



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 05:28 PM EST

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 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

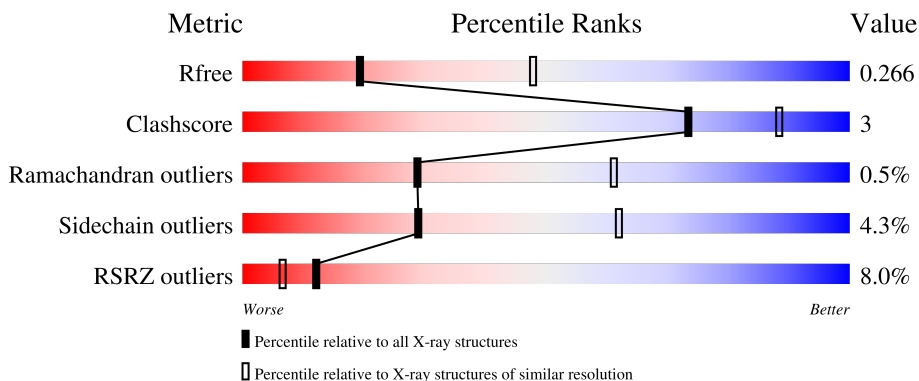
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.








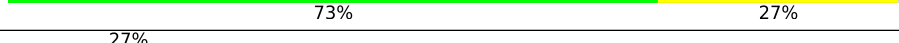

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of 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	A	906	
1	B	906	
1	C	906	
1	D	906	
2	E	18	

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Mol	Chain	Length	Quality of chain
2	G	18	 61% 33% 6%
2	I	18	 83% 17%
2	K	18	 17% 67% 28% 6%
3	F	15	 7% 80% 20%
3	H	15	 80% 13% 7%
3	J	15	 73% 27%
3	L	15	 27% 80% 20%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32383 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 protein called DNA polymerase.

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

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

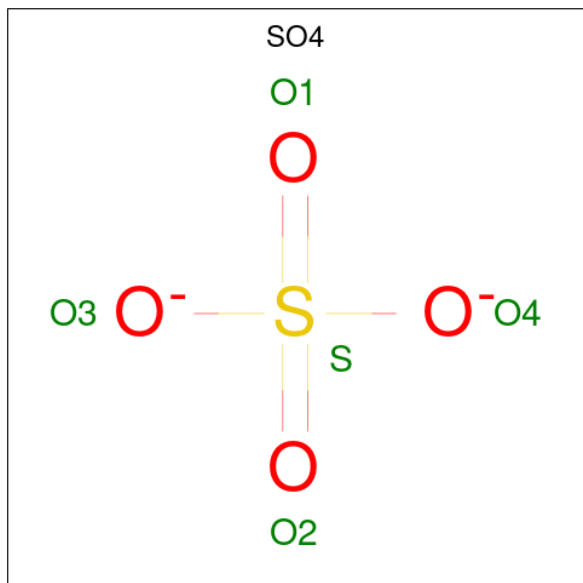
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3').

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: O<sub>4</sub>S).



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

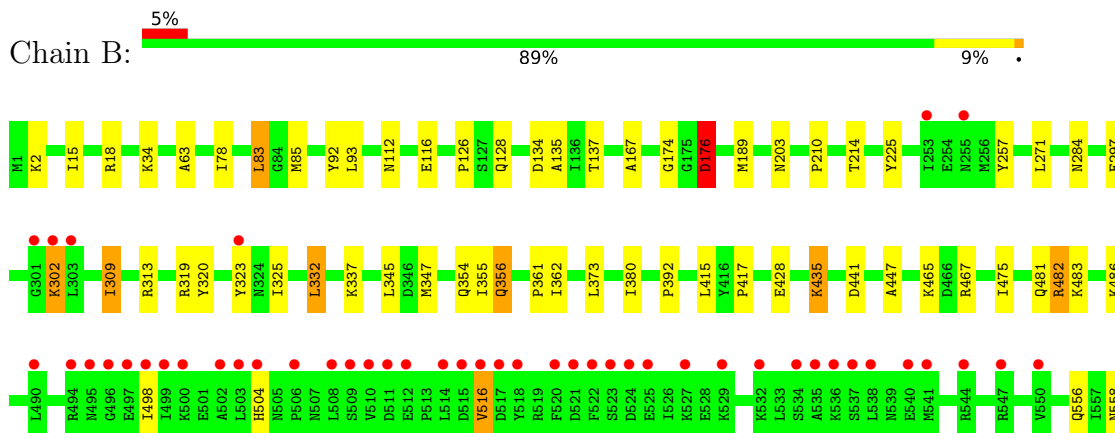
### 3 Residue-property plots

These plots are drawn for all protein, RNA, 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: DNA polymerase

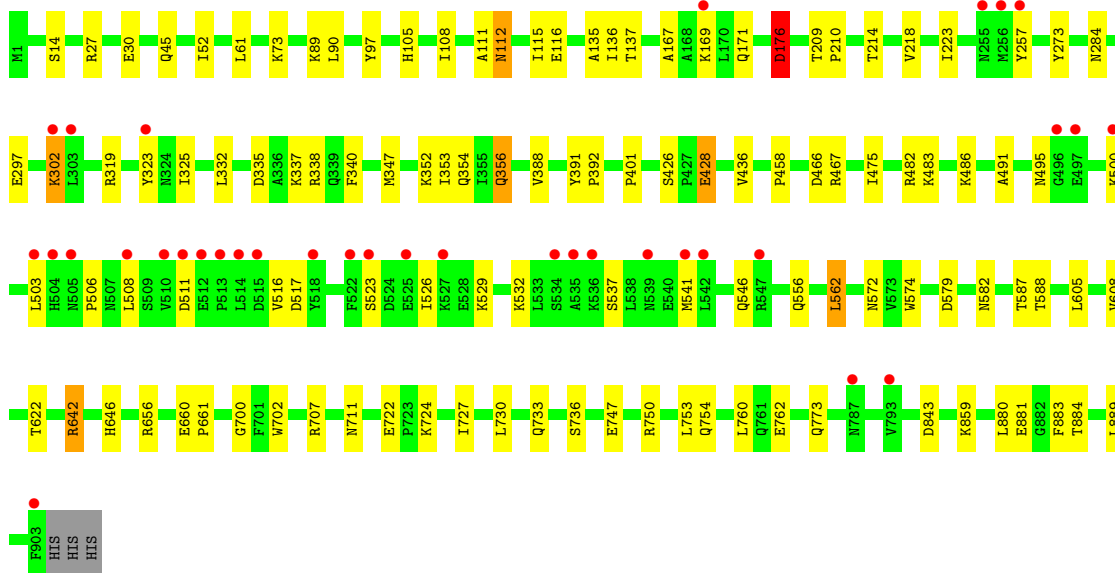
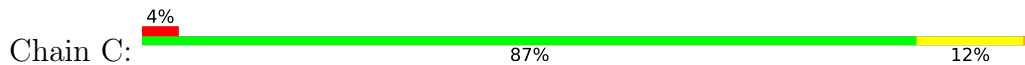


- Molecule 1: DNA polymerase

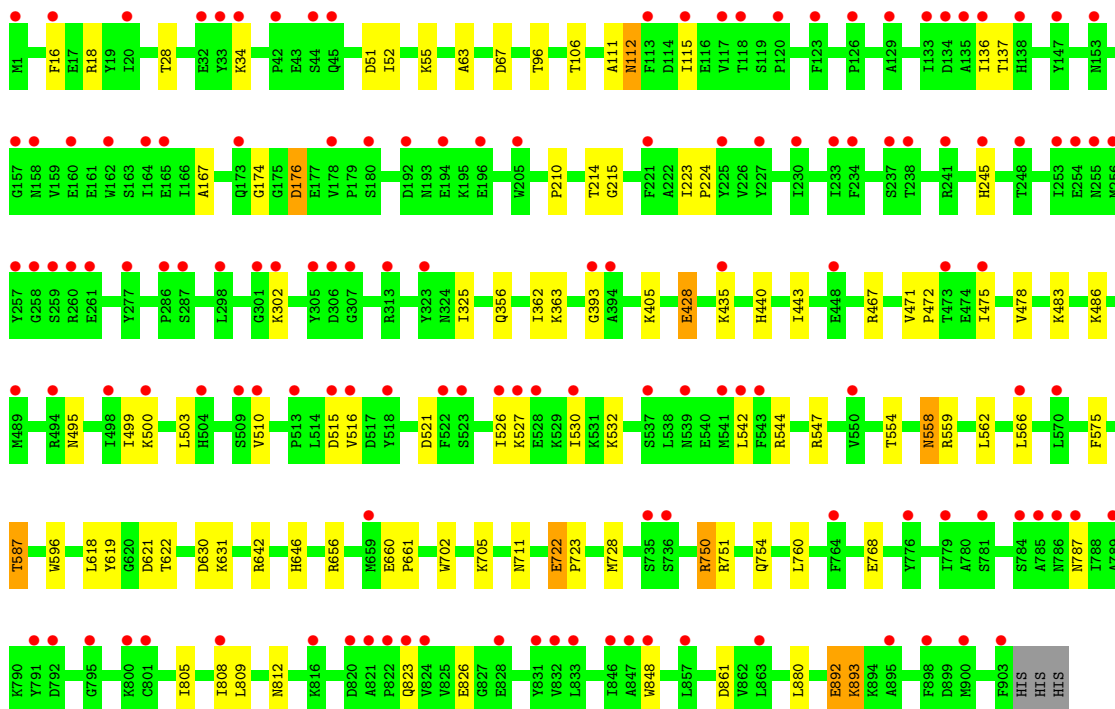
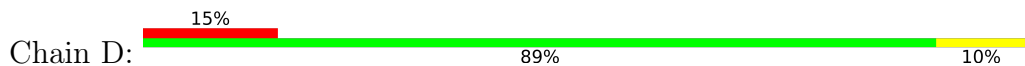




• Molecule 1: DNA polymerase




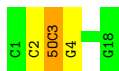
• Molecule 1: DNA polymerase





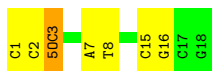
- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain E:  83% 11% 6%




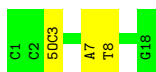
- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain G:  61% 33% 6%



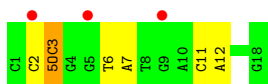
- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain I:  83% 17%




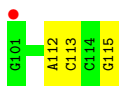
- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain K:  17% 67% 28% 6%




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

Chain F:  7% 80% 20%



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

Chain H:  80% 13% 7%




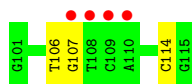
- Molecule 3: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*AP\*CP\*CP\*G)-3')

Chain J:  73% 27%



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

Chain L:  27% 80% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.6.0116, CNS	Depositor
R, $R_{free}$	0.232 , 0.281 0.220 , 0.266	Depositor DCC
$R_{free}$ test set	12706 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtrriage
Anisotropy	0.092	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtrriage'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.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 5OC

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 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7384	0	7274	59	0
1	B	7384	0	7274	50	0
1	C	7374	0	7267	46	0
1	D	7374	0	7267	39	0
2	E	366	0	201	3	0
2	G	370	0	200	6	0
2	I	366	0	201	2	0
2	K	366	0	201	4	0
3	F	304	0	170	3	0
3	H	304	0	170	2	0
3	J	304	0	170	2	0
3	L	304	0	170	3	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	4	0
5	B	71	0	0	0	0
5	C	39	0	0	0	0
5	D	10	0	0	1	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	30565	207	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 3.

All (207) 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:D:112:ASN:HB3	1:D:214:THR:HG23	1.45	0.94
1:A:112:ASN:HB3	1:A:214:THR:HG23	1.53	0.91
1:B:112:ASN:HB3	1:B:214:THR:HG23	1.54	0.90
1:B:361:PRO:HG2	2:G:2:DC:H5''	1.62	0.82
1:A:392:PRO:O	1:A:587:THR:HG21	1.88	0.73
1:B:392:PRO:O	1:B:587:THR:HG21	1.89	0.72
1:A:8:VAL:HG11	1:A:93:LEU:HD21	1.72	0.71
1:B:415:LEU:HD22	1:B:623:ASP:HB3	1.76	0.68
1:B:302:LYS:H	1:B:302:LYS:HD2	1.60	0.66
1:C:90:LEU:HD11	1:C:353:ILE:HG22	1.79	0.65
1:C:112:ASN:HB3	1:C:214:THR:HG23	1.79	0.65
1:C:482:ARG:HE	1:C:556:GLN:HE21	1.45	0.64
1:B:642:ARG:HE	1:B:646:HIS:CE1	2.14	0.64
1:A:655:ALA:O	1:A:660:GLU:HG2	1.98	0.64
1:A:171:GLN:HE21	1:A:319:ARG:HH22	1.45	0.63
1:B:656:ARG:HA	1:B:660:GLU:HG3	1.80	0.63
1:A:52:ILE:HD12	1:A:428:GLU:HG3	1.78	0.63
1:A:170:LEU:H	1:A:173:GLN:HE21	1.47	0.62
1:D:18:ARG:HG2	1:D:28:THR:HG22	1.81	0.62
1:D:656:ARG:HA	1:D:660:GLU:HG3	1.81	0.62
1:C:347:MET:HE3	1:C:562:LEU:HD13	1.82	0.62
1:B:116:GLU:HB2	1:B:135:ALA:HB3	1.80	0.61
1:C:167:ALA:HA	1:C:176:ASP:HB2	1.81	0.61
1:C:707:ARG:HD2	2:I:7:DA:H4'	1.83	0.60
1:A:412:LEU:HD13	1:A:415:LEU:HD13	1.83	0.59
1:C:572:ASN:HD22	1:C:574:TRP:H	1.51	0.58
1:C:171:GLN:HE21	1:C:319:ARG:HH22	1.48	0.58
1:C:656:ARG:HA	1:C:660:GLU:HG3	1.85	0.58
1:D:137:THR:HG21	1:D:325:ILE:HA	1.83	0.58
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.85	0.58
1:D:544:ARG:HA	1:D:547:ARG:HB3	1.84	0.58
1:D:34:LYS:HE3	1:D:63:ALA:HA	1.85	0.57
1:B:711:ASN:HD21	1:B:754:GLN:HE21	1.53	0.57
1:D:892:GLU:O	1:D:893:LYS:HB2	2.04	0.57
1:D:516:VAL:HG21	1:D:526:ILE:HG21	1.86	0.56
1:A:57:CYS:HB3	5:A:923:HOH:O	2.04	0.56
1:B:707:ARG:HH22	1:B:731:GLU:CD	2.09	0.56
1:C:115:ILE:HG22	1:C:136:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ALA:HA	1:D:176:ASP:HB2	1.88	0.56
1:A:27:ARG:HH21	1:B:189:MET:HB3	1.71	0.55
1:B:655:ALA:O	1:B:660:GLU:HG2	2.07	0.55
1:C:660:GLU:HB2	1:C:661:PRO:HD3	1.89	0.55
1:D:711:ASN:HD21	1:D:754:GLN:HE21	1.55	0.54
1:B:319:ARG:HD2	1:B:323:TYR:CE1	2.43	0.54
1:C:711:ASN:HD21	1:C:754:GLN:HE21	1.56	0.54
1:A:711:ASN:HD21	1:A:754:GLN:HE21	1.55	0.54
1:B:486:LYS:HG2	1:B:556:GLN:HG3	1.89	0.54
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.89	0.53
1:A:738:PRO:O	1:A:742:GLN:HB2	2.08	0.53
1:C:572:ASN:ND2	1:C:574:TRP:H	2.06	0.53
1:D:554:THR:O	1:D:558:ASN:HB2	2.09	0.53
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.90	0.53
1:D:111:ALA:HB3	1:D:210:PRO:HB3	1.91	0.53
2:G:15:DC:H2'	2:G:16:DG:C8	2.44	0.53
1:B:112:ASN:HB3	1:B:214:THR:CG2	2.35	0.53
1:D:440:HIS:HA	1:D:443:ILE:HD12	1.91	0.53
1:B:660:GLU:HB2	1:B:661:PRO:HD3	1.92	0.52
1:C:112:ASN:HB3	1:C:214:THR:CG2	2.40	0.52
1:C:491:ALA:O	1:C:495:ASN:HB2	2.10	0.52
1:C:319:ARG:HD2	1:C:323:TYR:CE1	2.46	0.51
1:A:112:ASN:HD21	1:A:332:LEU:HD11	1.76	0.51
1:C:97:TYR:O	1:C:352:LYS:HE2	2.10	0.51
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.92	0.51
1:B:167:ALA:HA	1:B:176:ASP:HB2	1.92	0.51
1:C:302:LYS:H	1:C:302:LYS:HD2	1.75	0.51
3:J:102:DC:H2''	3:J:103:DG:C8	2.45	0.51
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.94	0.50
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.94	0.50
1:B:126:PRO:HA	1:B:225:TYR:CD2	2.46	0.50
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:655:ALA:HA	1:A:659:MET:HB2	1.94	0.49
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.94	0.49
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.13	0.49
1:B:83:LEU:HD23	1:B:83:LEU:H	1.78	0.49
1:C:503:LEU:HA	1:C:506:PRO:HG3	1.93	0.49
1:A:101:ILE:HD12	1:A:352:LYS:HG2	1.95	0.49
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.95	0.49
1:B:354:GLN:HB3	1:B:356:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ASN:ND2	1:B:754:GLN:HE21	2.11	0.48
1:D:478:VAL:HG13	1:D:559:ARG:HD3	1.94	0.48
1:A:814:ALA:HB1	1:A:858:ILE:HG21	1.94	0.48
1:C:605:LEU:HA	1:C:608:VAL:HG22	1.94	0.48
1:D:728:MET:HG3	3:L:114:DC:H5''	1.95	0.48
1:B:126:PRO:HA	1:B:225:TYR:HD2	1.78	0.48
1:C:529:LYS:HD3	1:C:532:LYS:HD2	1.95	0.48
1:B:34:LYS:HE3	1:B:63:ALA:HA	1.96	0.48
1:D:500:LYS:HA	1:D:503:LEU:HB2	1.95	0.48
1:A:157:GLY:O	1:A:313:ARG:NH2	2.46	0.48
1:A:368:ILE:HD13	1:A:562:LEU:HD21	1.96	0.48
1:B:297:GLU:O	1:B:337:LYS:HE2	2.12	0.48
1:A:355:ILE:HD12	1:A:355:ILE:H	1.78	0.48
3:H:101:DG:H2''	3:H:102:DC:OP2	2.13	0.47
1:D:115:ILE:HG22	1:D:136:ILE:HG12	1.96	0.47
1:D:711:ASN:ND2	1:D:754:GLN:HE21	2.11	0.47
1:A:202:LEU:O	1:A:206:GLN:HG2	2.14	0.47
1:B:116:GLU:HB3	1:B:320:TYR:OH	2.15	0.47
1:A:350:TYR:HE1	1:A:481:GLN:HE22	1.61	0.47
1:D:809:LEU:HD23	1:D:812:ASN:HD22	1.79	0.47
1:A:364:THR:HG22	1:A:368:ILE:HD11	1.97	0.47
1:C:297:GLU:O	1:C:337:LYS:HE2	2.15	0.47
1:C:727:ILE:HG23	1:C:730:LEU:HD12	1.96	0.47
1:D:660:GLU:HB2	1:D:661:PRO:HD3	1.97	0.47
1:A:725:LEU:HD11	1:A:750:ARG:HG3	1.98	0.46
1:A:555:ALA:O	1:A:559:ARG:HG2	2.16	0.46
1:B:435:LYS:NZ	1:B:435:LYS:HA	2.31	0.46
1:D:475:ILE:HD13	1:D:566:LEU:HD22	1.97	0.46
1:A:166:ILE:HA	1:A:169:LYS:HD3	1.97	0.46
1:B:482:ARG:HH11	1:B:556:GLN:HG2	1.81	0.46
1:B:345:LEU:HD23	1:B:355:ILE:HG12	1.98	0.46
1:A:273:TYR:OH	1:A:335:ASP:HA	2.15	0.46
1:A:8:VAL:HG13	1:A:354:GLN:HE21	1.81	0.45
1:B:15:ILE:HD11	1:B:92:TYR:CZ	2.51	0.45
1:B:18:ARG:NH2	1:B:210:PRO:O	2.47	0.45
1:B:481:GLN:HB3	1:B:559:ARG:HH11	1.82	0.45
1:C:14:SER:OG	1:C:30:GLU:HG2	2.16	0.45
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
1:A:868:TYR:O	1:A:872:LEU:N	2.46	0.45
1:B:362:ILE:HG12	2:G:2:DC:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:DA:H2''	2:G:8:DT:H5'	1.99	0.45
1:C:273:TYR:OH	1:C:335:ASP:HA	2.17	0.45
2:E:3:5OC:O2	3:F:115:DG:N2	2.41	0.45
1:D:16:PHE:HB3	1:D:245:HIS:CE1	2.52	0.45
1:B:78:ILE:H	1:B:78:ILE:HG13	1.66	0.45
1:D:705:LYS:HB2	2:K:7:DA:H5'	1.97	0.45
1:D:722:GLU:HG3	1:D:723:PRO:HD2	1.99	0.44
1:A:642:ARG:H	1:A:642:ARG:HG2	1.59	0.44
1:B:134:ASP:HB2	1:B:313:ARG:NH1	2.32	0.44
1:C:579:ASP:HB3	1:C:582:ASN:HB2	1.99	0.44
1:C:711:ASN:ND2	1:C:754:GLN:HE21	2.15	0.44
1:A:38:PHE:HB3	5:A:923:HOH:O	2.17	0.44
1:A:745:LEU:HD22	1:A:883:PHE:HE2	1.82	0.44
1:C:218:VAL:HG22	1:C:223:ILE:HG13	2.00	0.44
1:D:393:GLY:HA2	1:D:587:THR:HG21	1.99	0.44
1:B:15:ILE:C	1:B:15:ILE:HD12	2.38	0.44
1:B:309:ILE:H	1:B:309:ILE:HG13	1.56	0.44
1:C:642:ARG:HH11	1:C:646:HIS:CE1	2.36	0.44
1:C:747:GLU:OE2	1:C:750:ARG:NH1	2.51	0.44
1:D:362:ILE:HG23	1:D:575:PHE:HD1	1.83	0.44
1:A:482:ARG:HH11	1:A:556:GLN:HG2	1.83	0.44
1:A:711:ASN:ND2	1:A:754:GLN:HE21	2.16	0.44
1:A:115:ILE:HG22	1:A:136:ILE:HG12	1.99	0.43
1:A:848:TRP:HB2	1:A:849:PRO:HD2	1.99	0.43
1:B:572:ASN:ND2	1:B:574:TRP:H	2.15	0.43
1:D:750:ARG:HH12	1:D:751:ARG:HG3	1.83	0.43
2:K:2:DC:H2'	2:K:3:5OC:H6	2.00	0.43
1:A:449:ARG:HA	1:A:450:PRO:HD3	1.89	0.43
1:D:52:ILE:HD12	1:D:428:GLU:HG3	2.00	0.43
1:C:354:GLN:HB3	1:C:356:GLN:OE1	2.19	0.43
1:A:52:ILE:HB	1:A:428:GLU:HG2	2.00	0.43
1:A:736:SER:OG	3:F:112:DA:H5''	2.19	0.43
1:D:642:ARG:HH21	1:D:646:HIS:CE1	2.37	0.43
1:D:495:ASN:O	1:D:499:ILE:HG12	2.19	0.43
1:A:313:ARG:HD2	5:A:930:HOH:O	2.19	0.43
1:A:599:ARG:HH12	1:A:600:LYS:HE2	1.84	0.43
2:E:2:DC:H2'	2:E:3:5OC:H6	2.01	0.42
1:B:137:THR:HG21	1:B:325:ILE:HA	2.01	0.42
1:D:805:ILE:HA	1:D:808:ILE:HD12	2.01	0.42
1:B:784:SER:HA	1:B:829:LYS:HA	2.01	0.42
1:A:441:ASP:HB3	1:A:447:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HG	1:A:340:PHE:HB3	2.00	0.42
1:C:111:ALA:HB3	1:C:210:PRO:HB3	2.00	0.42
1:B:176:ASP:OD1	1:B:176:ASP:N	2.52	0.42
1:D:499:ILE:HG21	1:D:542:LEU:HB2	2.02	0.42
1:B:663:ILE:HG21	1:B:683:MET:HB3	2.02	0.42
1:C:52:ILE:HD12	1:C:428:GLU:HG3	2.02	0.42
1:C:884:THR:HB	1:C:889:LEU:O	2.20	0.42
1:A:105:HIS:HA	1:A:108:ILE:HD12	2.02	0.42
1:A:303:LEU:HG	1:A:323:TYR:CZ	2.55	0.42
1:A:747:GLU:OE2	1:A:750:ARG:NH1	2.53	0.42
1:B:373:LEU:HD12	1:B:380:ILE:HG22	2.02	0.41
1:C:105:HIS:HA	1:C:108:ILE:HD12	2.02	0.41
1:B:271:LEU:HD11	1:B:355:ILE:CG2	2.51	0.41
2:K:6:DT:H2''	2:K:7:DA:H8	1.84	0.41
1:B:85:MET:HA	1:B:380:ILE:HD11	2.01	0.41
2:G:7:DA:H2'	2:G:8:DT:C6	2.55	0.41
1:C:176:ASP:OD1	1:C:319:ARG:HD3	2.20	0.41
1:C:537:SER:O	1:C:541:MET:HG2	2.20	0.41
1:D:527:LYS:O	1:D:530:ILE:HG22	2.19	0.41
1:A:734:LYS:HG2	3:F:113:DC:H5'	2.01	0.41
1:C:338:ARG:HB3	1:C:340:PHE:CZ	2.55	0.41
1:B:417:PRO:HB3	1:B:475:ILE:HG12	2.02	0.41
1:C:137:THR:HG21	1:C:325:ILE:HA	2.02	0.41
1:A:302:LYS:H	1:A:302:LYS:HD2	1.85	0.41
1:C:736:SER:HB3	3:J:112:DA:H5''	2.03	0.41
1:D:619:TYR:CE2	1:D:621:ASP:HB2	2.56	0.41
1:A:862:VAL:C	1:A:864:HIS:H	2.22	0.41
1:C:209:THR:HA	1:C:210:PRO:HD3	1.86	0.41
1:C:523:SER:HB3	1:C:526:ILE:HG12	2.03	0.41
1:C:700:GLY:HA2	1:C:753:LEU:HD22	2.03	0.41
1:A:345:LEU:HD23	1:A:355:ILE:HG12	2.03	0.41
2:E:3:5OC:H2'	2:E:4:DG:C8	2.56	0.41
1:B:112:ASN:HD21	1:B:332:LEU:CD1	2.34	0.41
1:B:347:MET:CE	1:B:558:ASN:HD22	2.32	0.41
1:D:51:ASP:HB2	5:D:910:HOH:O	2.21	0.41
1:D:223:ILE:N	1:D:224:PRO:HD2	2.36	0.41
1:A:482:ARG:HD2	1:A:556:GLN:HG2	2.02	0.41
1:A:663:ILE:HG21	1:A:683:MET:HB3	2.01	0.41
1:C:587:THR:HG22	1:C:588:THR:N	2.35	0.41
1:B:112:ASN:HD21	1:B:332:LEU:HD11	1.85	0.40
1:B:465:LYS:HE2	1:B:677:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3:5OC:O2	3:H:115:DG:N2	2.45	0.40
1:D:728:MET:HG3	3:L:114:DC:OP1	2.20	0.40
1:A:16:PHE:HB3	1:A:245:HIS:CE1	2.57	0.40
1:A:137:THR:HG21	1:A:325:ILE:HA	2.04	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 [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	
1	A	902/906 (100%)	858 (95%)	41 (4%)	3 (0%)	41	72
1	B	902/906 (100%)	859 (95%)	39 (4%)	4 (0%)	34	66
1	C	901/906 (99%)	864 (96%)	32 (4%)	5 (1%)	25	56
1	D	901/906 (99%)	855 (95%)	41 (5%)	5 (1%)	25	56
All	All	3606/3624 (100%)	3436 (95%)	153 (4%)	17 (0%)	29	61

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

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Mol	Chain	Res	Type
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 [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	
1	A	801/803 (100%)	763 (95%)	38 (5%)	26	59
1	B	801/803 (100%)	773 (96%)	28 (4%)	36	70
1	C	800/803 (100%)	760 (95%)	40 (5%)	24	56
1	D	800/803 (100%)	767 (96%)	33 (4%)	30	64
All	All	3202/3212 (100%)	3063 (96%)	139 (4%)	29	62

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	112	ASN
1	A	131	HIS
1	A	153	ASN
1	A	158	ASN
1	A	171	GLN
1	A	173	GLN
1	A	207	GLN
1	A	245	HIS
1	A	284	ASN
1	A	285	GLN
1	A	354	GLN
1	A	389	GLN
1	A	481	GLN
1	A	572	ASN
1	A	675	ASN
1	A	678	GLN
1	A	711	ASN
1	B	40	HIS
1	B	112	ASN
1	B	128	GLN
1	B	131	HIS
1	B	153	ASN
1	B	158	ASN
1	B	203	ASN
1	B	284	ASN
1	B	285	GLN
1	B	324	ASN
1	B	481	GLN
1	B	558	ASN
1	B	572	ASN
1	B	646	HIS
1	B	675	ASN
1	B	678	GLN
1	B	711	ASN
1	B	787	ASN
1	B	818	ASN
1	C	40	HIS
1	C	45	GLN
1	C	112	ASN
1	C	131	HIS
1	C	153	ASN

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Mol	Chain	Res	Type
1	C	158	ASN
1	C	171	GLN
1	C	173	GLN
1	C	203	ASN
1	C	207	GLN
1	C	284	ASN
1	C	285	GLN
1	C	539	ASN
1	C	556	GLN
1	C	558	ASN
1	C	572	ASN
1	C	646	HIS
1	C	675	ASN
1	C	711	ASN
1	C	773	GLN
1	D	131	HIS
1	D	158	ASN
1	D	173	GLN
1	D	207	GLN
1	D	285	GLN
1	D	481	GLN
1	D	539	ASN
1	D	556	GLN
1	D	675	ASN
1	D	711	ASN
1	D	812	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	I	3	2	18,21,22	0.36	0	25,30,33	1.16	1 (4%)
2	5OC	G	3	2	18,21,22	0.39	0	25,30,33	1.16	1 (4%)
2	5OC	E	3	2	18,21,22	0.36	0	25,30,33	1.15	1 (4%)
2	5OC	K	3	2	18,21,22	0.37	0	25,30,33	1.16	1 (4%)

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	I	3	2	-	0/7/21/22	0/2/2/2
2	5OC	G	3	2	-	0/7/21/22	0/2/2/2
2	5OC	E	3	2	-	0/7/21/22	0/2/2/2
2	5OC	K	3	2	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	5OC	O5-C5-C4	5.40	122.57	114.43
2	G	3	5OC	O5-C5-C4	5.38	122.55	114.43
2	I	3	5OC	O5-C5-C4	5.36	122.51	114.43
2	E	3	5OC	O5-C5-C4	5.35	122.50	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	5OC	1	0
2	E	3	5OC	3	0
2	K	3	5OC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	G	19	-	4,4,4	0.36	0	6,6,6	0.08	0
4	SO4	E	19	-	4,4,4	0.35	0	6,6,6	0.10	0
4	SO4	K	19	-	4,4,4	0.34	0	6,6,6	0.04	0
4	SO4	I	19	-	4,4,4	0.35	0	6,6,6	0.06	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	K	1
2	I	1
2	G	1
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	3:5OC	OP2	4:DG	P	6.52
1	I	3:5OC	OP2	4:DG	P	6.37
1	G	3:5OC	OP2	4:DG	P	6.30
1	E	3:5OC	OP2	4:DG	P	6.29

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	904/906 (99%)	0.53	73 (8%) 12 6	48, 84, 166, 266	0
1	B	904/906 (99%)	0.32	48 (5%) 26 17	35, 63, 156, 343	0
1	C	903/906 (99%)	0.28	35 (3%) 39 29	38, 68, 137, 233	0
1	D	903/906 (99%)	0.89	136 (15%) 2 1	69, 115, 201, 249	0
2	E	17/18 (94%)	-0.04	0 100 100	69, 88, 133, 141	0
2	G	17/18 (94%)	-0.43	0 100 100	37, 52, 71, 72	0
2	I	17/18 (94%)	-0.31	0 100 100	50, 57, 78, 81	0
2	K	17/18 (94%)	1.19	3 (17%) 1 1	87, 123, 145, 148	0
3	F	15/15 (100%)	0.09	1 (6%) 17 10	65, 97, 160, 162	0
3	H	15/15 (100%)	-0.44	0 100 100	40, 53, 77, 82	0
3	J	15/15 (100%)	-0.31	0 100 100	45, 66, 98, 100	0
3	L	15/15 (100%)	1.73	4 (26%) 0 0	104, 145, 162, 163	0
All	All	3742/3756 (99%)	0.49	300 (8%) 12 6	35, 82, 181, 343	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	MET	12.6
1	D	135	ALA	12.4
1	B	510	VAL	10.1
1	D	847	ALA	9.5
1	D	789	ALA	9.1
1	B	499	ILE	8.4
1	A	256	MET	8.0
1	D	257	TYR	7.2
1	B	302	LYS	7.2
1	A	257	TYR	7.2
1	A	770	GLU	7.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	511	ASP	6.6
1	C	512	GLU	6.5
1	B	508	LEU	6.4
1	A	507	ASN	6.0
1	B	895	ALA	5.8
1	B	502	ALA	5.8
1	C	503	LEU	5.8
1	B	509	SER	5.7
1	A	847	ALA	5.5
1	A	500	LYS	5.5
1	B	516	VAL	5.5
1	D	254	GLU	5.5
1	A	799	PRO	5.4
1	D	253	ILE	5.4
1	D	823	GLN	5.4
1	A	523	SER	5.4
1	C	500	LYS	5.3
1	A	528	GLU	5.3
1	D	165	GLU	5.1
3	L	108	DT	5.0
1	A	504	HIS	5.0
1	B	498	ILE	4.9
1	D	786	ASN	4.9
1	C	303	LEU	4.9
1	B	534	SER	4.8
1	D	117	VAL	4.8
1	A	862	VAL	4.8
1	A	508	LEU	4.7
1	A	537	SER	4.7
1	D	192	ASP	4.7
1	D	779	ILE	4.7
1	D	787	ASN	4.7
1	A	800	LYS	4.6
1	B	522	PHE	4.6
1	D	543	PHE	4.6
1	A	858	ILE	4.5
1	D	831	TYR	4.5
1	B	517	ASP	4.5
1	D	301	GLY	4.5
1	B	497	GLU	4.5
1	D	306	ASP	4.4
1	D	828	GLU	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	863	LEU	4.4
1	D	530	ILE	4.4
1	D	277	TYR	4.4
1	D	134	ASP	4.4
1	A	530	ILE	4.4
1	A	532	LYS	4.4
1	B	535	ALA	4.3
1	D	800	LYS	4.3
1	A	543	PHE	4.3
1	A	531	LYS	4.2
1	A	805	ILE	4.2
1	D	286	PRO	4.2
1	D	261	GLU	4.2
1	D	900	MET	4.1
1	D	513	PRO	4.1
1	A	514	LEU	4.1
1	C	535	ALA	4.1
1	D	305	TYR	4.1
1	A	37	LEU	4.1
1	A	542	LEU	4.1
1	D	801	CYS	4.1
1	B	537	SER	4.0
1	D	821	ALA	4.0
1	A	301	GLY	4.0
1	B	511	ASP	4.0
1	C	508	LEU	4.0
1	D	515	ASP	4.0
1	B	536	LYS	4.0
1	A	501	GLU	4.0
1	D	255	ASN	4.0
1	C	525	GLU	3.9
1	D	795	GLY	3.9
3	L	109	DC	3.9
1	D	158	ASN	3.9
1	C	302	LYS	3.8
1	D	785	ALA	3.8
1	C	522	PHE	3.8
1	A	823	GLN	3.8
1	D	848	TRP	3.8
1	D	178	VAL	3.8
1	D	857	LEU	3.7
1	A	253	ILE	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	164	ILE	3.7
1	A	254	GLU	3.7
1	C	513	PRO	3.6
1	D	162	TRP	3.6
1	A	533	LEU	3.6
1	B	495	ASN	3.6
1	D	129	ALA	3.5
1	B	503	LEU	3.5
1	D	115	ILE	3.5
1	A	302	LYS	3.5
1	C	515	ASP	3.5
1	B	518	TYR	3.4
1	D	194	GLU	3.4
1	D	509	SER	3.4
1	A	498	ILE	3.4
1	D	160	GLU	3.4
1	D	138	HIS	3.4
1	A	496	GLY	3.4
1	B	521	ASP	3.4
1	D	500	LYS	3.4
1	D	393	GLY	3.3
1	D	824	VAL	3.3
1	D	550	VAL	3.3
1	D	298	LEU	3.3
1	B	500	LYS	3.3
1	A	535	ALA	3.3
3	L	110	DA	3.3
1	C	514	LEU	3.3
1	A	511	ASP	3.2
1	D	526	ILE	3.2
2	K	2	DC	3.2
1	C	536	LYS	3.2
1	D	259	SER	3.2
1	B	538	LEU	3.2
1	B	527	LYS	3.2
1	D	820	ASP	3.2
1	D	233	ILE	3.2
1	D	784	SER	3.1
1	D	173	GLN	3.1
1	C	541	MET	3.1
1	D	736	SER	3.1
1	A	491	ALA	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	57	CYS	3.1
1	D	120	PRO	3.0
1	D	118	THR	3.0
1	A	524	ASP	3.0
1	C	169	LYS	3.0
1	D	153	ASN	3.0
1	B	504	HIS	3.0
1	D	33	TYR	3.0
1	A	787	ASN	3.0
1	C	527	LYS	3.0
1	C	256	MET	2.9
1	D	258	GLY	2.9
1	D	504	HIS	2.9
1	C	518	TYR	2.9
1	D	44	SER	2.9
1	B	512	GLU	2.9
1	A	503	LEU	2.9
1	D	241	ARG	2.9
1	D	473	THR	2.9
1	D	225	TYR	2.9
1	C	903	PHE	2.9
1	B	541	MET	2.9
1	C	523	SER	2.8
1	D	230	ILE	2.8
1	D	808	ILE	2.8
1	B	520	PHE	2.8
1	D	113	PHE	2.8
1	C	505	ASN	2.8
1	D	302	LYS	2.8
1	A	495	ASN	2.8
1	D	45	GLN	2.8
1	D	16	PHE	2.8
1	A	819	ILE	2.7
1	A	506	PRO	2.7
1	A	82	ALA	2.7
1	B	529	LYS	2.7
1	C	323	TYR	2.7
1	A	252	VAL	2.7
1	C	534	SER	2.7
1	D	816	LYS	2.7
1	C	496	GLY	2.7
1	D	32	GLU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	539	ASN	2.7
1	A	774	LEU	2.7
1	B	496	GLY	2.7
1	D	498	ILE	2.7
1	A	846	ILE	2.7
1	D	791	TYR	2.7
1	C	497	GLU	2.6
1	B	524	ASP	2.6
1	A	518	TYR	2.6
1	D	542	LEU	2.6
1	D	42	PRO	2.6
1	D	566	LEU	2.6
2	K	5	DG	2.6
1	C	257	TYR	2.6
1	A	525	GLU	2.6
1	A	541	MET	2.6
1	D	776	TYR	2.6
1	A	785	ALA	2.6
1	D	903	PHE	2.6
1	A	49	TYR	2.6
1	D	147	TYR	2.6
1	D	260	ARG	2.6
1	D	898	PHE	2.6
1	D	20	ILE	2.5
1	D	528	GLU	2.5
1	D	123	PHE	2.5
1	C	255	ASN	2.5
1	D	245	HIS	2.5
1	B	532	LYS	2.5
1	C	504	HIS	2.5
1	A	832	VAL	2.5
1	A	255	ASN	2.5
1	D	516	VAL	2.5
1	C	793	VAL	2.5
1	D	133	ILE	2.5
1	D	659	MET	2.4
1	A	536	LYS	2.4
1	B	544	ARG	2.4
1	C	542	LEU	2.4
1	D	136	ILE	2.4
1	D	196	GLU	2.4
1	D	833	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	506	PRO	2.4
1	B	514	LEU	2.4
1	D	846	ILE	2.4
3	L	107	DG	2.4
1	D	792	ASP	2.4
1	A	534	SER	2.4
1	D	523	SER	2.4
1	A	77	ASP	2.4
1	D	735	SER	2.4
1	A	497	GLU	2.3
1	D	234	PHE	2.3
1	D	764	PHE	2.3
1	A	516	VAL	2.3
1	D	527	LYS	2.3
1	D	1	MET	2.3
1	B	323	TYR	2.3
1	A	512	GLU	2.3
1	B	255	ASN	2.3
1	C	539	ASN	2.3
1	D	34	LYS	2.3
1	B	515	ASP	2.3
1	D	541	MET	2.3
1	B	301	GLY	2.3
1	D	522	PHE	2.3
1	D	781	SER	2.3
1	B	547	ARG	2.3
1	C	787	ASN	2.2
1	B	523	SER	2.2
1	D	435	LYS	2.2
1	B	494	ARG	2.2
1	D	313	ARG	2.2
2	K	9	DG	2.2
1	A	261	GLU	2.2
1	D	895	ALA	2.2
1	D	489	MET	2.2
1	A	98	ASN	2.2
1	A	258	GLY	2.2
1	D	323	TYR	2.2
1	D	287	SER	2.2
1	D	570	LEU	2.2
1	B	253	ILE	2.2
1	D	822	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	525	GLU	2.2
1	D	180	SER	2.2
1	D	832	VAL	2.2
1	B	490	LEU	2.2
1	D	475	ILE	2.2
1	D	238	THR	2.2
1	C	547	ARG	2.2
1	A	786	ASN	2.2
1	D	248	THR	2.2
1	D	227	TYR	2.2
1	D	863	LEU	2.1
1	A	505	ASN	2.1
1	A	804	HIS	2.1
1	A	62	PHE	2.1
3	F	101	DG	2.1
1	A	833	LEU	2.1
1	D	237	SER	2.1
1	D	510	VAL	2.1
1	A	808	ILE	2.1
1	D	221	PHE	2.1
1	D	518	TYR	2.1
1	A	492	ALA	2.1
1	A	651	LEU	2.1
1	D	205	TRP	2.1
1	D	537	SER	2.1
1	D	307	GLY	2.1
1	D	448	GLU	2.1
1	D	126	PRO	2.1
1	D	157	GLY	2.0
1	B	540	GLU	2.0
1	B	550	VAL	2.0
1	B	303	LEU	2.0
1	A	52	ILE	2.0
1	A	544	ARG	2.0
1	D	394	ALA	2.0
1	C	510	VAL	2.0
1	D	494	ARG	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. 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
2	5OC	K	3	20/21	0.82	0.47	112,114,118,119	0
2	5OC	E	3	20/21	0.92	0.17	69,76,81,82	0
2	5OC	I	3	20/21	0.95	0.15	56,60,62,64	0
2	5OC	G	3	20/21	0.97	0.18	38,40,43,44	0

### 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, 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
4	SO4	E	19	5/5	0.87	0.21	99,101,101,104	0
4	SO4	K	19	5/5	0.88	0.15	126,126,126,128	0
4	SO4	G	19	5/5	0.92	0.18	77,78,81,85	0
4	SO4	I	19	5/5	0.97	0.13	84,86,87,90	0

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

There are no such residues in this entry.