Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:16 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

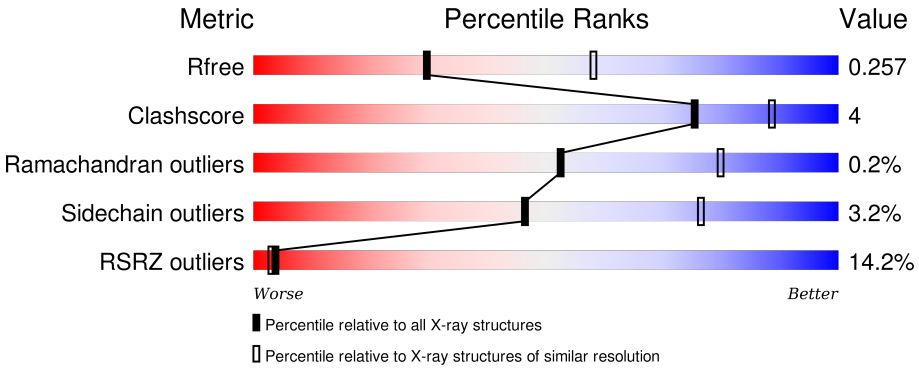
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	11% 56% 44%
1	G	18	39% 44% 44% 6% 6%
1	I	18	72% 22% 6%
1	K	18	56% 72% 11% 17%
2	F	15	7% 60% 33% 7%

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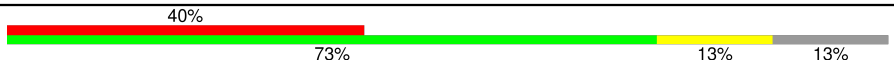
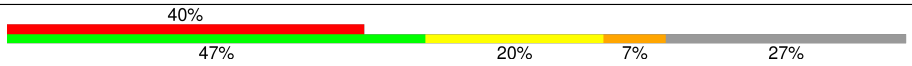
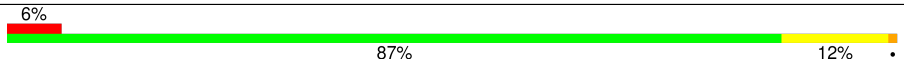
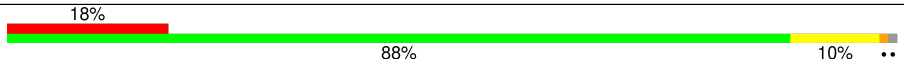
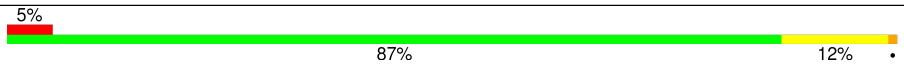
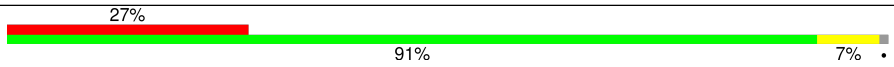
Mol	Chain	Length	Quality of chain
2	H	15	
2	J	15	
2	L	15	
3	A	906	
3	B	906	
3	C	906	
3	D	906	

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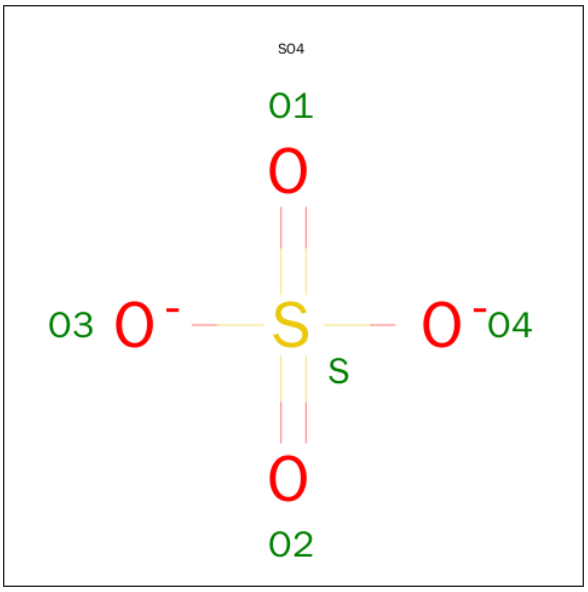
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	898	Total	C	N	O	S	0	0	0
			7328	4706	1221	1369	32			

There are 20 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

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

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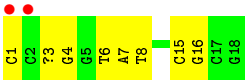
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	71	Total O 71 71	0	0
5	D	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

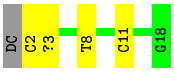
• Molecule 1: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain E:



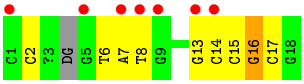
• Molecule 1: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:



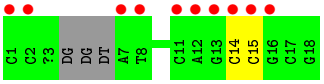
• Molecule 1: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:



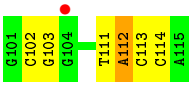
• Molecule 1: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:



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

Chain F:

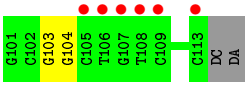


• Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

Chain J:

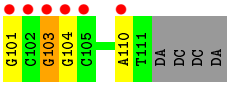
• Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

Chain H:



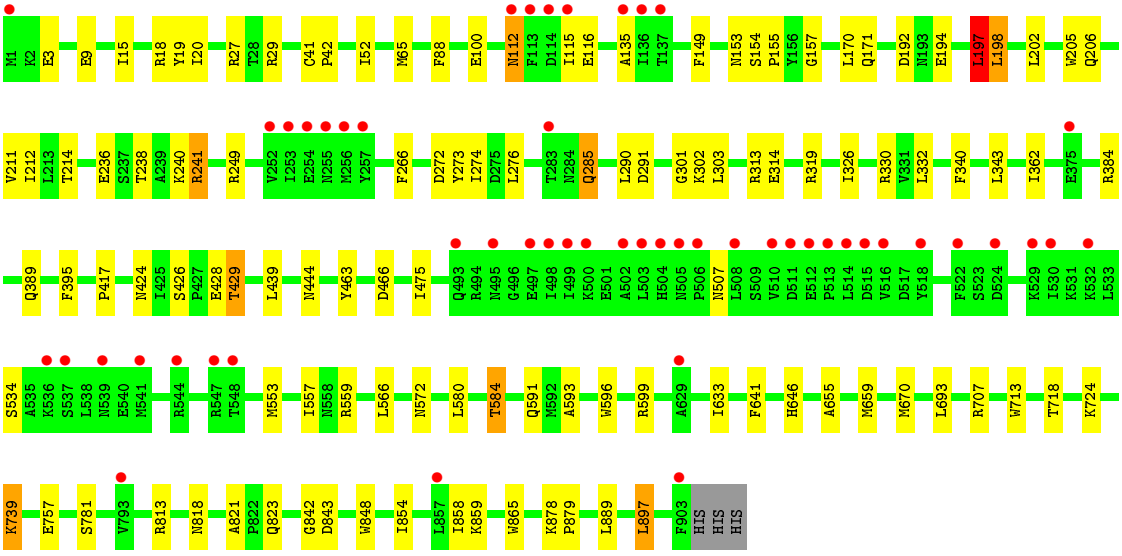
• Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

Chain L:



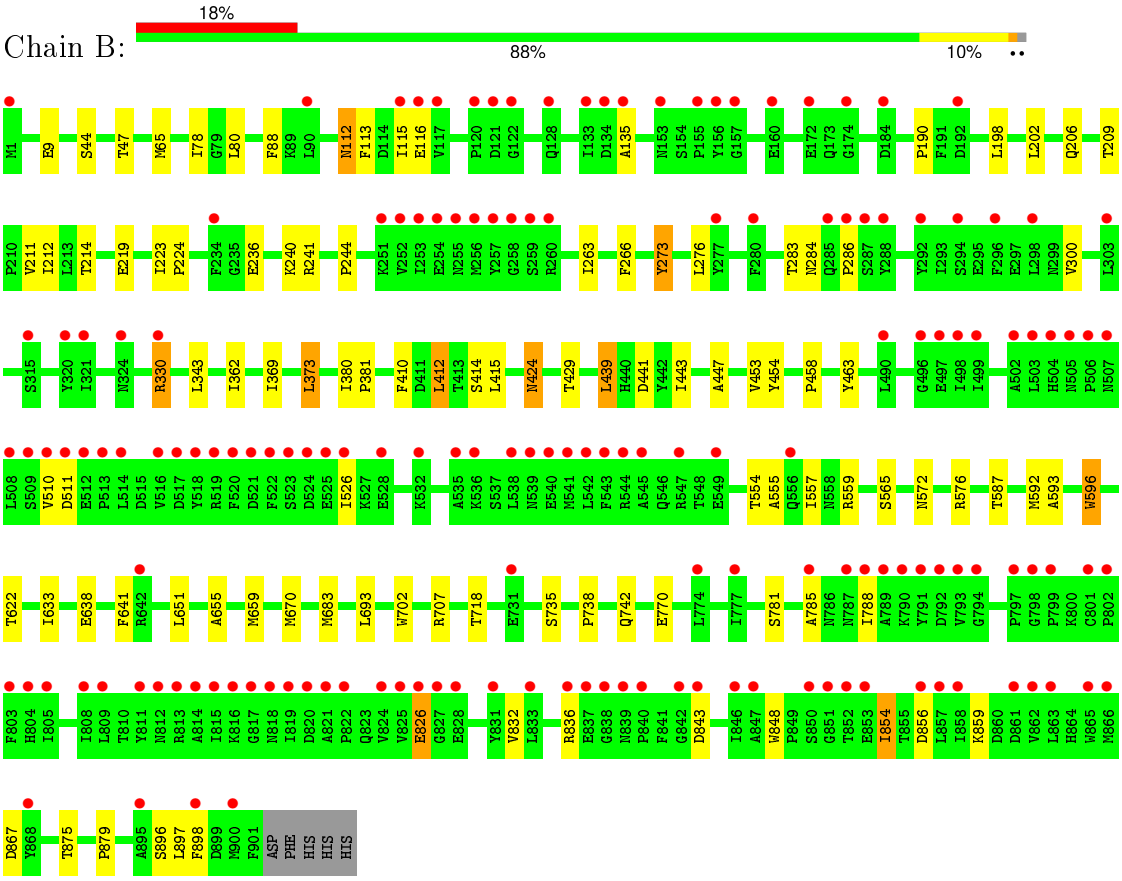
• Molecule 3: DNA polymerase

Chain A:



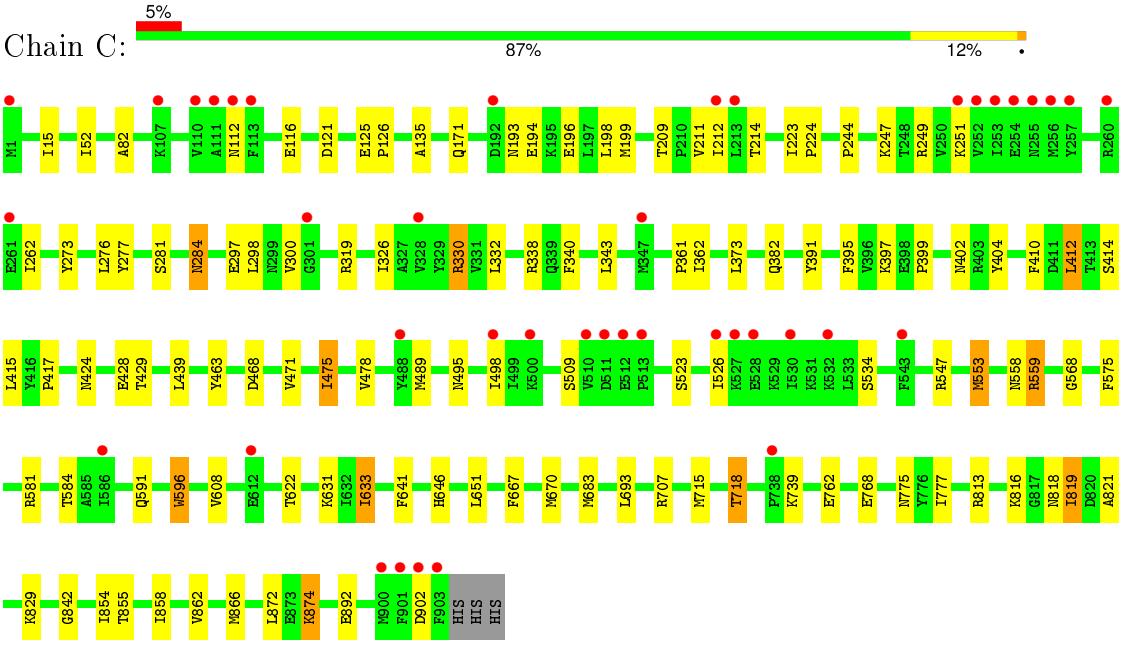
• Molecule 3: DNA polymerase

Chain B:



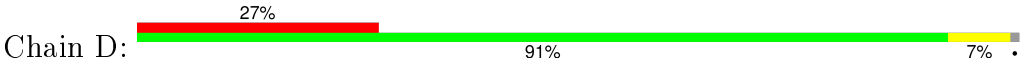
• Molecule 3: DNA polymerase

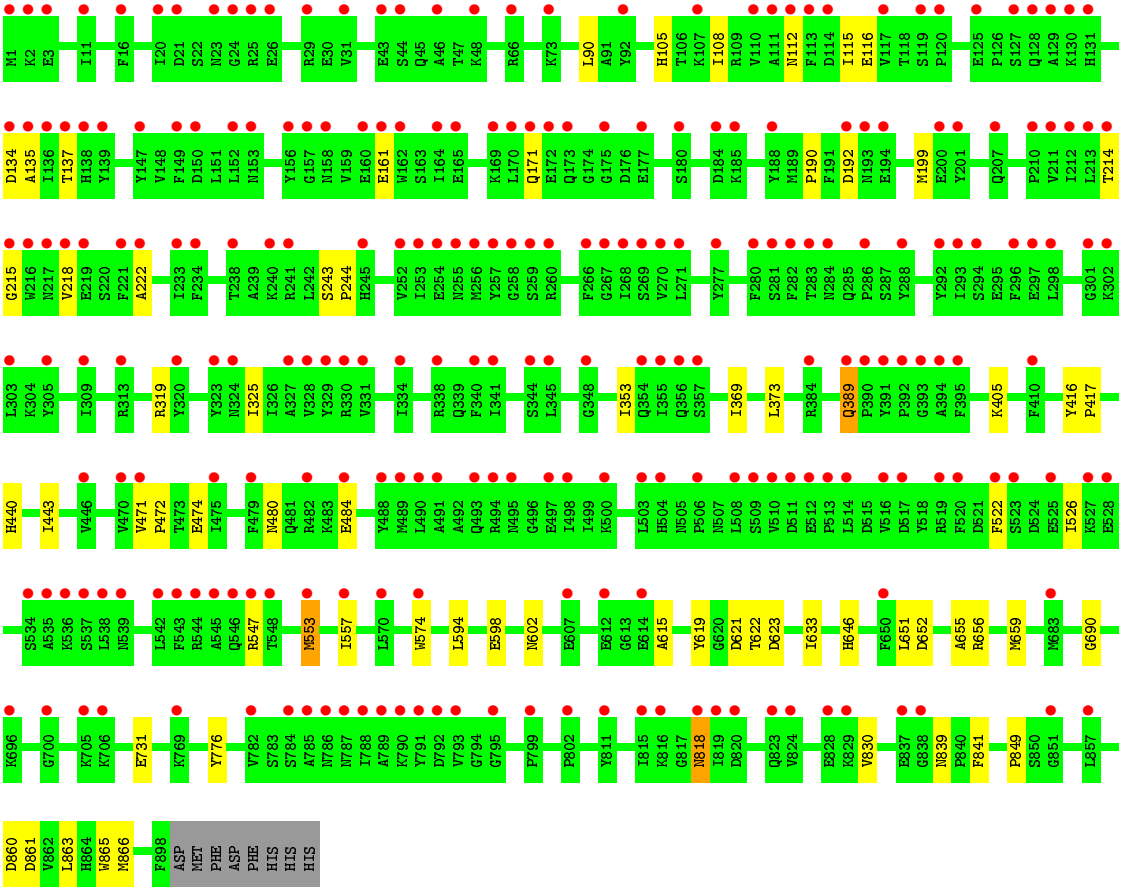
Chain C:



• Molecule 3: DNA polymerase

Chain D:




M1 K2 E3 I11 F16 I20 D21 S22 N23 G24 R25 E26 R29 E30 V31 E43 S44 Q45 A46 T47 K48 R66 K73 L90 A91 Y92 H105 T106 K107 I108 R109 V110 A111 N112 F113 D114 I115 E116 V117 T118 S119 P120 E125 P126 S127 Q128 A129 K130 H131
D134 A135 I136 T137 H138 Y139 Y147 V148 F149 D150 L151 L152 N153 Y156 G157 N158 V159 E160 E161 W162 S163 I164 E165 K169 L170 Q171 E172 Q173 G174 G175 D176 E177 S180 D184 K185 Y188 M189 P190 F191 D192 N193 E194 M199 E200 Y201 Q207 P210 V211 I212 L213 T214
G215 W216 N217 V218 E219 S220 F221 A222 I233 F234 T238 A239 K240 R241 L242 S243 P244 H245 V252 I253 E254 N255 M256 Y257 G258 S259 R260 F266 G267 I268 S269 V270 L271 Y277 F280 S281 F282 T283 N284 Q285 P286 S287 Y288 Y292 I293 S294 E295 F296 E297 L298 G301 K302
L303 K304 Y305 I309 R313 R319 Y320 Y323 N324 I325 I326 A327 V328 Y329 R330 V331 I334 R338 Q339 F340 I341 S344 L345 G348 I353 Q354 I355 Q356 S357 I369 L373 R384 Q389 P390 Y391 P392 G393 A394 F395 K405 F410 Y416 P417
H440 I443 V446 V470 V471 P472 T473 E474 I475 F479 N480 Q481 R482 K483 E484 Y488 M489 L490 A491 A492 Q493 R494 N495 G496 E497 I498 I499 K500 L503 H504 N505 P506 N507 L508 S509 V510 D511 E512 P513 L514 D515 V516 D517 Y518 R519 F520 D521 F522 S523 D524 E525 I526 K527 E528
S534 A535 K536 S537 L538 N539 L542 F543 R544 A545 Q546 R547 T548 M553 I557 L570 W574 L594 E598 N602 E607 E612 G613 E614 A615 Y619 G620 D621 T622 D623 I633 H646 F650 L651 D652 A655 R656 M659 M683 G690
K696 G700 K705 K706 E731 K769 Y776 V782 S783 S784 A785 N786 N787 I788 A789 K790 Y791 D792 V793 G794 G795 F799 P802 Y811 I815 K816 G817 N818 I819 D820 Q823 Y824 E828 K829 V830 E837 G838 N839 P840 F841 P849 S850 G851 L857
D860 D861 V862 L863 H864 W865 M866 F898 ASP MET PHE ASP PHE HIS HIS HIS

4 Data and refinement statistics (i)

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 30.31 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.71) 98.1 (30.31-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.224 , 0.268 0.216 , 0.257	Depositor DCC
R_{free} test set	13797 reflections (10.71%)	DCC
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 142606 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	E	0.23	0/387	0.84	0/593
1	G	0.24	0/345	0.80	1/529 (0.2%)
1	I	0.29	0/369	0.78	0/565
1	K	0.21	0/298	0.74	0/456
2	F	0.23	0/319	0.89	1/491 (0.2%)
2	H	0.23	0/294	0.81	0/452
2	J	0.27	0/339	0.83	0/521
2	L	0.23	0/249	0.97	3/383 (0.8%)
3	A	0.43	4/7555 (0.1%)	0.53	1/10209 (0.0%)
3	B	0.42	3/7535 (0.0%)	0.49	0/10182
3	C	0.42	1/7555 (0.0%)	0.51	0/10209
3	D	0.41	2/7507 (0.0%)	0.46	0/10145
All	All	0.41	10/32752 (0.0%)	0.54	6/44735 (0.0%)

All (10) bond length outliers are listed below:

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

All (6) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:641:PHE:HD1	3:C:646:HIS:HD2	1.47	0.62
3:C:424:ASN:O	3:C:429:THR:HG21	2.00	0.62
3:B:211:VAL:HG12	3:B:212:ILE:HD12	1.80	0.62
1:G:13:DG:H2"	1:G:14:DC:H5"	1.81	0.62
3:C:489:MET:SD	3:C:553:MET:HG2	2.40	0.61
3:B:439:LEU:HD13	3:B:443:ILE:HD11	1.83	0.61
1:E:8:DT:H4'	3:A:707:ARG:HD2	1.83	0.60
3:A:285:GLN:HE21	3:A:285:GLN:HA	1.66	0.60
1:I:2:DC:O4'	1:I:2:DC:O2	2.19	0.59
3:A:112:ASN:HB3	3:A:214:THR:HG23	1.85	0.59
2:J:101:DG:H2'	2:J:102:DC:C6	2.37	0.59
1:I:11:DC:OP1	3:C:874:LYS:HE2	2.02	0.59
3:A:202:LEU:O	3:A:206:GLN:HG2	2.03	0.58
3:A:475:ILE:HD12	3:A:566:LEU:HD23	1.85	0.57
3:C:818:ASN:HD22	3:C:821:ALA:HB2	1.69	0.57
3:A:417:PRO:HB3	3:A:475:ILE:CD1	2.35	0.57
3:B:224:PRO:HA	3:B:263:ILE:HD12	1.87	0.57
3:C:343:LEU:HD12	3:C:558:ASN:HD21	1.70	0.57
3:B:236:GLU:HG2	3:B:240:LYS:HE2	1.86	0.57
3:B:209:THR:HG21	3:B:244:PRO:HG3	1.86	0.56
3:B:424:ASN:O	3:B:429:THR:HG21	2.05	0.56
3:D:830:VAL:HG12	3:D:849:PRO:HA	1.88	0.56
3:A:641:PHE:HD1	3:A:646:HIS:HD2	1.52	0.55
3:B:373:LEU:HD23	3:B:380:ILE:HG22	1.88	0.55
3:A:236:GLU:O	3:A:240:LYS:HG2	2.07	0.55
3:D:137:THR:HG21	3:D:325:ILE:HA	1.88	0.55
2:F:102:DC:H2"	2:F:103:DG:C8	2.42	0.55
2:J:114:DC:H2"	2:J:115:DA:OP2	2.07	0.54
3:A:313:ARG:HD2	5:A:917:HOH:O	2.07	0.54
3:B:738:PRO:O	3:B:742:GLN:HB2	2.07	0.54
3:C:862:VAL:O	3:C:866:MET:HG3	2.07	0.54
1:G:16:DG:H2'	1:G:17:DC:O4'	2.07	0.54
3:D:171:GLN:HE21	3:D:319:ARG:HH22	1.56	0.54
2:L:103:DG:H2"	2:L:104:DG:C8	2.42	0.54
3:B:9:GLU:HG2	3:B:266:PHE:HD2	1.73	0.53
1:E:15:DC:H2"	1:E:16:DG:C8	2.44	0.53
1:G:2:DC:C2'	1:G:2:DC:O2	2.47	0.53
3:C:171:GLN:HE21	3:C:319:ARG:HH22	1.57	0.53
3:A:314:GLU:HG3	5:A:923:HOH:O	2.09	0.53
3:A:757:GLU:HB2	3:A:889:LEU:HD22	1.91	0.53
3:A:897:LEU:CD2	3:A:897:LEU:H	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:27:ARG:NH2	3:B:190:PRO:O	2.42	0.52
3:C:343:LEU:HD12	3:C:558:ASN:ND2	2.24	0.52
3:B:555:ALA:O	3:B:559:ARG:HG2	2.09	0.52
3:C:395:PHE:HB2	3:C:591:GLN:HG2	1.90	0.52
3:A:9:GLU:HG2	3:A:266:PHE:HD2	1.75	0.52
3:B:202:LEU:O	3:B:206:GLN:HG2	2.10	0.52
3:A:854:ILE:HD12	3:A:859:LYS:HA	1.92	0.51
3:C:391:TYR:HB2	3:C:584:THR:HG22	1.91	0.51
3:D:652:ASP:CG	3:D:656:ARG:HH12	2.14	0.51
3:C:523:SER:H	3:C:526:ILE:HD12	1.76	0.51
3:B:788:ILE:HD12	3:B:826:GLU:HG2	1.93	0.51
3:D:480:ASN:O	3:D:484:GLU:HB2	2.10	0.50
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.93	0.50
3:A:596:TRP:HB3	3:A:670:MET:HE2	1.92	0.50
3:C:414:SER:HB3	3:C:417:PRO:HG2	1.93	0.50
3:C:641:PHE:HD1	3:C:646:HIS:CD2	2.29	0.50
3:C:209:THR:HG21	3:C:244:PRO:HG3	1.94	0.50
1:I:3:5OC:OP2	3:C:361:PRO:HD2	2.11	0.50
3:C:818:ASN:O	3:C:819:ILE:C	2.50	0.49
3:B:458:PRO:HG3	3:B:592:MET:SD	2.53	0.49
3:B:655:ALA:HA	3:B:659:MET:HB2	1.93	0.49
1:G:8:DT:H4'	3:B:707:ARG:HD2	1.94	0.49
3:D:416:TYR:HB2	3:D:417:PRO:HD3	1.95	0.49
3:C:715:MET:O	3:C:718:THR:HG23	2.12	0.49
3:B:116:GLU:HB2	3:B:135:ALA:HB3	1.94	0.49
3:B:65:MET:CE	3:B:88:PHE:CB	2.90	0.49
3:C:193:ASN:ND2	3:C:196:GLU:H	2.11	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
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:C:52:ILE:HD12	3:C:428:GLU:HB3	1.96	0.48
3:B:781:SER:HB2	3:B:832:VAL:HB	1.96	0.48
3:A:3:GLU:HB2	3:A:20:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:DC:H4'	1:I:3:5OC:O5'	2.12	0.47
3:A:157:GLY:O	3:A:313:ARG:NH2	2.47	0.47
3:B:286:PRO:HA	3:B:735:SER:HB3	1.95	0.47
3:A:580:LEU:O	3:A:584:THR:HG23	2.14	0.47
3:C:211:VAL:HG12	3:C:212:ILE:HD12	1.97	0.47
3:A:301:GLY:O	3:A:330:ARG:NH1	2.47	0.47
3:A:593:ALA:HA	3:A:670:MET:CE	2.45	0.47
3:C:509:SER:HB2	3:C:534:SER:HB3	1.96	0.47
3:C:284:ASN:HD21	3:C:829:LYS:NZ	2.11	0.47
3:A:290:LEU:HD23	3:A:302:LYS:HE3	1.96	0.47
3:C:495:ASN:HA	3:C:498:ILE:HD12	1.97	0.47
3:C:247:LYS:NZ	3:C:249:ARG:HH21	2.13	0.47
3:C:326:ILE:O	3:C:330:ARG:HG2	2.15	0.47
3:C:298:LEU:HB2	3:C:300:VAL:HG22	1.98	0.46
3:D:633:ILE:HD11	3:D:651:LEU:HD11	1.97	0.46
3:B:856:ASP:HA	3:B:859:LYS:HB3	1.97	0.46
3:A:818:ASN:HD22	3:A:821:ALA:HB2	1.81	0.46
3:C:641:PHE:CD1	3:C:646:HIS:HD2	2.30	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:B:236:GLU:O	3:B:240:LYS:HG2	2.16	0.46
1:E:1:DC:H4'	3:A:572:ASN:HD21	1.81	0.46
3:B:638:GLU:HA	3:B:641:PHE:HD2	1.80	0.46
3:D:522:PHE:HB3	3:D:526:ILE:HB	1.98	0.46
3:A:897:LEU:N	3:A:897:LEU:HD23	2.25	0.45
3:A:149:PHE:HB3	3:A:197:LEU:HD13	1.98	0.45
3:D:621:ASP:O	3:D:623:ASP:N	2.49	0.45
3:B:596:TRP:HB3	3:B:670:MET:HE2	1.97	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:C:125:GLU:HA	3:C:126:PRO:HD3	1.81	0.45
3:C:410:PHE:HB3	3:C:683:MET:HG2	1.98	0.45
3:A:9:GLU:CG	3:A:266:PHE:HD2	2.29	0.45
3:B:286:PRO:HA	3:B:735:SER:CB	2.47	0.45
3:B:412:LEU:HG	3:B:415:LEU:HD13	1.98	0.45
3:C:768:GLU:HG2	3:C:872:LEU:HD21	1.99	0.45
3:C:251:LYS:HB3	3:C:262:ILE:HG13	1.98	0.44
3:B:65:MET:HE2	3:B:88:PHE:CB	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:641:PHE:HD1	3:A:646:HIS:CD2	2.33	0.44
3:A:238:THR:O	3:A:241:ARG:HB2	2.18	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
3:C:596:TRP:HB3	3:C:670:MET:HE2	2.00	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:D:471:VAL:HB	3:D:472:PRO:HD3	2.00	0.44
3:C:277:TYR:O	3:C:281:SER:HB3	2.17	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:B:343:LEU:HD12	3:B:554:THR:HG23	2.00	0.43
3:A:395:PHE:HB2	3:A:591:GLN:HG2	2.00	0.43
3:C:429:THR:HG23	3:C:463:TYR:HD1	1.84	0.43
3:D:161:GLU:HG2	3:D:190:PRO:HG3	2.00	0.43
3:A:153:ASN:HB2	3:A:192:ASP:O	2.19	0.43
3:A:897:LEU:CD2	3:A:897:LEU:N	2.81	0.43
3:C:194:GLU:HG2	3:C:198:LEU:HD13	2.01	0.43
3:B:369:ILE:HG22	3:B:373:LEU:HD22	2.00	0.42
3:D:116:GLU:HB2	3:D:135:ALA:HB3	2.00	0.42
3:A:197:LEU:HD12	3:A:197:LEU:C	2.39	0.42
3:C:284:ASN:HD21	3:C:829:LYS:HZ3	1.67	0.42
3:A:507:ASN:O	3:A:534:SER:HA	2.19	0.42
3:C:330:ARG:HG2	3:C:330:ARG:H	1.67	0.42
3:A:116:GLU:HB2	3:A:135:ALA:HB3	2.02	0.42
3:D:863:LEU:HA	3:D:866:MET:HG3	2.01	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:A:52:ILE:HD12	3:A:428:GLU:HB3	2.02	0.42

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:244:PRO:HD2	3:B:266:PHE:O	2.21	0.40
3:B:78:ILE:HD12	3:B:80:LEU:HD12	2.03	0.40
3:D:90:LEU:HD22	3:D:353:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	901/906 (99%)	875 (97%)	25 (3%)	1 (0%)	56	83
3	B	899/906 (99%)	858 (95%)	38 (4%)	3 (0%)	46	74
3	C	901/906 (99%)	873 (97%)	27 (3%)	1 (0%)	56	83
3	D	896/906 (99%)	855 (95%)	39 (4%)	2 (0%)	52	80
All	All	3597/3624 (99%)	3461 (96%)	129 (4%)	7 (0%)	52	80

All (7) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	800/803 (100%)	769 (96%)	31 (4%)	39	69
3	B	798/803 (99%)	769 (96%)	29 (4%)	42	72
3	C	800/803 (100%)	771 (96%)	29 (4%)	42	72
3	D	795/803 (99%)	783 (98%)	12 (2%)	72	91
All	All	3193/3212 (99%)	3092 (97%)	101 (3%)	46	76

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

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

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

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

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

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (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	$\#\|Z\| > 2$
1	5OC	E	3	1	12,21,22	1.30	1 (8%)	12,30,33	0.36	0
1	5OC	G	3	1	0,3,22	0.00	-	0,3,33	0.00	-
1	5OC	I	3	1	12,21,22	1.34	1 (8%)	12,30,33	0.62	0
1	5OC	K	3	1	0,3,22	0.00	-	0,3,33	0.00	-

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	3	5OC	C6-C5	-3.85	1.34	1.39
1	E	3	5OC	C6-C5	-3.75	1.34	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	907	-	4,4,4	0.40	0	6,6,6	0.17	0
4	SO4	C	907	-	4,4,4	0.38	0	6,6,6	0.09	0
4	SO4	F	3	-	4,4,4	0.36	0	6,6,6	0.06	0
4	SO4	H	2	-	4,4,4	0.37	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	907	-	-	0/0/0/0	0/0/0/0
4	SO4	C	907	-	-	0/0/0/0	0/0/0/0
4	SO4	F	3	-	-	0/0/0/0	0/0/0/0
4	SO4	H	2	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.40	2 (11%) 6 5	57, 89, 126, 143	0
1	G	16/18 (88%)	1.96	7 (43%) 0 0	62, 114, 138, 155	0
1	I	16/18 (88%)	-0.29	0 100 100	37, 50, 70, 94	0
1	K	14/18 (77%)	3.02	10 (71%) 0 0	53, 162, 197, 200	0
2	F	15/15 (100%)	0.82	1 (6%) 21 20	72, 87, 138, 141	0
2	H	13/15 (86%)	2.29	6 (46%) 0 0	94, 116, 140, 141	0
2	J	15/15 (100%)	-0.26	0 100 100	36, 61, 87, 87	0
2	L	11/15 (73%)	2.39	6 (54%) 0 0	158, 169, 173, 174	0
3	A	903/906 (99%)	0.32	52 (5%) 26 26	30, 54, 146, 263	0
3	B	901/906 (99%)	1.00	159 (17%) 2 1	34, 80, 218, 286	0
3	C	903/906 (99%)	0.30	41 (4%) 37 36	28, 62, 135, 197	0
3	D	898/906 (99%)	1.44	243 (27%) 1 1	84, 135, 213, 253	0
All	All	3722/3756 (99%)	0.78	527 (14%) 4 3	28, 78, 201, 286	0

All (527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	819	ILE	19.3
3	B	821	ALA	13.1
3	B	820	ASP	12.4
3	B	862	VAL	11.2
3	D	257	TYR	11.1
3	D	111	ALA	11.0
3	B	256	MET	10.3
3	A	505	ASN	9.5
3	B	286	PRO	9.2
3	D	789	ALA	9.1
3	A	256	MET	9.1

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Mol	Chain	Res	Type	RSRZ
3	D	395	PHE	8.6
3	D	522	PHE	8.2
3	D	523	SER	8.0
3	D	215	GLY	7.8
3	B	798	GLY	7.7
3	D	282	PHE	7.7
3	B	812	ASN	7.6
3	B	857	LEU	7.4
3	B	516	VAL	7.3
3	D	256	MET	7.1
3	B	507	ASN	7.0
3	D	788	ILE	7.0
3	B	257	TYR	6.8
3	D	394	ALA	6.8
3	D	504	HIS	6.8
3	B	528	GLU	6.8
3	C	510	VAL	6.7
3	B	818	ASN	6.7
3	D	792	ASP	6.6
3	D	787	ASN	6.6
3	B	801	CYS	6.5
3	B	541	MET	6.5
3	D	506	PRO	6.4
3	B	499	ILE	6.4
3	D	1	MET	6.4
3	B	539	ASN	6.3
3	B	865	TRP	6.3
3	D	491	ALA	6.3
3	A	516	VAL	6.2
3	D	258	GLY	6.2
3	D	510	VAL	6.1
3	A	498	ILE	6.0
3	B	287	SER	6.0
3	B	816	LYS	6.0
3	B	809	LEU	6.0
1	G	7	DA	5.9
3	B	799	PRO	5.9
3	B	811	TYR	5.8
1	K	2	DC	5.8
3	D	391	TYR	5.7
3	B	847	ALA	5.7
3	D	214	THR	5.7

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Mol	Chain	Res	Type	RSRZ
3	B	498	ILE	5.7
3	D	269	SER	5.6
3	D	254	GLU	5.5
3	D	520	PHE	5.5
3	D	165	GLU	5.5
3	B	846	ILE	5.5
3	D	503	LEU	5.5
3	B	510	VAL	5.4
3	B	789	ALA	5.4
3	D	46	ALA	5.4
3	B	513	PRO	5.4
3	B	840	PRO	5.4
3	A	515	ASP	5.3
3	B	817	GLY	5.3
3	D	498	ILE	5.2
3	A	257	TYR	5.2
3	B	813	ARG	5.2
3	B	514	LEU	5.1
3	D	270	VAL	5.1
3	D	305	TYR	5.1
3	D	210	PRO	5.1
3	B	852	THR	5.1
3	D	511	ASP	5.1
3	B	255	ASN	5.0
3	A	532	LYS	5.0
3	D	160	GLU	5.0
3	A	495	ASN	5.0
3	D	137	THR	5.0
3	D	138	HIS	5.0
3	B	805	ILE	4.9
3	B	254	GLU	4.9
3	B	791	TYR	4.9
3	B	839	ASN	4.9
3	B	858	ILE	4.9
3	D	328	VAL	4.8
3	B	825	VAL	4.8
3	A	514	LEU	4.8
3	D	528	GLU	4.8
1	K	8	DT	4.7
3	B	298	LEU	4.7
3	B	504	HIS	4.7
3	A	503	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
3	B	824	VAL	4.7
3	A	530	ILE	4.7
3	B	785	ALA	4.7
3	B	792	ASP	4.7
1	K	1	DC	4.7
3	B	505	ASN	4.7
3	B	538	LEU	4.7
3	B	822	PRO	4.6
3	B	793	VAL	4.6
3	B	863	LEU	4.6
3	B	526	ILE	4.6
3	B	838	GLY	4.5
3	B	160	GLU	4.5
2	H	108	DT	4.5
3	B	184	ASP	4.5
3	A	253	ILE	4.5
3	D	164	ILE	4.5
3	B	288	TYR	4.5
3	B	866	MET	4.5
3	B	861	ASP	4.4
3	D	131	HIS	4.4
3	C	256	MET	4.4
3	B	521	ASP	4.4
3	D	241	ARG	4.4
3	B	128	GLN	4.4
3	B	260	ARG	4.4
3	B	802	PRO	4.4
3	D	517	ASP	4.4
3	D	253	ILE	4.4
3	B	790	LYS	4.4
3	D	120	PRO	4.4
3	A	497	GLU	4.4
3	D	207	GLN	4.3
3	B	851	GLY	4.3
3	D	114	ASP	4.3
1	K	13	DG	4.3
3	D	488	TYR	4.3
3	D	162	TRP	4.3
3	D	255	ASN	4.3
3	D	180	SER	4.2
3	D	823	GLN	4.2
1	K	14	DC	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	829	LYS	4.2
3	D	188	TYR	4.2
3	B	815	ILE	4.2
3	D	16	PHE	4.2
3	B	856	ASP	4.1
3	D	192	ASP	4.1
3	B	192	ASP	4.1
3	A	254	GLU	4.1
3	B	804	HIS	4.1
3	D	482	ARG	4.0
2	H	105	DC	4.0
3	A	508	LEU	4.0
3	D	268	ILE	4.0
3	D	547	ARG	4.0
3	D	267	GLY	4.0
3	A	541	MET	4.0
3	D	252	VAL	4.0
3	D	546	GLN	4.0
3	D	340	PHE	4.0
1	K	7	DA	4.0
3	D	293	ILE	4.0
3	A	504	HIS	4.0
3	B	797	PRO	4.0
3	B	512	GLU	4.0
3	D	200	GLU	4.0
3	C	530	ILE	4.0
3	B	827	GLY	3.9
1	K	15	DC	3.9
3	D	169	LYS	3.9
3	D	44	SER	3.9
3	C	511	ASP	3.9
3	D	297	GLU	3.8
3	D	791	TYR	3.8
3	B	155	PRO	3.8
3	D	393	GLY	3.8
3	D	537	SER	3.8
3	D	543	PHE	3.8
3	B	540	GLU	3.8
3	B	1	MET	3.8
3	D	66	ARG	3.8
3	B	517	ASP	3.8
3	D	245	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	103	DG	3.7
3	B	508	LEU	3.7
3	D	334	ILE	3.7
3	D	323	TYR	3.7
1	G	1	DC	3.7
3	A	1	MET	3.7
3	D	384	ARG	3.7
3	D	129	ALA	3.7
3	B	157	GLY	3.7
3	D	130	LYS	3.7
3	D	139	TYR	3.7
3	D	277	TYR	3.7
3	B	156	TYR	3.6
3	A	536	LYS	3.6
3	A	903	PHE	3.6
3	D	280	PHE	3.6
2	L	101	DG	3.6
2	H	107	DG	3.6
3	D	26	GLU	3.6
3	A	500	LYS	3.6
3	D	793	VAL	3.6
3	B	518	TYR	3.6
3	D	553	MET	3.6
1	K	11	DC	3.6
3	B	828	GLU	3.6
3	D	112	ASN	3.5
3	B	121	ASP	3.5
3	D	21	ASP	3.5
3	D	527	LYS	3.5
3	D	152	LEU	3.5
3	D	296	PHE	3.5
3	B	253	ILE	3.5
3	D	238	THR	3.5
3	A	502	ALA	3.5
3	D	156	TYR	3.5
3	B	542	LEU	3.5
3	B	837	GLU	3.5
3	D	284	ASN	3.4
3	C	257	TYR	3.4
3	D	824	VAL	3.4
3	B	303	LEU	3.4
1	G	8	DT	3.4

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Mol	Chain	Res	Type	RSRZ
3	D	545	ALA	3.4
3	B	172	GLU	3.4
3	D	784	SER	3.4
3	D	514	LEU	3.4
3	D	828	GLU	3.4
3	A	537	SER	3.4
3	B	544	ARG	3.4
3	D	48	LYS	3.4
3	D	508	LEU	3.4
2	H	113	DC	3.4
3	D	338	ARG	3.3
3	B	258	GLY	3.3
3	D	73	LYS	3.3
2	L	105	DC	3.3
3	A	513	PRO	3.3
3	B	522	PHE	3.3
3	D	509	SER	3.3
3	D	286	PRO	3.3
3	D	785	ALA	3.3
3	D	259	SER	3.3
2	H	106	DT	3.3
3	B	117	VAL	3.3
3	D	107	LYS	3.3
3	D	769	LYS	3.3
3	C	111	ALA	3.3
3	D	150	ASP	3.3
3	D	819	ILE	3.3
3	B	808	ILE	3.2
3	D	24	GLY	3.2
3	D	217	ASN	3.2
3	C	254	GLU	3.2
3	B	524	ASP	3.2
3	D	153	ASN	3.2
3	B	519	ARG	3.2
1	K	12	DA	3.2
3	D	219	GLU	3.2
3	B	503	LEU	3.2
3	B	234	PHE	3.2
3	D	799	PRO	3.2
3	B	842	GLY	3.2
3	A	512	GLU	3.2
3	D	266	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
3	B	259	SER	3.2
3	D	696	LYS	3.2
3	B	803	PHE	3.2
3	D	127	SER	3.2
3	D	161	GLU	3.2
3	D	345	LEU	3.1
3	D	392	PRO	3.1
3	B	252	VAL	3.1
3	B	532	LYS	3.1
3	D	281	SER	3.1
3	B	831	TYR	3.1
3	A	522	PHE	3.1
3	B	787	ASN	3.1
3	C	112	ASN	3.1
3	B	523	SER	3.1
3	D	500	LYS	3.1
3	D	11	ILE	3.1
3	D	212	ILE	3.1
3	D	113	PHE	3.1
3	D	574	TRP	3.1
3	D	92	TYR	3.1
3	D	128	GLN	3.1
3	D	356	GLN	3.1
3	B	296	PHE	3.1
3	D	344	SER	3.1
3	A	112	ASN	3.1
3	D	446	VAL	3.1
3	D	288	TYR	3.0
3	B	545	ALA	3.0
3	C	1	MET	3.0
3	D	173	GLN	3.0
3	D	313	ARG	3.0
3	C	612	GLU	3.0
3	A	518	TYR	3.0
3	B	285	GLN	3.0
3	C	213	LEU	3.0
3	D	330	ARG	3.0
3	B	826	GLU	3.0
3	D	271	LEU	3.0
3	B	294	SER	3.0
3	A	544	ARG	3.0
3	B	543	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	329	TYR	3.0
3	A	511	ASP	3.0
3	D	516	VAL	3.0
3	D	837	GLU	2.9
3	D	147	TYR	2.9
3	D	292	TYR	2.9
3	B	292	TYR	2.9
3	D	820	ASP	2.9
3	C	500	LYS	2.9
3	B	320	TYR	2.9
3	C	513	PRO	2.9
3	D	136	ILE	2.9
3	D	519	ARG	2.9
3	D	612	GLU	2.9
3	D	542	LEU	2.9
3	D	240	LYS	2.9
3	A	857	LEU	2.8
3	D	3	GLU	2.8
2	L	104	DG	2.8
3	B	315	SER	2.8
3	A	135	ALA	2.8
3	B	277	TYR	2.8
3	C	260	ARG	2.8
3	D	298	LEU	2.8
3	D	211	VAL	2.8
3	C	543	PHE	2.8
3	B	174	GLY	2.8
1	E	1	DC	2.8
3	D	471	VAL	2.8
1	G	13	DG	2.8
3	A	137	THR	2.8
3	D	23	ASN	2.8
3	D	134	ASP	2.8
3	D	495	ASN	2.8
3	D	320	TYR	2.8
3	B	497	GLU	2.8
3	A	547	ARG	2.8
3	D	811	TYR	2.7
3	A	115	ILE	2.7
3	D	25	ARG	2.7
3	D	544	ARG	2.7
3	D	857	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	233	ILE	2.7
3	D	213	LEU	2.7
3	C	253	ILE	2.7
3	D	185	LYS	2.7
3	A	113	PHE	2.7
3	D	221	PHE	2.7
3	D	548	THR	2.7
3	C	498	ILE	2.7
3	D	110	VAL	2.7
3	C	488	TYR	2.7
3	D	234	PHE	2.7
3	B	731	GLU	2.7
3	C	512	GLU	2.7
3	D	172	GLU	2.7
3	D	171	GLN	2.7
3	B	120	PRO	2.7
3	B	900	MET	2.7
3	A	283	THR	2.7
3	D	283	THR	2.7
3	D	570	LEU	2.6
3	B	556	GLN	2.6
3	B	280	PHE	2.6
3	B	868	TYR	2.6
3	D	302	LYS	2.6
3	D	20	ILE	2.6
3	D	497	GLU	2.6
3	D	348	GLY	2.6
3	A	524	ASP	2.6
3	B	549	GLU	2.6
3	D	355	ILE	2.6
3	C	301	GLY	2.6
3	D	484	GLU	2.6
3	D	331	VAL	2.6
3	A	548	THR	2.6
3	D	158	ASN	2.6
3	D	790	LYS	2.6
3	C	192	ASP	2.6
2	L	110	DA	2.6
3	C	527	LYS	2.6
3	B	134	ASP	2.6
3	B	843	ASP	2.6
3	D	354	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	110	VAL	2.6
3	C	586	ILE	2.6
3	D	149	PHE	2.6
3	D	795	GLY	2.5
3	D	389	GLN	2.5
3	B	116	GLU	2.5
3	D	705	LYS	2.5
3	D	175	GLY	2.5
3	A	539	ASN	2.5
3	D	303	LEU	2.5
3	B	506	PRO	2.5
3	A	255	ASN	2.5
3	B	535	ALA	2.5
3	B	895	ALA	2.5
3	D	324	ASN	2.5
3	D	194	GLU	2.5
3	D	216	TRP	2.5
3	B	135	ALA	2.5
3	C	900	MET	2.5
3	D	341	ILE	2.5
1	G	14	DC	2.5
3	D	851	GLY	2.5
3	D	327	ALA	2.5
3	D	525	GLU	2.5
3	D	539	ASN	2.5
3	D	786	ASN	2.5
3	B	536	LYS	2.4
3	A	499	ILE	2.4
3	B	525	GLU	2.4
3	D	818	ASN	2.4
3	A	136	ILE	2.4
3	B	502	ALA	2.4
3	D	218	VAL	2.4
3	B	794	GLY	2.4
3	D	390	PRO	2.4
3	D	43	GLU	2.4
3	D	260	ARG	2.4
3	B	133	ILE	2.4
3	D	157	GLY	2.4
3	A	375	GLU	2.4
3	C	902	ASP	2.4
3	D	494	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	252	VAL	2.4
3	D	222	ALA	2.4
3	B	321	ILE	2.4
3	B	251	LYS	2.4
3	B	833	LEU	2.3
2	H	109	DC	2.3
3	C	526	ILE	2.3
3	B	520	PHE	2.3
3	B	330	ARG	2.3
3	D	29	ARG	2.3
3	D	119	SER	2.3
3	A	793	VAL	2.3
3	D	31	VAL	2.3
3	D	538	LEU	2.3
3	B	642	ARG	2.3
1	E	2	DC	2.3
3	C	532	LYS	2.3
3	D	301	GLY	2.3
3	C	347	MET	2.3
3	A	114	ASP	2.3
3	D	557	ILE	2.3
3	D	309	ILE	2.3
3	D	700	GLY	2.3
3	A	506	PRO	2.3
1	G	5	DG	2.3
3	D	489	MET	2.3
3	A	629	ALA	2.3
3	B	814	ALA	2.3
3	D	535	ALA	2.3
3	D	410	PHE	2.3
3	D	607	GLU	2.3
3	B	324	ASN	2.3
3	D	193	ASN	2.3
3	D	294	SER	2.2
2	F	104	DG	2.2
3	D	782	VAL	2.2
2	L	102	DC	2.2
3	C	528	GLU	2.2
3	D	117	VAL	2.2
3	D	534	SER	2.2
3	D	650	PHE	2.2
3	B	853	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	B	490	LEU	2.2
3	B	547	ARG	2.2
3	D	170	LEU	2.2
3	D	479	PHE	2.2
3	D	815	ILE	2.2
3	D	177	GLU	2.2
3	C	107	LYS	2.2
3	D	706	LYS	2.2
3	B	511	ASP	2.2
3	D	490	LEU	2.1
3	D	493	GLN	2.1
3	B	850	SER	2.1
3	C	212	ILE	2.1
3	C	903	PHE	2.1
3	D	184	ASP	2.1
3	D	816	LYS	2.1
3	B	777	ILE	2.1
3	D	838	GLY	2.1
3	C	901	PHE	2.1
3	B	122	GLY	2.1
3	B	788	ILE	2.1
3	D	475	ILE	2.1
3	D	135	ALA	2.1
3	B	509	SER	2.1
3	D	125	GLU	2.1
3	D	683	MET	2.1
3	D	512	GLU	2.1
3	A	252	VAL	2.1
3	C	255	ASN	2.1
3	C	328	VAL	2.1
3	B	115	ILE	2.1
3	C	113	PHE	2.1
3	C	251	LYS	2.1
3	C	738	PRO	2.1
3	D	357	SER	2.0
3	B	153	ASN	2.0
3	A	510	VAL	2.0
3	D	2	LYS	2.0
3	D	470	VAL	2.0
3	D	513	PRO	2.0
3	D	802	PRO	2.0
3	C	261	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	614	GLU	2.0
3	A	493	GLN	2.0
3	B	90	LEU	2.0
3	D	201	TYR	2.0
3	D	536	LYS	2.0
1	G	9	DG	2.0
1	K	16	DG	2.0
3	B	836	ARG	2.0
3	B	496	GLY	2.0
3	A	529	LYS	2.0
3	B	774	LEU	2.0
3	B	898	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	5OC	G	3	4/21	0.96	0.12	-	108,111,111,113	0
1	5OC	I	3	20/21	0.90	0.22	-	78,91,100,100	0
1	5OC	K	3	4/21	0.65	0.32	-	123,130,134,136	0
1	5OC	E	3	20/21	0.62	0.35	-	148,155,160,160	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	C	907	5/5	0.87	0.20	-0.42	112,115,116,120	0
4	SO4	B	907	5/5	0.93	0.32	-	83,85,88,88	0
4	SO4	H	2	5/5	0.80	0.24	-	126,128,128,130	0
4	SO4	F	3	5/5	0.90	0.16	-	121,121,123,124	0

6.5 Other polymers (i)

There are no such residues in this entry.