



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 3TAE / pdb_00003tae
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

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

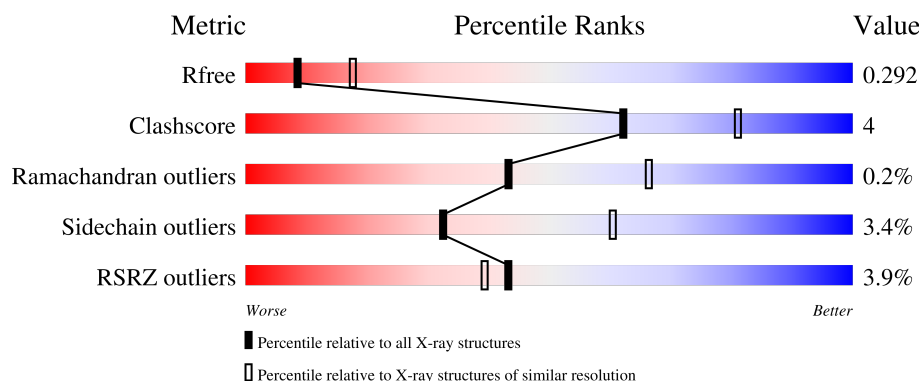
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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 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	E	18	
1	G	18	
1	I	18	
1	K	18	
2	F	15	

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Mol	Chain	Length	Quality of chain
2	H	15	
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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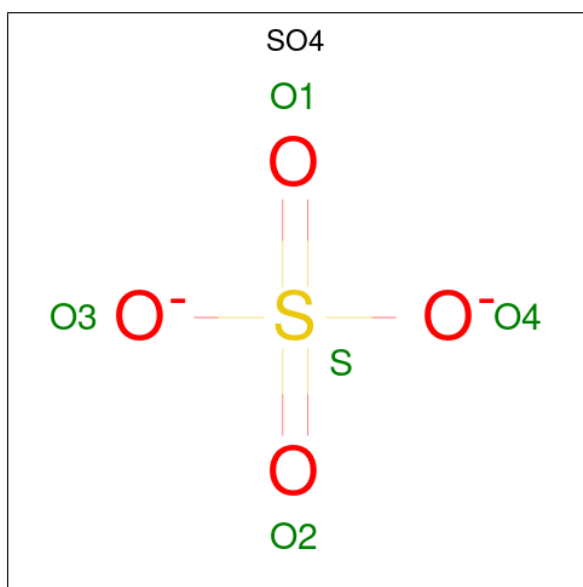
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	898	Total	C	N	O	S	0	0	0
			7328	4706	1221	1369	32			

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 (CCD ID: SO4) (formula: O₄S).



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	O	0	0
			71	71		
5	D	4	Total	O	0	0
			4	4		

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.

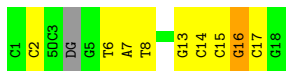
- Molecule 1: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')



- 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')

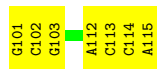


- Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

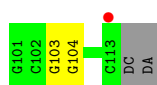
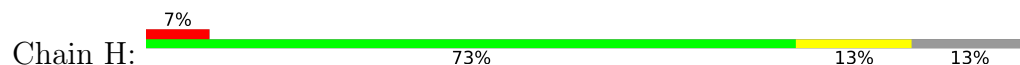




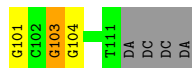
- Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')



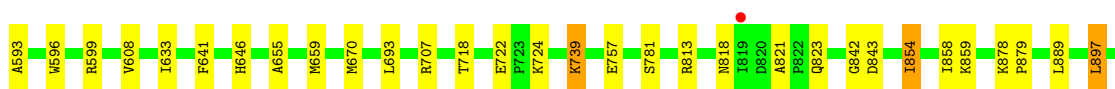
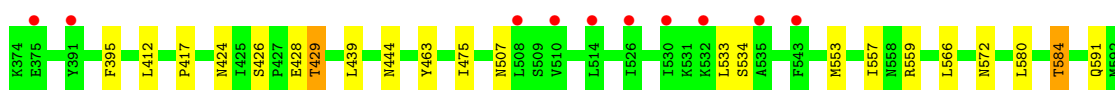
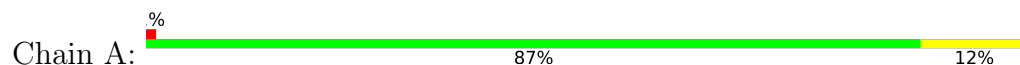
- Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')



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

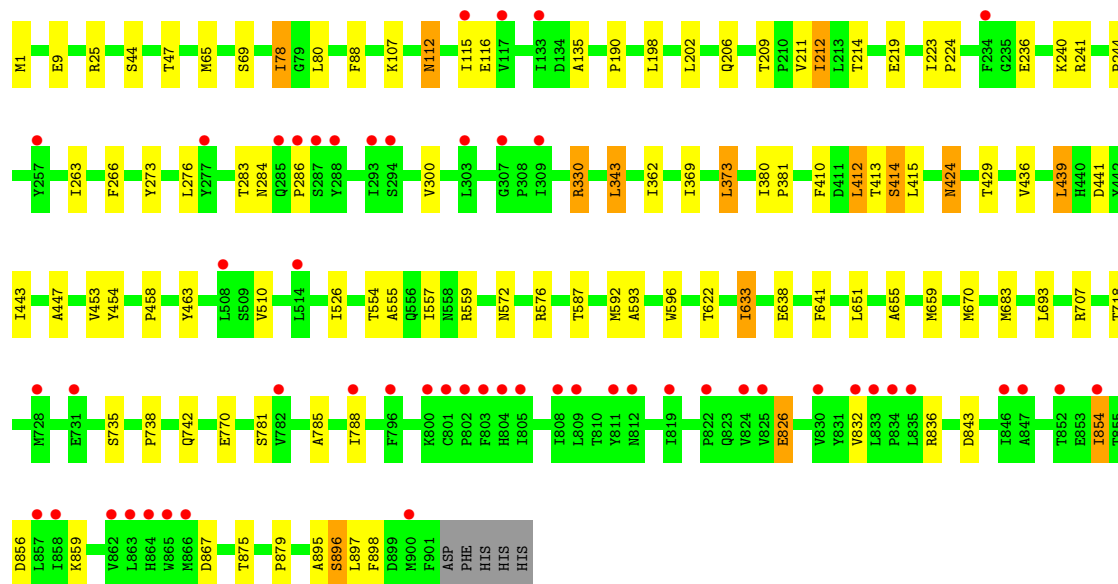


- Molecule 3: DNA polymerase



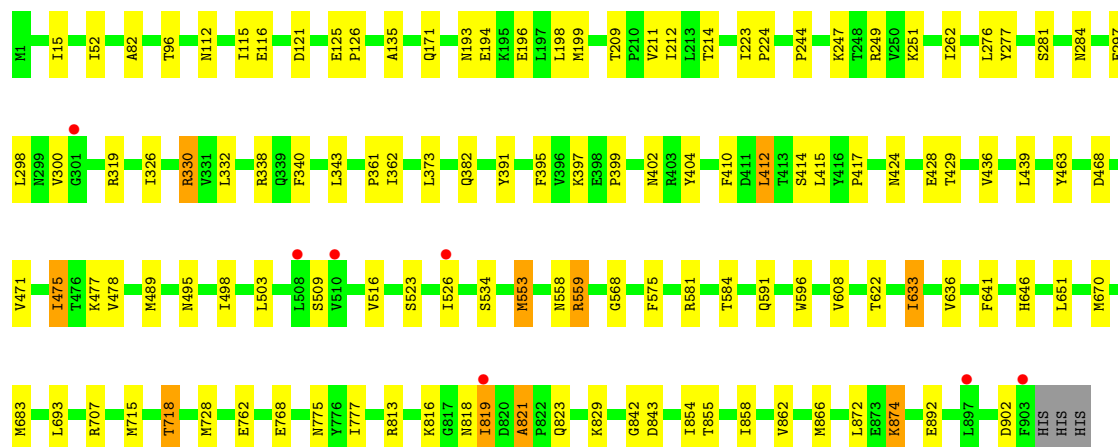
- Molecule 3: DNA polymerase

Chain B: 

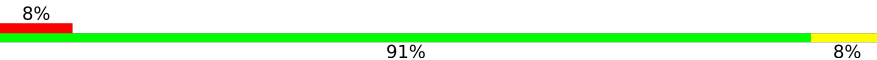


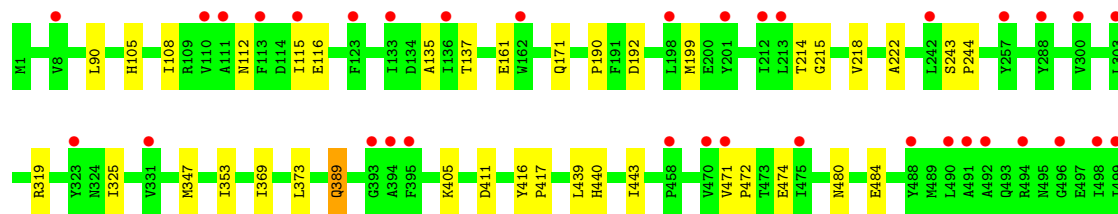
• Molecule 3: DNA polymerase

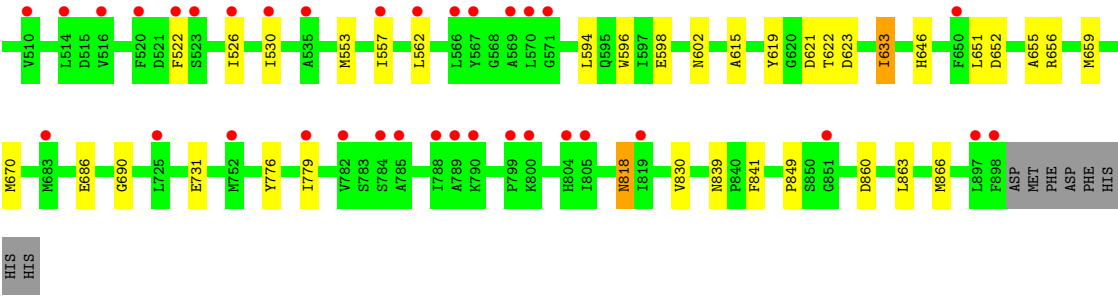
Chain C: 



• Molecule 3: DNA polymerase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.27Å 123.71Å 165.90Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	30.00 – 2.71 30.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.71) 98.0 (30.00-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0116, CNS	Depositor
R, R_{free}	0.224 , 0.268 (Not available) , 0.292	Depositor DCC
R_{free} test set	13797 reflections (9.48%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.8	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	32066	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

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	E	0.28	0/387	0.68	0/593
1	G	0.28	0/345	0.63	1/529 (0.2%)
1	I	0.31	0/369	0.70	0/565
1	K	0.28	0/298	0.56	0/456
2	F	0.28	0/319	0.74	1/491 (0.2%)
2	H	0.28	0/294	0.66	0/452
2	J	0.30	0/339	0.72	0/521
2	L	0.28	0/249	0.81	2/383 (0.5%)
3	A	0.53	0/7555	0.80	2/10209 (0.0%)
3	B	0.52	0/7535	0.77	0/10182
3	C	0.53	0/7555	0.79	2/10209 (0.0%)
3	D	0.51	0/7507	0.76	0/10145
All	All	0.51	0/32752	0.77	8/44735 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	103	DG	P-O3'-C3'	6.03	129.25	120.20
3	C	821	ALA	N-CA-C	-5.58	102.75	109.83
3	A	189	MET	CA-C-N	5.47	125.67	120.31
3	A	189	MET	C-N-CA	5.47	125.67	120.31
2	L	101	DG	P-O3'-C3'	5.18	127.97	120.20
3	C	843	ASP	N-CA-C	5.12	115.80	108.74
2	F	112	DA	O3'-P-O5'	5.09	111.64	104.00
1	G	16	DG	P-O3'-C3'	5.08	127.83	120.20

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	8	0
2	L	223	0	126	1	0
3	A	7374	0	7267	67	0
3	B	7355	0	7254	60	0
3	C	7374	0	7267	61	0
3	D	7328	0	7232	36	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
5	I	6	0	0	0	0
5	J	4	0	0	0	0
All	All	32066	0	30325	252	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 (252) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H2'	1:G:2:DC:O2	1.73	0.87
3:A:65:MET:HE3	3:A:88:PHE:HB2	1.55	0.86
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: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:65:MET:HE3	3:A:88:PHE:CB	2.13	0.78
3:A:813:ARG:HH21	3:A:842:GLY:HA3	1.49	0.77
3:B:65:MET:HE2	3:B:88:PHE:HB2	1.69	0.75
1:E:6:DT:H2''	1:E:7:DA:H5''	1.69	0.75
3:A:593:ALA:HA	3:A:670:MET:HE1	1.69	0.73
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
3:A:65:MET:CE	3:A:88:PHE:HB2	2.19	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
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:199:MET:HE2	3:B:25:ARG:CZ	2.25	0.66
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
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
1:I:2:DC:O4'	1:I:2:DC:O2	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:101:DG:H2'	2:J:102:DC:C6	2.37	0.59
3:A:112:ASN:HB3	3:A:214:THR:HG23	1.85	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:593:ALA:HA	3:B:670:MET:HE1	1.87	0.56
3:B:424:ASN:O	3:B:429:THR:HG21	2.05	0.56
3:D:652:ASP:CG	3:D:656:ARG:HH12	2.14	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:C:818:ASN:O	3:C:819:ILE:C	2.50	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
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:D:171:GLN:HE21	3:D:319:ARG:HH22	1.56	0.54
3:B:9:GLU:HG2	3:B:266:PHE:HD2	1.73	0.53
3:C:596:TRP:CG	3:C:670:MET:HE2	2.43	0.53
1:E:15:DC:H2''	1:E:16:DG:C8	2.44	0.53
1:G:2:DC:O2	1:G:2:DC:C2'	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
3:A:897:LEU:H	3:A:897:LEU:CD2	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:343:LEU:HD12	3:C:558:ASN:ND2	2.24	0.52
3:C:395:PHE:HB2	3:C:591:GLN:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:523:SER:H	3:C:526:ILE:HD12	1.76	0.51
3:A:596:TRP:CG	3:A:670:MET:HE2	2.46	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:B:65:MET:HE3	3:B:88:PHE:HB3	1.93	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:B:458:PRO:HG3	3:B:592:MET:SD	2.53	0.49
1:G:8:DT:H4'	3:B:707:ARG:HD2	1.94	0.49
3:B:655:ALA:HA	3:B:659:MET:HB2	1.93	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:65:MET:CE	3:B:88:PHE:CB	2.90	0.49
3:B:633:ILE:HD11	3:B:651:LEU:HD11	1.95	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
1:G:6:DT:H2''	1:G:7:DA:H5''	1.94	0.49
3:D:440:HIS:HA	3:D:443:ILE:HD12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:197:LEU:C	3:A:197:LEU:HD12	2.39	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:B:592:MET:HE3	3:B:670:MET:SD	2.55	0.46
3:C:298:LEU:HB2	3:C:300:VAL:HG22	1.98	0.46
3:D:347:MET:HE1	3:D:562:LEU:HD11	1.97	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:9:GLU:CG	3:B:266:PHE:HD2	2.27	0.46
3:B:343:LEU:HD11	3:B:557:ILE:HD11	1.98	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
3:B:362:ILE:HD11	3:B:572:ASN:CG	2.41	0.46
1:E:1:DC:H4'	3:A:572:ASN:HD21	1.81	0.46
3:A:596:TRP:HB3	3:A:670:MET:HE2	1.97	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:HD23	3:A:897:LEU:N	2.25	0.45
3:B:65:MET:HE3	3:B:88:PHE:CB	2.46	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
2:J:102:DC:H2''	2:J:103:DG:C8	2.51	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
3:A:362:ILE:HD11	3:A:572:ASN:CG	2.41	0.45
3:C:125:GLU:HA	3:C:126:PRO:HD3	1.81	0.45
3:C:247:LYS:HZ1	3:C:249:ARG:HH21	1.65	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:B:596:TRP:HB3	3:B:670:MET:HE2	1.98	0.44
3:C:251:LYS:HB3	3:C:262:ILE:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:238:THR:O	3:A:241:ARG:HB2	2.18	0.44
3:A:641:PHE:HD1	3:A:646:HIS:CD2	2.33	0.44
1:I:2:DC:H2''	3:C:362:ILE:HD12	1.99	0.44
3:A:641:PHE:CD1	3:A:646:HIS:HD2	2.33	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:813:ARG:HH21	3:C:842:GLY:HA3	1.81	0.44
1:K:14:DC:H2'	1:K:15:DC:H6	1.82	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
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:D:411:ASP:CG	3:D:686:GLU:HG3	2.44	0.42
3:A:507:ASN:O	3:A:534:SER:HA	2.19	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:52:ILE:HD12	3:A:428:GLU:HB3	2.02	0.42
3:A:194:GLU:HG2	3:A:198:LEU:HD22	2.02	0.42
3:A:878:LYS:HB3	3:A:879:PRO:HD3	2.02	0.42
3:B:895:ALA:O	3:B:896:SER:C	2.62	0.42
3:D:863:LEU:HA	3:D:866:MET:HG3	2.01	0.42
2:H:103:DG:H2''	2:H:104:DG:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:426:SER:O	3:A:429:THR:HG22	2.19	0.42
2:F:114:DC:N4	5:F:204:HOH:O	2.50	0.42
3:B:112:ASN:HB3	3:B:214:THR:HG23	2.01	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: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
2:F:112:DA:C3'	2:F:113:DC:H5''	2.50	0.41
3:C:112:ASN:HD21	3:C:332:LEU:HG	1.85	0.41
3:D:779:ILE:HD11	3:D:866:MET:HE1	2.02	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:A:255:ASN:C	3:A:257:TYR:H	2.29	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:D:596:TRP:CD1	3:D:670:MET:HE2	2.55	0.41
3:B:381:PRO:HG2	3:B:576:ARG:HG2	2.01	0.41
3:B:413:THR:O	3:B:414:SER:C	2.64	0.41
3:B:836:ARG:HG3	3:B:867:ASP:HB2	2.03	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:A:593:ALA:HA	3:A:670:MET:CE	2.45	0.40
3:B:1:MET:HE1	3:B:107:LYS:HD2	2.03	0.40
3:B:429:THR:HG23	3:B:463:TYR:HD2	1.86	0.40
3:B:439:LEU:HD13	3:B:443:ILE:CD1	2.51	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:347:MET:HA	3:D:347:MET:HE3	2.03	0.40
3:D:594:LEU:O	3:D:598:GLU:HB2	2.21	0.40
3:D:818:ASN:H	3:D:818:ASN:HD22	1.69	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)
2:J:114:DC:OP2	3:C:728:MET:HE2	2.21	0.40
3:B:78:ILE:HD12	3:B:80:LEU:HD12	2.03	0.40
3:B:244:PRO:HD2	3:B:266:PHE:O	2.21	0.40
3:B:596:TRP:CG	3:B:670:MET:HE2	2.57	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%)	48	72
3	B	899/906 (99%)	858 (95%)	38 (4%)	3 (0%)	36	59
3	C	901/906 (99%)	873 (97%)	27 (3%)	1 (0%)	48	72
3	D	896/906 (99%)	855 (95%)	39 (4%)	2 (0%)	43	66
All	All	3597/3624 (99%)	3461 (96%)	129 (4%)	7 (0%)	43	66

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 ⓘ

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%)	764 (96%)	36 (4%)	24	50
3	B	798/803 (99%)	767 (96%)	31 (4%)	28	56
3	C	800/803 (100%)	768 (96%)	32 (4%)	28	55
3	D	795/803 (99%)	784 (99%)	11 (1%)	59	80
All	All	3193/3212 (99%)	3083 (97%)	110 (3%)	32	60

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	15	ILE
3	A	45	GLN
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	219	GLU
3	A	241	ARG
3	A	263	ILE
3	A	285	GLN
3	A	291	ASP
3	A	309	ILE
3	A	319	ARG
3	A	342	ASN
3	A	343	LEU
3	A	373	LEU
3	A	412	LEU
3	A	429	THR
3	A	439	LEU
3	A	533	LEU
3	A	559	ARG
3	A	584	THR

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Mol	Chain	Res	Type
3	A	608	VAL
3	A	633	ILE
3	A	693	LEU
3	A	718	THR
3	A	722	GLU
3	A	724	LYS
3	A	739	LYS
3	A	781	SER
3	A	823	GLN
3	A	843	ASP
3	A	854	ILE
3	A	897	LEU
3	B	44	SER
3	B	47	THR
3	B	69	SER
3	B	78	ILE
3	B	112	ASN
3	B	115	ILE
3	B	198	LEU
3	B	212	ILE
3	B	241	ARG
3	B	283	THR
3	B	284	ASN
3	B	300	VAL
3	B	330	ARG
3	B	343	LEU
3	B	373	LEU
3	B	412	LEU
3	B	414	SER
3	B	436	VAL
3	B	439	LEU
3	B	510	VAL
3	B	526	ILE
3	B	587	THR
3	B	633	ILE
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

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Mol	Chain	Res	Type
3	B	898	PHE
3	C	15	ILE
3	C	96	THR
3	C	115	ILE
3	C	121	ASP
3	C	199	MET
3	C	330	ARG
3	C	373	LEU
3	C	412	LEU
3	C	436	VAL
3	C	439	LEU
3	C	468	ASP
3	C	475	ILE
3	C	477	LYS
3	C	503	LEU
3	C	516	VAL
3	C	553	MET
3	C	559	ARG
3	C	581	ARG
3	C	608	VAL
3	C	633	ILE
3	C	636	VAL
3	C	693	LEU
3	C	718	THR
3	C	762	GLU
3	C	816	LYS
3	C	823	GLN
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	199	MET
3	D	373	LEU
3	D	389	GLN
3	D	439	LEU
3	D	530	ILE
3	D	633	ILE
3	D	646	HIS
3	D	731	GLU

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Mol	Chain	Res	Type
3	D	818	ASN
3	D	860	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	40	HIS
3	A	98	ASN
3	A	112	ASN
3	A	158	ASN
3	A	193	ASN
3	A	285	GLN
3	A	444	ASN
3	A	504	HIS
3	A	646	HIS
3	A	733	GLN
3	A	818	ASN
3	A	823	GLN
3	A	864	HIS
3	B	40	HIS
3	B	112	ASN
3	B	153	ASN
3	B	193	ASN
3	B	284	ASN
3	B	285	GLN
3	B	339	GLN
3	B	342	ASN
3	B	382	GLN
3	B	386	HIS
3	B	389	GLN
3	B	424	ASN
3	B	481	GLN
3	B	485	HIS
3	B	493	GLN
3	B	504	HIS
3	B	646	HIS
3	B	773	GLN
3	B	823	GLN
3	C	171	GLN
3	C	193	ASN
3	C	284	ASN
3	C	285	GLN

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Mol	Chain	Res	Type
3	C	382	GLN
3	C	386	HIS
3	C	440	HIS
3	C	444	ASN
3	C	485	HIS
3	C	558	ASN
3	C	646	HIS
3	C	775	ASN
3	C	786	ASN
3	C	818	ASN
3	C	823	GLN
3	C	839	ASN
3	D	64	ASN
3	D	131	HIS
3	D	171	GLN
3	D	299	ASN
3	D	371	ASN
3	D	389	GLN
3	D	485	HIS
3	D	602	ASN
3	D	606	ASN
3	D	646	HIS
3	D	679	HIS
3	D	786	ASN
3	D	818	ASN
3	D	823	GLN

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	I	3	1	18,21,22	0.41	0	24,30,33	0.93	1 (4%)
1	5OC	K	3	1	0,3,22	-	-	0,3,33	-	-
1	5OC	G	3	1	0,3,22	-	-	0,3,33	-	-
1	5OC	E	3	1	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
1	5OC	I	3	1	-	0/7/21/22	0/2/2/2
1	5OC	E	3	1	-	2/7/21/22	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	3	5OC	O5-C5-C4	3.74	122.60	114.82
1	E	3	5OC	O5-C5-C4	3.69	122.51	114.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 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	F	3	-	4,4,4	0.44	0	6,6,6	0.06	0
4	SO4	C	907	-	4,4,4	0.44	0	6,6,6	0.10	0
4	SO4	H	2	-	4,4,4	0.44	0	6,6,6	0.07	0
4	SO4	B	907	-	4,4,4	0.45	0	6,6,6	0.14	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
1	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3:5OC	OP2	4:DG	P	7.44
1	E	3:5OC	OP2	4:DG	P	6.90

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	17/18 (94%)	-0.00	1 (5%) 28 25	57, 89, 126, 143	0
1	G	16/18 (88%)	0.61	0 100 100	62, 114, 138, 155	0
1	I	16/18 (88%)	-0.65	0 100 100	37, 50, 70, 94	0
1	K	14/18 (77%)	0.59	0 100 100	53, 162, 197, 200	0
2	F	15/15 (100%)	0.07	0 100 100	72, 87, 138, 141	0
2	H	13/15 (86%)	0.79	1 (7%) 19 17	94, 116, 140, 141	0
2	J	15/15 (100%)	-0.53	0 100 100	36, 61, 87, 87	0
2	L	11/15 (73%)	0.68	0 100 100	158, 169, 173, 174	0
3	A	903/906 (99%)	-0.20	13 (1%) 73 71	30, 54, 146, 263	0
3	B	901/906 (99%)	0.37	53 (5%) 28 25	34, 80, 218, 286	0
3	C	903/906 (99%)	-0.14	7 (0%) 82 81	28, 62, 135, 197	0
3	D	898/906 (99%)	0.73	70 (7%) 19 17	84, 135, 213, 253	0
All	All	3722/3756 (99%)	0.19	145 (3%) 43 39	28, 78, 201, 286	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	862	VAL	6.8
3	B	286	PRO	5.4
3	A	508	LEU	5.2
3	B	802	PRO	4.9
3	B	805	ILE	4.8
3	D	570	LEU	4.7
3	D	522	PHE	4.6
3	B	846	ILE	4.2
3	B	800	LYS	3.9
3	D	898	PHE	3.9
3	A	510	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
3	B	847	ALA	3.9
3	B	809	LEU	3.8
3	B	808	ILE	3.7
3	B	857	LEU	3.7
3	D	498	ILE	3.6
3	D	113	PHE	3.6
3	B	788	ILE	3.6
3	B	858	ILE	3.6
3	D	523	SER	3.6
3	B	309	ILE	3.6
3	B	819	ILE	3.5
3	B	863	LEU	3.5
3	B	824	VAL	3.5
3	D	115	ILE	3.4
3	B	825	VAL	3.4
3	D	569	ALA	3.3
3	B	782	VAL	3.3
3	D	784	SER	3.2
3	B	303	LEU	3.1
3	D	394	ALA	3.1
3	D	471	VAL	3.1
3	B	514	LEU	3.0
3	D	788	ILE	3.0
3	D	514	LEU	3.0
3	D	530	ILE	3.0
3	C	508	LEU	2.9
3	A	375	GLU	2.9
3	B	833	LEU	2.9
3	D	475	ILE	2.9
3	B	852	THR	2.9
3	B	865	TRP	2.9
3	B	811	TYR	2.9
3	D	458	PRO	2.8
3	B	812	ASN	2.8
3	B	288	TYR	2.8
3	D	790	LYS	2.8
3	C	903	PHE	2.8
3	B	731	GLU	2.8
3	B	287	SER	2.8
3	C	526	ILE	2.8
3	D	393	GLY	2.8
3	D	789	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	B	834	PRO	2.8
3	B	854	ILE	2.8
3	B	801	CYS	2.7
3	A	530	ILE	2.7
3	D	198	LEU	2.7
3	D	496	GLY	2.7
3	D	526	ILE	2.7
3	D	490	LEU	2.7
3	D	566	LEU	2.6
3	D	470	VAL	2.6
3	B	796	PHE	2.6
3	D	133	ILE	2.6
3	A	514	LEU	2.6
3	D	242	LEU	2.6
3	D	897	LEU	2.6
3	D	257	TYR	2.6
3	B	804	HIS	2.6
3	C	510	VAL	2.5
3	D	288	TYR	2.5
3	B	803	PHE	2.5
3	B	835	LEU	2.5
3	D	212	ILE	2.5
3	D	331	VAL	2.5
3	D	800	LYS	2.4
3	B	133	ILE	2.4
3	B	864	HIS	2.4
3	D	8	VAL	2.4
3	C	897	LEU	2.4
3	B	866	MET	2.4
3	B	900	MET	2.4
3	B	257	TYR	2.4
3	C	819	ILE	2.4
3	B	822	PRO	2.4
3	B	117	VAL	2.4
3	B	508	LEU	2.4
2	H	113	DC	2.4
3	D	571	GLY	2.4
3	D	395	PHE	2.4
3	D	562	LEU	2.3
3	D	510	VAL	2.3
3	B	234	PHE	2.3
3	D	111	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	779	ILE	2.3
3	A	532	LYS	2.3
3	D	300	VAL	2.3
3	A	543	PHE	2.3
3	D	162	TRP	2.3
3	D	516	VAL	2.3
3	D	725	LEU	2.3
3	D	323	TYR	2.2
3	D	110	VAL	2.2
3	A	526	ILE	2.2
3	D	851	GLY	2.2
3	D	782	VAL	2.2
3	D	491	ALA	2.2
3	B	277	TYR	2.2
3	D	213	LEU	2.2
3	D	488	TYR	2.2
3	D	683	MET	2.2
3	B	293	ILE	2.2
3	D	499	ILE	2.2
3	D	123	PHE	2.2
3	D	520	PHE	2.2
3	D	201	TYR	2.1
3	B	832	VAL	2.1
3	D	804	HIS	2.1
3	A	903	PHE	2.1
1	E	2	DC	2.1
3	B	285	GLN	2.1
3	C	301	GLY	2.1
3	D	557	ILE	2.1
3	B	294	SER	2.1
3	A	535	ALA	2.1
3	D	303	LEU	2.1
3	D	805	ILE	2.1
3	D	494	ARG	2.1
3	D	799	PRO	2.1
3	B	115	ILE	2.1
3	D	567	TYR	2.1
3	D	785	ALA	2.0
3	A	253	ILE	2.0
3	A	819	ILE	2.0
3	B	307	GLY	2.0
3	D	136	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	391	TYR	2.0
3	B	830	VAL	2.0
3	D	650	PHE	2.0
3	D	492	ALA	2.0
3	D	535	ALA	2.0
3	B	728	MET	2.0
3	D	752	MET	2.0
3	D	819	ILE	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
1	5OC	E	3	20/21	0.31	0.14	148,155,160,160	0
1	5OC	K	3	4/21	0.50	0.14	123,130,134,136	0
1	5OC	G	3	4/21	0.82	0.10	108,111,111,113	0
1	5OC	I	3	20/21	0.86	0.13	78,91,100,100	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	F	3	5/5	0.75	0.09	121,121,123,124	0
4	SO4	H	2	5/5	0.79	0.10	126,128,128,130	0
4	SO4	B	907	5/5	0.86	0.20	83,85,88,88	0
4	SO4	C	907	5/5	0.88	0.15	112,115,116,120	0

6.5 Other polymers ⓘ

There are no such residues in this entry.