



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:57 AM UTC

PDB ID : 3TAB / pdb_00003tab
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

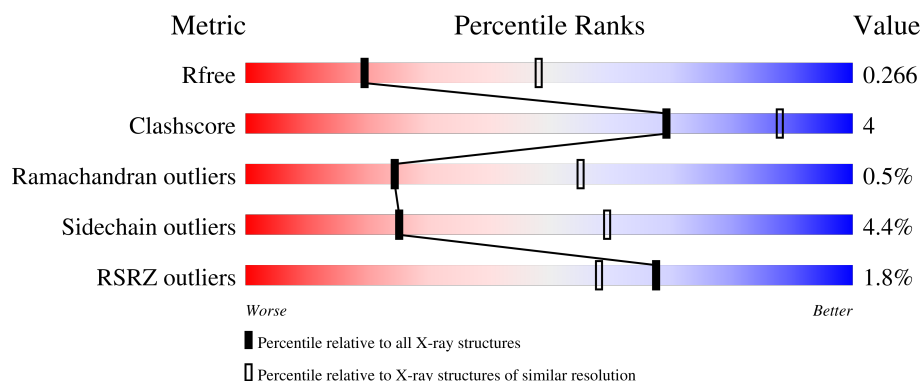
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	 67%28%6%
2	I	18	 83%17%
2	K	18	 67%28%6%
3	F	15	 80%20%
3	H	15	 80%20%
3	J	15	 73%27%
3	L	15	 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
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

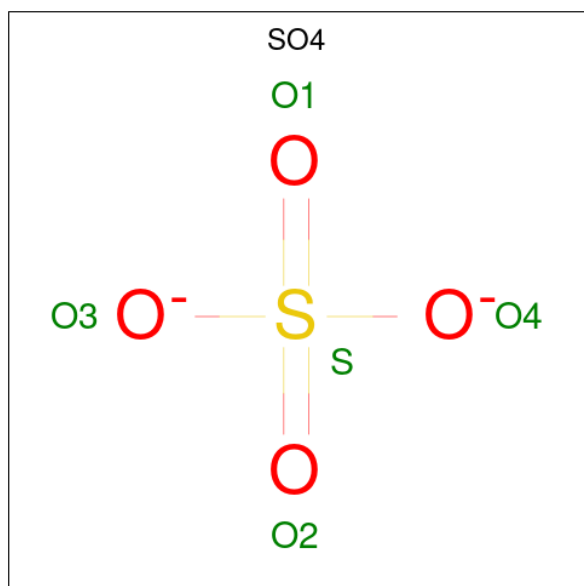
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

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 (CCD ID: 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

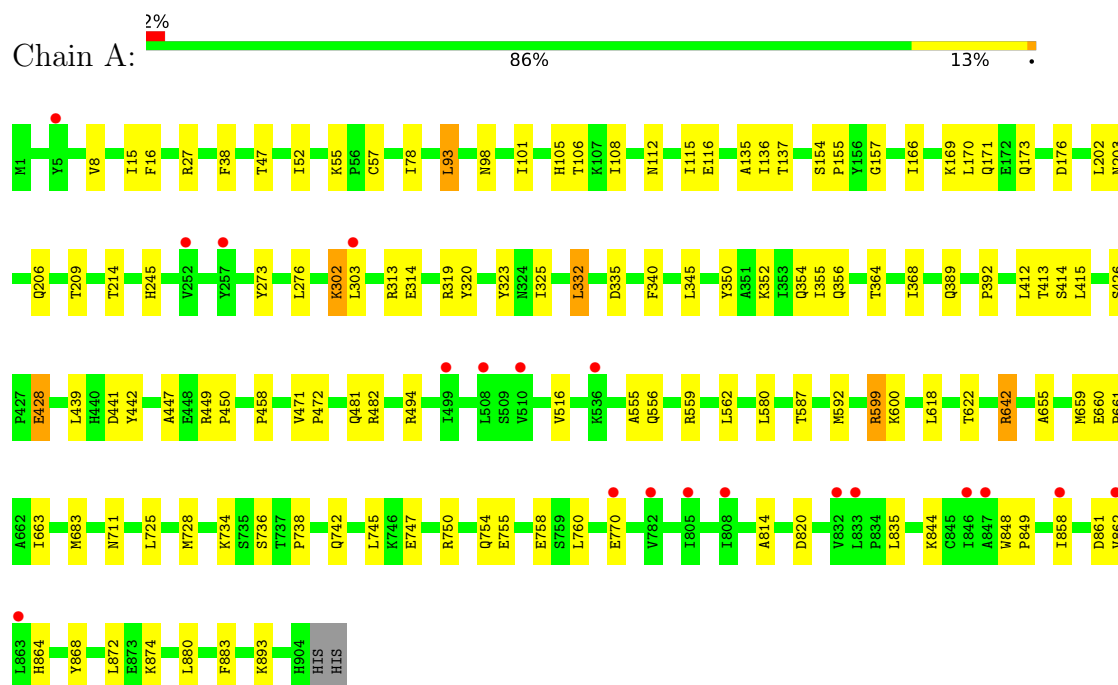
- Molecule 5 is water.

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

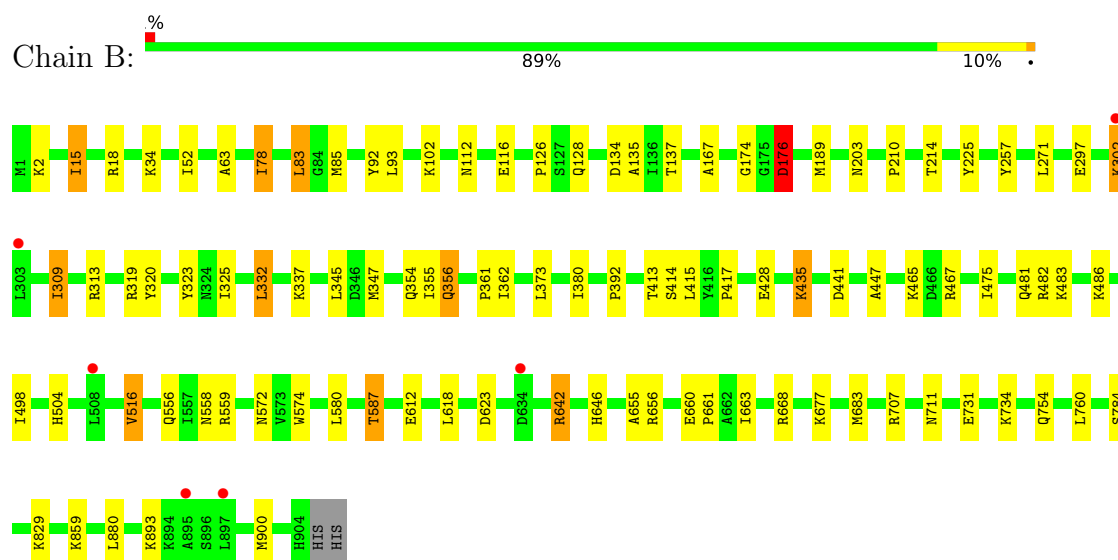
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

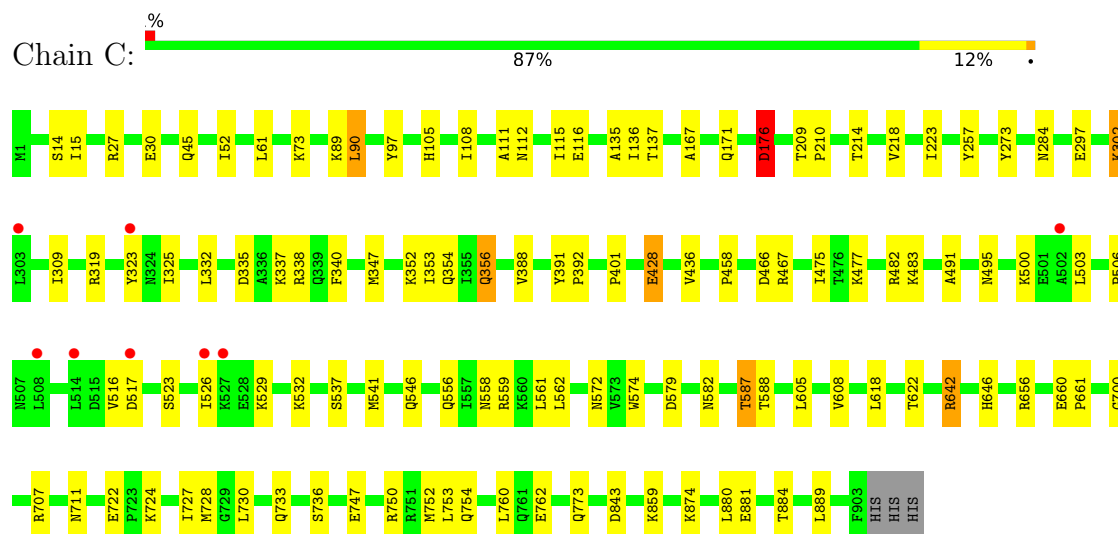
• Molecule 1: DNA polymerase



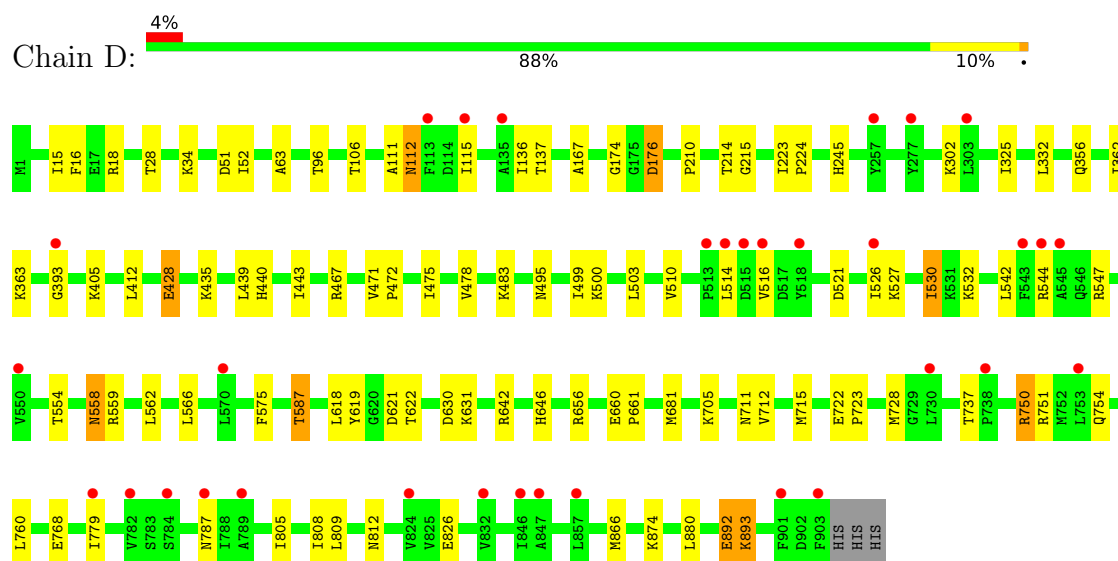
• Molecule 1: DNA polymerase



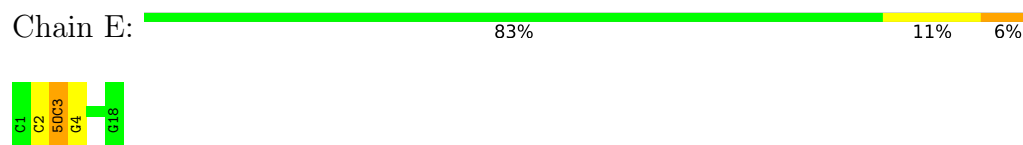
- Molecule 1: DNA polymerase



- Molecule 1: DNA polymerase

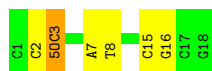


- Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')



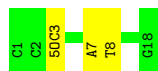
- Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')





- 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: 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: 80% 20%



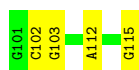
- Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain H: 80% 20%



- 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: 80% 20%



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 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.80) 99.9 (30.00-2.80)	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, CNS	Depositor
R, R_{free}	0.232 , 0.281 0.220 , 0.266	Depositor DCC
R_{free} test set	12706 reflections (9.29%)	wwPDB-VP
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 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/7566	0.76	0/10224
1	B	0.52	0/7566	0.77	0/10224
1	C	0.50	0/7555	0.75	0/10209
1	D	0.51	0/7555	0.75	0/10209
2	E	0.28	0/387	0.57	0/593
2	G	0.29	0/391	0.66	0/597
2	I	0.29	0/387	0.66	0/593
2	K	0.27	0/387	0.56	0/593
3	F	0.28	0/340	0.62	0/523
3	H	0.28	0/340	0.72	0/523
3	J	0.30	0/340	0.71	0/523
3	L	0.28	0/340	0.64	0/523
All	All	0.50	0/33154	0.75	0/45334

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7384	0	7274	53	0
1	C	7374	0	7267	49	0
1	D	7374	0	7267	42	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	3	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	1	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	220	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 (220) 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:442:TYR:HB3	1:A:592:MET:HE2	1.67	0.76
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:B:347:MET:HE2	1:B:558:ASN:HD22	1.54	0.72
1:A:8:VAL:HG11	1:A:93:LEU:HD21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:MET:HE2	1:C:558:ASN:ND2	2.11	0.65
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: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:B:707:ARG:HH22	1:B:731:GLU:CD	2.09	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:A:412:LEU:HG	1:A:683:MET:HE3	1.85	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:C:347:MET:HE2	1:C:558:ASN:HD22	1.70	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:C:115:ILE:HG22	1:C:136:ILE:HG12	1.88	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:347:MET:HE2	1:B:558:ASN:ND2	2.21	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
1:B:734:LYS:NZ	5:B:976:HOH:O	2.29	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:D:681:MET:HE2	1:D:681:MET:HA	1.93	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:C:752:MET:HE3	1:C:889:LEU:HD11	1.93	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
1:B:15:ILE:C	1:B:15:ILE:HD12	2.38	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:458:PRO:HB3	1:A:592:MET:HE3	1.95	0.47
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:A:862:VAL:C	1:A:864:HIS:H	2.22	0.47
1:D:712:VAL:HG11	1:D:715:MET:HE2	1.97	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: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:413:THR:O	1:A:414:SER:C	2.62	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:B:413:THR:O	1:B:414:SER:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:HB3	1:A:447:ALA:HB2	2.02	0.42
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:C:728:MET:HE2	3:J:115:DG:OP2	2.20	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: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: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:D:779:ILE:HD11	1:D:866:MET:HE1	2.03	0.41
1:B:112:ASN:HD21	1:B:332:LEU:HD11	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LYS:HE2	1:B:677:LYS:HA	2.03	0.40
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%)	36	66
1	B	902/906 (100%)	859 (95%)	39 (4%)	4 (0%)	30	60
1	C	901/906 (99%)	864 (96%)	32 (4%)	5 (1%)	21	51
1	D	901/906 (99%)	855 (95%)	41 (5%)	5 (1%)	21	51
All	All	3606/3624 (100%)	3436 (95%)	153 (4%)	17 (0%)	24	55

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

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Mol	Chain	Res	Type
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%)	767 (96%)	34 (4%)	26	61
1	B	801/803 (100%)	769 (96%)	32 (4%)	28	63
1	C	800/803 (100%)	758 (95%)	42 (5%)	20	52
1	D	800/803 (100%)	766 (96%)	34 (4%)	26	60
All	All	3202/3212 (100%)	3060 (96%)	142 (4%)	25	59

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	47	THR
1	A	55	LYS
1	A	78	ILE
1	A	93	LEU
1	A	98	ASN
1	A	106	THR
1	A	203	ASN
1	A	209	THR
1	A	302	LYS
1	A	314	GLU
1	A	332	LEU
1	A	356	GLN

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Mol	Chain	Res	Type
1	A	389	GLN
1	A	426	SER
1	A	428	GLU
1	A	439	LEU
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	728	MET
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	874	LYS
1	A	880	LEU
1	B	2	LYS
1	B	15	ILE
1	B	52	ILE
1	B	78	ILE
1	B	83	LEU
1	B	93	LEU
1	B	102	LYS
1	B	128	GLN
1	B	176	ASP
1	B	203	ASN
1	B	257	TYR
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	483	LYS
1	B	498	ILE
1	B	504	HIS

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Mol	Chain	Res	Type
1	B	516	VAL
1	B	580	LEU
1	B	587	THR
1	B	612	GLU
1	B	618	LEU
1	B	642	ARG
1	B	668	ARG
1	B	760	LEU
1	B	859	LYS
1	B	880	LEU
1	B	900	MET
1	C	15	ILE
1	C	27	ARG
1	C	45	GLN
1	C	61	LEU
1	C	73	LYS
1	C	89	LYS
1	C	90	LEU
1	C	176	ASP
1	C	257	TYR
1	C	284	ASN
1	C	302	LYS
1	C	309	ILE
1	C	332	LEU
1	C	356	GLN
1	C	388	VAL
1	C	428	GLU
1	C	436	VAL
1	C	467	ARG
1	C	475	ILE
1	C	477	LYS
1	C	483	LYS
1	C	500	LYS
1	C	516	VAL
1	C	517	ASP
1	C	546	GLN
1	C	559	ARG
1	C	561	LEU
1	C	562	LEU
1	C	587	THR
1	C	618	LEU
1	C	642	ARG

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Mol	Chain	Res	Type
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	874	LYS
1	C	880	LEU
1	C	881	GLU
1	D	15	ILE
1	D	96	THR
1	D	106	THR
1	D	112	ASN
1	D	302	LYS
1	D	332	LEU
1	D	356	GLN
1	D	363	LYS
1	D	405	LYS
1	D	412	LEU
1	D	428	GLU
1	D	435	LYS
1	D	439	LEU
1	D	467	ARG
1	D	483	LYS
1	D	510	VAL
1	D	514	LEU
1	D	521	ASP
1	D	530	ILE
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	737	THR
1	D	750	ARG
1	D	760	LEU
1	D	768	GLU
1	D	787	ASN

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Mol	Chain	Res	Type
1	D	826	GLU
1	D	874	LYS
1	D	880	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	64	ASN
1	A	98	ASN
1	A	112	ASN
1	A	131	HIS
1	A	158	ASN
1	A	171	GLN
1	A	173	GLN
1	A	203	ASN
1	A	207	GLN
1	A	245	HIS
1	A	284	ASN
1	A	285	GLN
1	A	354	GLN
1	A	481	GLN
1	A	495	ASN
1	A	595	GLN
1	A	606	ASN
1	A	675	ASN
1	A	678	GLN
1	A	711	ASN
1	A	733	GLN
1	B	40	HIS
1	B	112	ASN
1	B	128	GLN
1	B	153	ASN
1	B	203	ASN
1	B	245	HIS
1	B	284	ASN
1	B	285	GLN
1	B	324	ASN
1	B	386	HIS
1	B	389	GLN
1	B	440	HIS
1	B	481	GLN

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Mol	Chain	Res	Type
1	B	505	ASN
1	B	539	ASN
1	B	558	ASN
1	B	572	ASN
1	B	582	ASN
1	B	645	ASN
1	B	646	HIS
1	B	675	ASN
1	B	678	GLN
1	B	711	ASN
1	B	733	GLN
1	B	786	ASN
1	B	787	ASN
1	C	40	HIS
1	C	128	GLN
1	C	131	HIS
1	C	158	ASN
1	C	171	GLN
1	C	173	GLN
1	C	203	ASN
1	C	207	GLN
1	C	245	HIS
1	C	284	ASN
1	C	285	GLN
1	C	333	GLN
1	C	386	HIS
1	C	539	ASN
1	C	556	GLN
1	C	558	ASN
1	C	572	ASN
1	C	591	GLN
1	C	646	HIS
1	C	675	ASN
1	C	711	ASN
1	C	761	GLN
1	C	773	GLN
1	C	775	ASN
1	C	787	ASN
1	D	98	ASN
1	D	158	ASN
1	D	207	GLN
1	D	284	ASN

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Mol	Chain	Res	Type
1	D	285	GLN
1	D	386	HIS
1	D	440	HIS
1	D	539	ASN
1	D	556	GLN
1	D	595	GLN
1	D	678	GLN
1	D	711	ASN
1	D	812	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	$\# Z > 2$
2	5OC	G	3	2	18,21,22	0.41	0	24,30,33	0.86	1 (4%)
2	5OC	I	3	2	18,21,22	0.39	0	24,30,33	0.86	1 (4%)
2	5OC	E	3	2	18,21,22	0.38	0	24,30,33	0.85	1 (4%)
2	5OC	K	3	2	18,21,22	0.39	0	24,30,33	0.85	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	G	3	2	-	0/7/21/22	0/2/2/2
2	5OC	I	3	2	-	0/7/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3.72	122.57	114.82
2	G	3	5OC	O5-C5-C4	3.71	122.55	114.82
2	I	3	5OC	O5-C5-C4	3.69	122.51	114.82
2	E	3	5OC	O5-C5-C4	3.69	122.50	114.82

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 oligosaccharides 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	I	19	-	4,4,4	0.45	0	6,6,6	0.08	0
4	SO4	K	19	-	4,4,4	0.44	0	6,6,6	0.06	0
4	SO4	G	19	-	4,4,4	0.46	0	6,6,6	0.09	0
4	SO4	E	19	-	4,4,4	0.45	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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%)	0.04	19 (2%) 63 54	48, 84, 166, 266	0
1	B	904/906 (99%)	-0.27	6 (0%) 84 77	35, 63, 156, 343	0
1	C	903/906 (99%)	-0.21	8 (0%) 81 74	38, 68, 137, 233	0
1	D	903/906 (99%)	0.38	33 (3%) 45 36	69, 115, 201, 249	0
2	E	17/18 (94%)	-0.13	0 100 100	69, 88, 133, 141	0
2	G	17/18 (94%)	-0.91	0 100 100	37, 52, 71, 72	0
2	I	17/18 (94%)	-0.81	0 100 100	50, 57, 78, 81	0
2	K	17/18 (94%)	0.27	0 100 100	87, 123, 145, 148	0
3	F	15/15 (100%)	0.01	0 100 100	65, 97, 160, 162	0
3	H	15/15 (100%)	-0.83	0 100 100	40, 53, 77, 82	0
3	J	15/15 (100%)	-0.68	0 100 100	45, 66, 98, 100	0
3	L	15/15 (100%)	0.34	0 100 100	104, 145, 162, 163	0
All	All	3742/3756 (99%)	-0.03	66 (1%) 67 58	35, 82, 181, 343	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	GLU	6.0
1	D	514	LEU	5.1
1	D	847	ALA	4.9
1	A	858	ILE	4.3
1	A	862	VAL	4.3
1	A	847	ALA	4.2
1	C	303	LEU	4.0
1	D	545	ALA	3.8
1	D	135	ALA	3.8
1	D	738	PRO	3.3
1	D	779	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	510	VAL	3.2
1	D	277	TYR	3.2
1	A	303	LEU	3.1
1	B	895	ALA	3.0
1	D	115	ILE	3.0
1	D	857	LEU	3.0
1	D	518	TYR	3.0
1	D	113	PHE	3.0
1	D	901	PHE	3.0
1	C	508	LEU	2.9
1	D	789	ALA	2.9
1	D	784	SER	2.9
1	D	513	PRO	2.8
1	D	903	PHE	2.8
1	D	516	VAL	2.8
1	C	514	LEU	2.8
1	C	527	LYS	2.8
1	A	832	VAL	2.7
1	B	303	LEU	2.7
1	A	508	LEU	2.7
1	A	846	ILE	2.6
1	D	526	ILE	2.6
1	B	508	LEU	2.6
1	D	303	LEU	2.5
1	D	832	VAL	2.5
1	C	502	ALA	2.5
1	B	634	ASP	2.4
1	D	570	LEU	2.4
1	D	550	VAL	2.4
1	C	517	ASP	2.4
1	D	515	ASP	2.4
1	A	863	LEU	2.4
1	D	730	LEU	2.4
1	D	543	PHE	2.3
1	B	897	LEU	2.3
1	B	302	LYS	2.3
1	D	824	VAL	2.3
1	D	393	GLY	2.3
1	C	323	TYR	2.2
1	D	257	TYR	2.2
1	A	536	LYS	2.2
1	A	833	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	526	ILE	2.1
1	D	787	ASN	2.1
1	D	782	VAL	2.1
1	A	5	TYR	2.1
1	D	544	ARG	2.1
1	A	808	ILE	2.1
1	D	846	ILE	2.1
1	A	499	ILE	2.1
1	A	252	VAL	2.1
1	D	753	LEU	2.0
1	A	805	ILE	2.0
1	A	257	TYR	2.0
1	A	782	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5OC	K	3	20/21	0.79	0.12	112,114,118,119	0
2	5OC	E	3	20/21	0.90	0.10	69,76,81,82	0
2	5OC	I	3	20/21	0.94	0.07	56,60,62,64	0
2	5OC	G	3	20/21	0.98	0.04	38,40,43,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	K	19	5/5	0.76	0.07	126,126,126,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	E	19	5/5	0.83	0.08	99,101,101,104	0
4	SO4	I	19	5/5	0.91	0.08	84,86,87,90	0
4	SO4	G	19	5/5	0.92	0.07	77,78,81,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.