C6	2.48	0.48
2:J:101:DG:H2''	2:J:102:DC:O5'	2.14	0.48
3:B:781:SER:HB2	3:B:832:VAL:HB	1.96	0.48
3:C:52:ILE:HD12	3:C:428:GLU:HB3	1.96	0.48
3:A:3:GLU:HB2	3:A:20:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:DC:H4'	1:I:3:5OC:O5'	2.12	0.47
3:A:157:GLY:O	3:A:313:ARG:NH2	2.47	0.47
3:A:580:LEU:O	3:A:584:THR:HG23	2.14	0.47
3:B:286:PRO:HA	3:B:735:SER:HB3	1.95	0.47
3:C:211:VAL:HG12	3:C:212:ILE:HD12	1.97	0.47
3:A:301:GLY:O	3:A:330:ARG:NH1	2.47	0.47
3:A:593:ALA:HA	3:A:670:MET:CE	2.45	0.47
3:C:284:ASN:HD21	3:C:829:LYS:NZ	2.11	0.47
3:C:509:SER:HB2	3:C:534:SER:HB3	1.96	0.47
3:A:290:LEU:HD23	3:A:302:LYS:HE3	1.96	0.47
3:C:495:ASN:HA	3:C:498:ILE:HD12	1.97	0.47
3:C:247:LYS:NZ	3:C:249:ARG:HH21	2.13	0.47
3:C:326:ILE:O	3:C:330:ARG:HG2	2.15	0.47
3:C:298:LEU:HB2	3:C:300:VAL:HG22	1.98	0.46
3:B:856:ASP:HA	3:B:859:LYS:HB3	1.97	0.46
3:D:633:ILE:HD11	3:D:651:LEU:HD11	1.97	0.46
3:A:818:ASN:HD22	3:A:821:ALA:HB2	1.81	0.46
3:B:343:LEU:HD11	3:B:557:ILE:HD11	1.98	0.46
3:B:9:GLU:CG	3:B:266:PHE:HD2	2.27	0.46
3:C:641:PHE:CD1	3:C:646:HIS:HD2	2.30	0.46
3:B:236:GLU:O	3:B:240:LYS:HG2	2.16	0.46
1:E:1:DC:H4'	3:A:572:ASN:HD21	1.81	0.46
3:B:638:GLU:HA	3:B:641:PHE:HD2	1.80	0.46
3:D:522:PHE:HB3	3:D:526:ILE:HB	1.98	0.46
3:A:149:PHE:HB3	3:A:197:LEU:HD13	1.98	0.45
3:A:897:LEU:N	3:A:897:LEU:HD23	2.25	0.45
3:B:596:TRP:HB3	3:B:670:MET:HE2	1.97	0.45
3:D:621:ASP:O	3:D:623:ASP:N	2.49	0.45
3:C:297:GLU:OE2	3:C:338:ARG:NH1	2.50	0.45
3:C:412:LEU:HG	3:C:415:LEU:HD13	1.99	0.45
3:A:276:LEU:HG	3:A:340:PHE:HB3	1.97	0.45
3:D:655:ALA:HA	3:D:659:MET:HB2	1.98	0.45
2:J:102:DC:H2"	2:J:103:DG:C8	2.51	0.45
3:C:125:GLU:HA	3:C:126:PRO:HD3	1.81	0.45
3:C:410:PHE:HB3	3:C:683:MET:HG2	1.98	0.45
3:A:9:GLU:CG	3:A:266:PHE:HD2	2.29	0.45
3:B:286:PRO:HA	3:B:735:SER:CB	2.47	0.45
3:B:412:LEU:HG	3:B:415:LEU:HD13	1.98	0.45
3:C:768:GLU:HG2	3:C:872:LEU:HD21	1.99	0.45
3:C:251:LYS:HB3	3:C:262:ILE:HG13	1.98	0.44
3:A:238:THR:O	3:A:241:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:641:PHE:HD1	3:A:646:HIS:CD2	2.33	0.44
3:B:65:MET:HE2	3:B:88:PHE:CB	2.39	0.44
3:A:641:PHE:CD1	3:A:646:HIS:HD2	2.33	0.44
1:I:2:DC:H2'	3:C:362:ILE:HD12	1.99	0.44
3:C:633:ILE:HD11	3:C:651:LEU:HD11	1.99	0.44
3:D:602:ASN:HD21	3:D:615:ALA:HA	1.83	0.44
3:B:854:ILE:HB	3:B:859:LYS:HB2	2.00	0.44
3:D:405:LYS:O	3:D:690:GLY:HA2	2.18	0.44
3:B:273:TYR:HA	3:B:276:LEU:HB2	2.00	0.44
3:C:596:TRP:HB3	3:C:670:MET:HE2	2.00	0.44
3:C:813:ARG:HH21	3:C:842:GLY:HA3	1.81	0.44
3:B:453:VAL:HG23	3:B:454:TYR:CD2	2.53	0.44
3:C:277:TYR:O	3:C:281:SER:HB3	2.17	0.44
3:D:471:VAL:HB	3:D:472:PRO:HD3	2.00	0.44
1:K:14:DC:H2'	1:K:15:DC:H6	1.82	0.44
3:A:171:GLN:HG3	5:A:981:HOH:O	2.16	0.43
3:D:553:MET:O	3:D:557:ILE:HG12	2.19	0.43
3:A:655:ALA:HA	3:A:659:MET:HB2	2.01	0.43
3:D:218:VAL:HA	3:D:222:ALA:HB3	2.00	0.43
3:A:303:LEU:HD22	3:A:326:ILE:HD12	2.00	0.43
3:A:112:ASN:HD21	3:A:332:LEU:HD21	1.83	0.43
3:C:362:ILE:HG23	3:C:575:PHE:HD1	1.84	0.43
3:C:775:ASN:HD21	3:C:777:ILE:HB	1.83	0.43
3:A:395:PHE:HB2	3:A:591:GLN:HG2	2.00	0.43
3:B:343:LEU:HD12	3:B:554:THR:HG23	2.00	0.43
3:C:429:THR:HG23	3:C:463:TYR:HD1	1.84	0.43
3:D:161:GLU:HG2	3:D:190:PRO:HG3	2.00	0.43
3:A:153:ASN:HB2	3:A:192:ASP:O	2.19	0.43
3:A:897:LEU:CD2	3:A:897:LEU:N	2.81	0.43
3:C:194:GLU:HG2	3:C:198:LEU:HD13	2.01	0.43
3:B:369:ILE:HG22	3:B:373:LEU:HD22	2.00	0.42
3:D:116:GLU:HB2	3:D:135:ALA:HB3	2.00	0.42
3:A:197:LEU:C	3:A:197:LEU:HD12	2.39	0.42
3:A:507:ASN:O	3:A:534:SER:HA	2.19	0.42
3:C:284:ASN:HD21	3:C:829:LYS:HZ3	1.67	0.42
3:A:116:GLU:HB2	3:A:135:ALA:HB3	2.02	0.42
3:C:330:ARG:HG2	3:C:330:ARG:H	1.67	0.42
3:A:194:GLU:HG2	3:A:198:LEU:HD22	2.02	0.42
3:A:52:ILE:HD12	3:A:428:GLU:HB3	2.02	0.42
3:A:878:LYS:HB3	3:A:879:PRO:HD3	2.02	0.42
3:D:863:LEU:HA	3:D:866:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:DG:H2"	2:H:104:DG:C8	2.55	0.42
3:A:426:SER:O	3:A:429:THR:HG22	2.19	0.42
3:B:112:ASN:HB3	3:B:214:THR:HG23	2.01	0.42
2:F:114:DC:N4	5:F:204:HOH:O	2.50	0.42
3:B:65:MET:HE3	3:B:88:PHE:HB3	2.02	0.42
3:C:276:LEU:HG	3:C:340:PHE:HB3	2.02	0.42
3:D:839:ASN:HD22	3:D:841:PHE:HB2	1.85	0.42
3:C:471:VAL:O	3:C:475:ILE:HG13	2.19	0.41
3:D:214:THR:OG1	3:D:215:GLY:N	2.52	0.41
3:A:41:CYS:HB2	3:A:42:PRO:HD2	2.01	0.41
3:B:219:GLU:HA	3:B:223:ILE:HD12	2.00	0.41
3:B:223:ILE:HB	3:B:224:PRO:HD3	2.01	0.41
3:C:667:PHE:CE1	3:C:670:MET:HE1	2.55	0.41
3:D:619:TYR:CE2	3:D:621:ASP:HB2	2.55	0.41
3:C:397:LYS:O	3:C:399:PRO:HD3	2.19	0.41
3:A:553:MET:O	3:A:557:ILE:HG12	2.20	0.41
3:D:389:GLN:HE21	3:D:389:GLN:HA	1.86	0.41
3:A:593:ALA:HA	3:A:670:MET:HE1	2.02	0.41
3:B:362:ILE:HD11	3:B:572:ASN:CG	2.41	0.41
3:B:593:ALA:HA	3:B:670:MET:CE	2.50	0.41
3:C:112:ASN:HD21	3:C:332:LEU:HG	1.85	0.41
2:F:112:DA:C3'	2:F:113:DC:H5"	2.50	0.41
3:B:330:ARG:H	3:B:330:ARG:HG2	1.57	0.41
3:C:402:ASN:HB3	3:C:404:TYR:CE2	2.56	0.41
3:A:154:SER:HB2	3:A:155:PRO:HD2	2.01	0.41
3:C:478:VAL:HG13	3:C:559:ARG:CG	2.51	0.41
3:C:775:ASN:ND2	3:C:777:ILE:HB	2.35	0.41
3:B:836:ARG:HG3	3:B:867:ASP:HB2	2.03	0.41
3:B:381:PRO:HG2	3:B:576:ARG:HG2	2.01	0.41
3:D:369:ILE:HG12	3:D:474:GLU:HG3	2.03	0.41
1:E:3:5OC:H2'A	1:E:4:DG:C8	2.56	0.41
3:A:272:ASP:OD1	3:A:274:ILE:HG22	2.21	0.40
3:B:439:LEU:HD13	3:B:443:ILE:CD1	2.51	0.40
3:B:429:THR:HG23	3:B:463:TYR:HD2	1.86	0.40
3:D:105:HIS:HA	3:D:108:ILE:HD12	2.02	0.40
3:D:243:SER:HA	3:D:244:PRO:HD3	1.97	0.40
3:D:594:LEU:O	3:D:598:GLU:HB2	2.21	0.40
3:D:818:ASN:HD22	3:D:818:ASN:H	1.69	0.40
3:A:362:ILE:HD11	3:A:572:ASN:CG	2.41	0.40
3:C:82:ALA:H	3:C:382:GLN:HE21	1.69	0.40
3:A:19:TYR:HE1	3:A:29:ARG:HG3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:244:PRO:HD2	3:B:266:PHE:O	2.21	0.40
3:B:78:ILE:HD12	3:B:80:LEU:HD12	2.03	0.40
3:D:90:LEU:HD22	3:D:353:ILE:HG22	2.03	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	
3	A	901/906 (99%)	875 (97%)	25 (3%)	1 (0%)	51	77
3	B	899/906 (99%)	858 (95%)	38 (4%)	3 (0%)	41	65
3	C	901/906 (99%)	873 (97%)	27 (3%)	1 (0%)	51	77
3	D	896/906 (99%)	855 (95%)	39 (4%)	2 (0%)	47	72
All	All	3597/3624 (99%)	3461 (96%)	129 (4%)	7 (0%)	47	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	819	ILE
3	D	192	ASP
3	D	622	THR
3	B	896	SER
3	B	424	ASN
3	B	622	THR
3	A	858	ILE

### 5.3.2 Protein sidechains [i](#)

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	
3	A	800/803 (100%)	769 (96%)	31 (4%)	32	59
3	B	798/803 (99%)	769 (96%)	29 (4%)	35	62
3	C	800/803 (100%)	771 (96%)	29 (4%)	35	62
3	D	795/803 (99%)	783 (98%)	12 (2%)	65	85
All	All	3193/3212 (99%)	3092 (97%)	101 (3%)	39	67

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

Mol	Chain	Res	Type
3	A	15	ILE
3	A	18	ARG
3	A	100	GLU
3	A	112	ASN
3	A	115	ILE
3	A	170	LEU
3	A	197	LEU
3	A	198	LEU
3	A	241	ARG
3	A	249	ARG
3	A	273	TYR
3	A	285	GLN
3	A	291	ASP
3	A	319	ARG
3	A	343	LEU
3	A	384	ARG
3	A	389	GLN
3	A	429	THR
3	A	439	LEU
3	A	466	ASP
3	A	559	ARG
3	A	584	THR
3	A	633	ILE
3	A	693	LEU
3	A	718	THR
3	A	724	LYS
3	A	739	LYS
3	A	781	SER

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Mol	Chain	Res	Type
3	A	823	GLN
3	A	843	ASP
3	A	897	LEU
3	B	44	SER
3	B	47	THR
3	B	112	ASN
3	B	113	PHE
3	B	115	ILE
3	B	198	LEU
3	B	241	ARG
3	B	273	TYR
3	B	283	THR
3	B	284	ASN
3	B	300	VAL
3	B	330	ARG
3	B	373	LEU
3	B	412	LEU
3	B	414	SER
3	B	439	LEU
3	B	510	VAL
3	B	511	ASP
3	B	526	ILE
3	B	565	SER
3	B	587	THR
3	B	693	LEU
3	B	718	THR
3	B	770	GLU
3	B	826	GLU
3	B	843	ASP
3	B	854	ILE
3	B	897	LEU
3	B	898	PHE
3	C	15	ILE
3	C	121	ASP
3	C	199	MET
3	C	273	TYR
3	C	284	ASN
3	C	330	ARG
3	C	373	LEU
3	C	412	LEU
3	C	439	LEU
3	C	468	ASP

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Mol	Chain	Res	Type
3	C	475	ILE
3	C	547	ARG
3	C	553	MET
3	C	559	ARG
3	C	581	ARG
3	C	608	VAL
3	C	631	LYS
3	C	633	ILE
3	C	693	LEU
3	C	718	THR
3	C	739	LYS
3	C	762	GLU
3	C	816	LYS
3	C	854	ILE
3	C	855	THR
3	C	858	ILE
3	C	874	LYS
3	C	892	GLU
3	C	902	ASP
3	D	115	ILE
3	D	134	ASP
3	D	199	MET
3	D	373	LEU
3	D	389	GLN
3	D	547	ARG
3	D	553	MET
3	D	646	HIS
3	D	731	GLU
3	D	818	ASN
3	D	860	ASP
3	D	861	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	40	HIS
3	A	70	GLN
3	A	98	ASN
3	A	112	ASN
3	A	193	ASN
3	A	285	GLN
3	A	444	ASN

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Mol	Chain	Res	Type
3	A	646	HIS
3	A	818	ASN
3	A	823	GLN
3	A	839	ASN
3	A	864	HIS
3	B	40	HIS
3	B	112	ASN
3	B	193	ASN
3	B	284	ASN
3	B	339	GLN
3	B	342	ASN
3	B	382	GLN
3	B	389	GLN
3	B	481	GLN
3	B	646	HIS
3	B	818	ASN
3	B	823	GLN
3	C	40	HIS
3	C	171	GLN
3	C	193	ASN
3	C	284	ASN
3	C	285	GLN
3	C	382	GLN
3	C	444	ASN
3	C	558	ASN
3	C	646	HIS
3	C	775	ASN
3	C	818	ASN
3	C	839	ASN
3	D	171	GLN
3	D	193	ASN
3	D	389	GLN
3	D	602	ASN
3	D	679	HIS
3	D	786	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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$
1	5OC	G	3	1	0,3,22	0.00	-	0,3,33	0.00	-
1	5OC	I	3	1	15,21,22	1.20	1 (6%)	15,30,33	1.05	1 (6%)
1	5OC	K	3	1	0,3,22	0.00	-	0,3,33	0.00	-
1	5OC	E	3	1	15,21,22	1.15	1 (6%)	15,30,33	0.95	1 (6%)

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
1	5OC	I	3	1	-	1/4/21/22	0/2/2/2
1	5OC	E	3	1	-	3/4/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	3	5OC	C6-C5	-3.67	1.34	1.39
1	E	3	5OC	C6-C5	-3.57	1.34	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	5OC	C2-N3-C4	3.30	120.00	116.02
1	I	3	5OC	C2-N3-C4	3.26	119.96	116.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	3	5OC	O4'-C1'-N1-C6
1	E	3	5OC	O4'-C1'-N1-C6
1	E	3	5OC	C3'-C4'-C5'-O5'
1	E	3	5OC	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	3	5OC	7	0
1	E	3	5OC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	B	907	-	4,4,4	0.36	0	6,6,6	0.11	0
4	SO4	C	907	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	H	2	-	4,4,4	0.34	0	6,6,6	0.05	0
4	SO4	F	3	-	4,4,4	0.33	0	6,6,6	0.07	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	17/18 (94%)	0.35	2 (11%) 4 3	57, 89, 126, 143	0
1	G	16/18 (88%)	1.89	6 (37%) 0 0	62, 114, 138, 155	0
1	I	16/18 (88%)	-0.32	0 100 100	37, 50, 70, 94	0
1	K	14/18 (77%)	2.90	9 (64%) 0 0	53, 162, 197, 200	0
2	F	15/15 (100%)	0.77	1 (6%) 17 16	72, 87, 138, 141	0
2	H	13/15 (86%)	2.24	6 (46%) 0 0	94, 116, 140, 141	0
2	J	15/15 (100%)	-0.29	0 100 100	36, 61, 87, 87	0
2	L	11/15 (73%)	2.32	6 (54%) 0 0	158, 169, 173, 174	0
3	A	903/906 (99%)	0.28	50 (5%) 25 24	30, 54, 146, 263	0
3	B	901/906 (99%)	0.95	152 (16%) 1 1	34, 80, 218, 286	0
3	C	903/906 (99%)	0.26	38 (4%) 36 35	28, 62, 135, 197	0
3	D	898/906 (99%)	1.39	235 (26%) 0 0	84, 135, 213, 253	0
All	All	3722/3756 (99%)	0.73	505 (13%) 3 2	28, 78, 201, 286	0

All (505) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	819	ILE	19.0
3	B	821	ALA	13.1
3	B	820	ASP	12.0
3	D	257	TYR	11.0
3	B	862	VAL	10.9
3	D	111	ALA	10.9
3	B	256	MET	9.9
3	A	505	ASN	9.4
3	B	286	PRO	9.3
3	D	789	ALA	9.1
3	A	256	MET	8.7

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Mol	Chain	Res	Type	RSRZ
3	D	395	PHE	8.5
3	D	522	PHE	8.1
3	D	523	SER	7.9
3	B	798	GLY	7.8
3	D	215	GLY	7.8
3	B	812	ASN	7.6
3	D	282	PHE	7.5
3	B	857	LEU	7.4
3	D	788	ILE	7.2
3	B	507	ASN	7.0
3	B	516	VAL	6.9
3	B	257	TYR	6.9
3	C	510	VAL	6.8
3	D	256	MET	6.8
3	D	394	ALA	6.7
3	B	528	GLU	6.6
3	D	504	HIS	6.6
3	B	818	ASN	6.6
3	D	792	ASP	6.6
3	D	506	PRO	6.5
3	B	541	MET	6.5
3	D	787	ASN	6.4
3	B	865	TRP	6.3
3	B	499	ILE	6.3
3	A	516	VAL	6.2
3	B	539	ASN	6.2
3	D	1	MET	6.1
3	D	491	ALA	6.1
3	B	801	CYS	6.1
3	D	258	GLY	6.0
3	D	510	VAL	6.0
3	A	498	ILE	6.0
3	B	816	LYS	5.9
3	B	809	LEU	5.9
3	B	799	PRO	5.9
3	B	287	SER	5.9
3	B	498	ILE	5.9
3	B	811	TYR	5.8
3	D	391	TYR	5.7
1	G	7	DA	5.7
3	B	847	ALA	5.6
1	K	2	DC	5.6

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Mol	Chain	Res	Type	RSRZ
3	D	214	THR	5.6
3	D	503	LEU	5.5
3	D	520	PHE	5.5
3	D	254	GLU	5.5
3	D	269	SER	5.5
3	B	510	VAL	5.4
3	D	165	GLU	5.4
3	B	846	ILE	5.3
3	B	513	PRO	5.3
3	D	46	ALA	5.2
3	A	515	ASP	5.2
3	B	840	PRO	5.2
3	B	813	ARG	5.1
3	D	498	ILE	5.1
3	A	257	TYR	5.1
3	B	789	ALA	5.1
3	B	805	ILE	5.1
3	B	817	GLY	5.0
3	A	495	ASN	5.0
3	B	839	ASN	5.0
3	D	270	VAL	5.0
3	D	305	TYR	5.0
3	B	255	ASN	5.0
3	D	210	PRO	5.0
3	B	858	ILE	4.9
3	B	852	THR	4.9
3	B	514	LEU	4.9
3	A	532	LYS	4.9
3	B	825	VAL	4.8
3	B	254	GLU	4.8
3	A	503	LEU	4.8
3	D	138	HIS	4.8
3	D	328	VAL	4.8
3	D	160	GLU	4.8
3	D	137	THR	4.8
3	D	528	GLU	4.7
3	B	791	TYR	4.7
1	K	8	DT	4.7
3	A	514	LEU	4.7
3	D	511	ASP	4.7
3	B	824	VAL	4.7
3	B	793	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
3	B	505	ASN	4.6
3	B	298	LEU	4.6
3	B	863	LEU	4.6
3	B	504	HIS	4.6
3	B	538	LEU	4.6
3	D	164	ILE	4.6
3	A	530	ILE	4.5
3	B	792	ASP	4.5
3	B	822	PRO	4.5
3	B	838	GLY	4.5
3	B	526	ILE	4.5
2	H	108	DT	4.5
3	B	160	GLU	4.5
3	A	253	ILE	4.4
3	B	785	ALA	4.4
3	B	861	ASP	4.4
3	D	517	ASP	4.4
1	K	1	DC	4.4
3	A	497	GLU	4.4
3	B	260	ARG	4.4
3	D	241	ARG	4.3
3	B	802	PRO	4.3
3	B	288	TYR	4.3
3	D	114	ASP	4.3
3	D	253	ILE	4.3
3	D	120	PRO	4.3
3	B	851	GLY	4.3
3	B	184	ASP	4.3
3	D	131	HIS	4.3
3	D	207	GLN	4.3
3	B	790	LYS	4.3
3	B	128	GLN	4.3
1	K	13	DG	4.2
3	D	488	TYR	4.2
3	B	521	ASP	4.2
3	D	255	ASN	4.2
3	D	188	TYR	4.2
3	D	180	SER	4.2
3	D	162	TRP	4.2
3	B	866	MET	4.2
3	C	256	MET	4.2
3	D	823	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	293	ILE	4.1
3	B	815	ILE	4.1
3	A	254	GLU	4.1
3	D	16	PHE	4.1
3	D	340	PHE	4.1
3	A	508	LEU	4.1
1	K	14	DC	4.1
3	D	829	LYS	4.0
3	B	192	ASP	4.0
3	B	827	GLY	4.0
3	D	268	ILE	4.0
3	B	797	PRO	4.0
3	D	192	ASP	4.0
3	B	804	HIS	4.0
3	C	530	ILE	4.0
3	D	546	GLN	4.0
3	D	547	ARG	3.9
3	D	252	VAL	3.9
3	D	267	GLY	3.9
3	D	482	ARG	3.9
3	A	504	HIS	3.9
3	B	856	ASP	3.9
3	D	44	SER	3.9
3	A	541	MET	3.9
3	D	537	SER	3.9
2	H	105	DC	3.9
3	D	543	PHE	3.9
3	B	512	GLU	3.8
3	B	155	PRO	3.8
3	D	200	GLU	3.8
3	C	511	ASP	3.8
3	D	791	TYR	3.8
3	B	157	GLY	3.8
3	D	169	LYS	3.8
3	B	540	GLU	3.8
3	D	245	HIS	3.8
1	K	7	DA	3.8
3	D	297	GLU	3.8
3	A	536	LYS	3.7
1	K	15	DC	3.7
3	D	334	ILE	3.7
3	D	393	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
3	B	1	MET	3.7
3	A	903	PHE	3.7
3	D	280	PHE	3.7
3	D	129	ALA	3.7
3	D	323	TYR	3.7
3	D	130	LYS	3.7
1	G	1	DC	3.6
2	L	103	DG	3.6
3	D	66	ARG	3.6
3	D	793	VAL	3.6
3	B	156	TYR	3.6
3	D	139	TYR	3.6
2	H	107	DG	3.6
3	B	508	LEU	3.6
3	D	384	ARG	3.6
2	L	101	DG	3.5
3	D	277	TYR	3.5
3	B	518	TYR	3.5
3	A	1	MET	3.5
3	D	26	GLU	3.5
3	A	500	LYS	3.5
3	B	517	ASP	3.5
3	D	156	TYR	3.5
3	D	152	LEU	3.5
3	D	514	LEU	3.5
3	B	828	GLU	3.4
3	D	828	GLU	3.4
3	D	553	MET	3.4
3	D	21	ASP	3.4
3	D	296	PHE	3.4
3	D	784	SER	3.4
3	B	303	LEU	3.4
3	A	537	SER	3.4
3	A	502	ALA	3.4
3	B	121	ASP	3.4
1	G	8	DT	3.4
3	D	238	THR	3.4
3	B	253	ILE	3.4
3	B	522	PHE	3.4
3	D	527	LYS	3.4
3	B	542	LEU	3.4
3	D	824	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	11	DC	3.4
3	D	284	ASN	3.4
3	D	112	ASN	3.3
3	D	48	LYS	3.3
3	B	837	GLU	3.3
3	B	544	ARG	3.3
3	C	257	TYR	3.3
2	H	113	DC	3.3
3	D	286	PRO	3.3
3	D	338	ARG	3.3
3	B	808	ILE	3.3
3	D	73	LYS	3.3
3	D	107	LYS	3.3
3	D	24	GLY	3.3
3	D	799	PRO	3.3
3	D	508	LEU	3.2
3	D	127	SER	3.2
3	D	153	ASN	3.2
3	D	259	SER	3.2
3	D	509	SER	3.2
2	H	106	DT	3.2
3	B	519	ARG	3.2
3	B	172	GLU	3.2
3	C	111	ALA	3.2
3	C	254	GLU	3.2
3	D	769	LYS	3.2
3	B	258	GLY	3.2
3	B	842	GLY	3.2
3	B	234	PHE	3.2
3	B	259	SER	3.2
2	L	105	DC	3.2
3	D	545	ALA	3.2
3	A	513	PRO	3.2
3	D	150	ASP	3.1
3	D	785	ALA	3.1
3	B	787	ASN	3.1
3	B	117	VAL	3.1
3	D	819	ILE	3.1
3	D	266	PHE	3.1
3	B	503	LEU	3.1
3	B	532	LYS	3.1
3	B	252	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	D	219	GLU	3.1
3	D	345	LEU	3.1
3	B	524	ASP	3.1
3	D	128	GLN	3.1
3	D	161	GLU	3.1
3	D	500	LYS	3.1
3	A	522	PHE	3.1
3	C	112	ASN	3.1
3	D	217	ASN	3.1
3	B	545	ALA	3.1
3	D	574	TRP	3.0
3	D	281	SER	3.0
1	K	12	DA	3.0
3	B	803	PHE	3.0
3	D	212	ILE	3.0
3	D	344	SER	3.0
3	D	11	ILE	3.0
3	A	512	GLU	3.0
3	D	113	PHE	3.0
3	D	92	TYR	3.0
3	C	213	LEU	3.0
3	D	392	PRO	3.0
3	D	356	GLN	3.0
3	A	112	ASN	3.0
3	B	296	PHE	3.0
3	B	831	TYR	3.0
3	D	519	ARG	3.0
3	D	173	GLN	3.0
3	D	446	VAL	3.0
3	D	288	TYR	2.9
3	D	696	LYS	2.9
3	B	826	GLU	2.9
3	C	612	GLU	2.9
3	B	523	SER	2.9
3	D	147	TYR	2.9
3	D	313	ARG	2.9
3	D	271	LEU	2.9
3	D	516	VAL	2.9
3	D	837	GLU	2.9
3	B	285	GLN	2.9
3	A	544	ARG	2.9
3	B	294	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	B	543	PHE	2.9
3	C	1	MET	2.9
3	D	330	ARG	2.9
3	D	820	ASP	2.9
3	D	292	TYR	2.9
3	C	513	PRO	2.8
3	B	292	TYR	2.8
3	D	136	ILE	2.8
3	A	511	ASP	2.8
3	D	612	GLU	2.8
3	B	320	TYR	2.8
3	D	329	TYR	2.8
3	A	857	LEU	2.8
3	D	298	LEU	2.8
3	A	518	TYR	2.8
3	B	277	TYR	2.8
2	L	104	DG	2.8
3	B	315	SER	2.8
3	D	3	GLU	2.8
3	D	811	TYR	2.8
3	A	135	ALA	2.8
3	C	500	LYS	2.8
3	D	471	VAL	2.7
3	A	137	THR	2.7
3	D	25	ARG	2.7
3	A	115	ILE	2.7
3	B	174	GLY	2.7
3	B	497	GLU	2.7
3	D	134	ASP	2.7
1	G	13	DG	2.7
3	C	543	PHE	2.7
3	D	213	LEU	2.7
3	D	495	ASN	2.7
3	D	857	LEU	2.7
3	C	498	ILE	2.7
3	D	240	LYS	2.7
3	D	542	LEU	2.7
3	A	547	ARG	2.7
3	D	211	VAL	2.7
3	D	23	ASN	2.7
3	D	320	TYR	2.7
3	C	260	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	110	VAL	2.7
3	D	283	THR	2.7
3	A	113	PHE	2.6
3	B	280	PHE	2.6
3	D	544	ARG	2.6
3	D	171	GLN	2.6
3	C	253	ILE	2.6
1	E	1	DC	2.6
3	B	120	PRO	2.6
3	D	548	THR	2.6
3	C	512	GLU	2.6
3	D	484	GLU	2.6
3	D	570	LEU	2.6
3	B	868	TYR	2.6
3	D	233	ILE	2.6
3	D	389	GLN	2.6
3	D	234	PHE	2.6
3	D	795	GLY	2.6
3	A	283	THR	2.6
3	B	900	MET	2.6
3	C	488	TYR	2.6
3	D	185	LYS	2.6
3	B	134	ASP	2.6
3	B	549	GLU	2.6
3	B	556	GLN	2.5
3	C	586	ILE	2.5
3	D	20	ILE	2.5
3	D	302	LYS	2.5
3	D	790	LYS	2.5
3	B	731	GLU	2.5
3	B	843	ASP	2.5
2	L	110	DA	2.5
3	D	355	ILE	2.5
3	A	524	ASP	2.5
3	D	175	GLY	2.5
3	D	348	GLY	2.5
3	D	172	GLU	2.5
3	B	135	ALA	2.5
3	C	110	VAL	2.5
3	D	303	LEU	2.5
3	D	331	VAL	2.5
3	D	221	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	255	ASN	2.5
3	D	705	LYS	2.5
3	D	851	GLY	2.5
3	D	216	TRP	2.5
3	D	354	GLN	2.5
3	C	192	ASP	2.5
3	C	301	GLY	2.5
3	B	506	PRO	2.4
3	B	535	ALA	2.4
3	D	324	ASN	2.4
3	C	527	LYS	2.4
3	A	548	THR	2.4
3	B	116	GLU	2.4
3	D	194	GLU	2.4
3	D	497	GLU	2.4
3	A	499	ILE	2.4
3	B	833	LEU	2.4
3	A	136	ILE	2.4
3	D	260	ARG	2.4
3	A	539	ASN	2.4
3	D	149	PHE	2.4
3	D	390	PRO	2.4
3	B	133	ILE	2.4
3	D	158	ASN	2.4
3	D	786	ASN	2.4
3	D	818	ASN	2.4
3	B	536	LYS	2.4
3	D	525	GLU	2.4
3	D	341	ILE	2.4
1	G	14	DC	2.3
3	B	794	GLY	2.3
3	B	321	ILE	2.3
3	D	327	ALA	2.3
3	D	29	ARG	2.3
3	D	218	VAL	2.3
3	C	900	MET	2.3
3	A	375	GLU	2.3
3	B	251	LYS	2.3
3	B	525	GLU	2.3
2	H	109	DC	2.3
3	B	895	ALA	2.3
3	D	539	ASN	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	A	793	VAL	2.3
3	C	252	VAL	2.3
3	D	650	PHE	2.3
3	D	43	GLU	2.3
3	C	902	ASP	2.3
3	D	157	GLY	2.3
3	D	538	LEU	2.3
3	B	502	ALA	2.3
3	D	535	ALA	2.3
3	B	520	PHE	2.3
3	D	309	ILE	2.3
3	D	557	ILE	2.3
3	D	700	GLY	2.3
3	D	119	SER	2.3
3	D	294	SER	2.3
3	D	193	ASN	2.2
3	B	814	ALA	2.2
3	D	222	ALA	2.2
3	C	526	ILE	2.2
1	G	5	DG	2.2
3	D	410	PHE	2.2
3	C	532	LYS	2.2
3	B	642	ARG	2.2
3	D	301	GLY	2.2
3	A	506	PRO	2.2
3	B	330	ARG	2.2
3	B	490	LEU	2.2
3	D	494	ARG	2.2
3	C	347	MET	2.2
3	A	114	ASP	2.2
1	E	2	DC	2.2
3	D	479	PHE	2.2
3	D	782	VAL	2.2
3	B	324	ASN	2.2
3	A	629	ALA	2.2
2	F	104	DG	2.2
3	D	31	VAL	2.2
3	D	490	LEU	2.2
3	D	607	GLU	2.2
3	B	511	ASP	2.2
3	B	547	ARG	2.2
3	D	489	MET	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	475	ILE	2.1
3	D	170	LEU	2.1
3	D	534	SER	2.1
3	C	528	GLU	2.1
3	D	706	LYS	2.1
3	B	853	GLU	2.1
3	D	177	GLU	2.1
3	C	901	PHE	2.1
2	L	102	DC	2.1
3	C	212	ILE	2.1
3	D	815	ILE	2.1
3	C	903	PHE	2.1
3	D	184	ASP	2.1
3	D	512	GLU	2.1
3	B	788	ILE	2.1
3	D	117	VAL	2.1
3	C	255	ASN	2.1
3	C	113	PHE	2.1
3	A	252	VAL	2.1
3	C	251	LYS	2.1
3	D	357	SER	2.0
3	D	794	GLY	2.0
3	C	107	LYS	2.0
3	B	115	ILE	2.0
3	B	850	SER	2.0
3	D	838	GLY	2.0
3	A	510	VAL	2.0
3	D	816	LYS	2.0
3	B	122	GLY	2.0
3	B	509	SER	2.0
3	D	493	GLN	2.0
3	D	683	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	5OC	E	3	20/21	0.62	0.35	148,155,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5OC	K	3	4/21	0.65	0.32	123,130,134,136	0
1	5OC	I	3	20/21	0.90	0.22	78,91,100,100	0
1	5OC	G	3	4/21	0.96	0.12	108,111,111,113	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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
4	SO4	H	2	5/5	0.81	0.22	126,128,128,130	0
4	SO4	C	907	5/5	0.87	0.20	112,115,116,120	0
4	SO4	F	3	5/5	0.90	0.17	121,121,123,124	0
4	SO4	B	907	5/5	0.93	0.32	83,85,88,88	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.