Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:14 PM GMT

PDB ID	:	3TAB
Title	:	5-hydroxycytosine paired with dGMP in RB69 gp43
Authors	:	Zahn, K.E.
Deposited on	:	2011-08-03
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

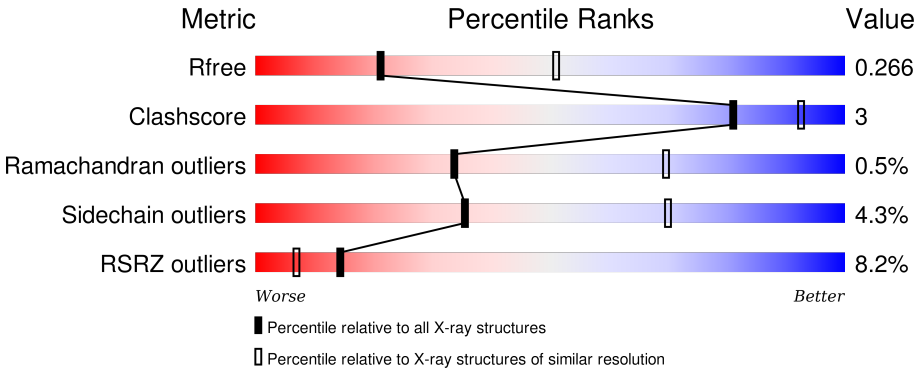
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	A	906	8% 86% 13%
1	B	906	6% 89% 9%
1	C	906	4% 87% 12%
1	D	906	15% 89% 10%
2	E	18	83% 17%

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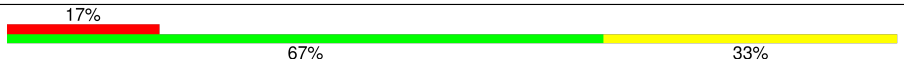
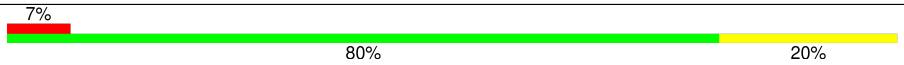
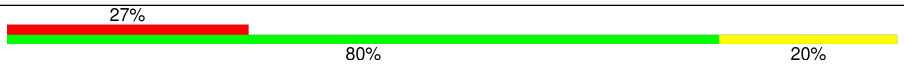
Mol	Chain	Length	Quality of chain
2	G	18	
2	I	18	
2	K	18	
3	F	15	
3	H	15	
3	J	15	
3	L	15	

2 Entry composition (i)

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

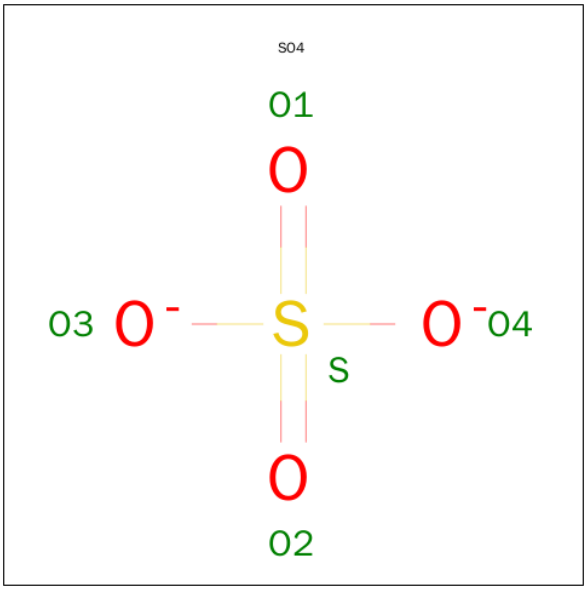
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

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 (three-letter code: SO4) (formula: O_4S).



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.

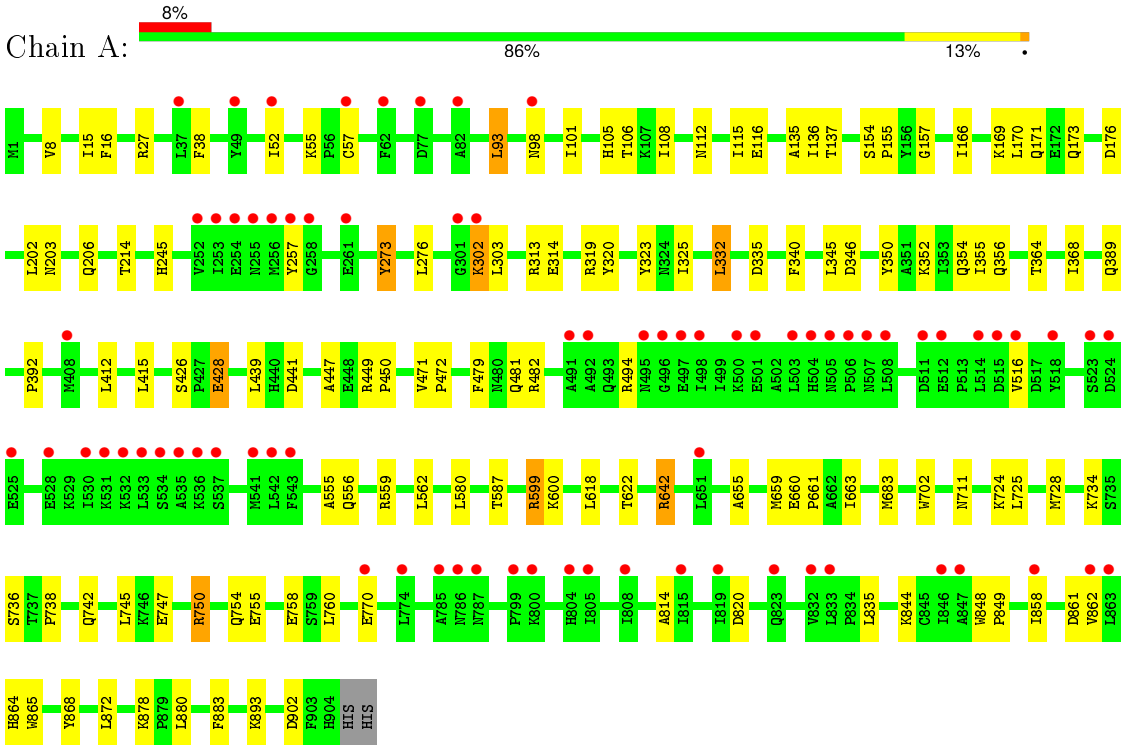
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	E	1	Total O 1 1	0	0
5	B	71	Total O 71 71	0	0
5	G	6	Total O 6 6	0	0
5	H	6	Total O 6 6	0	0
5	C	39	Total O 39 39	0	0
5	I	4	Total O 4 4	0	0
5	D	10	Total O 10 10	0	0
5	K	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

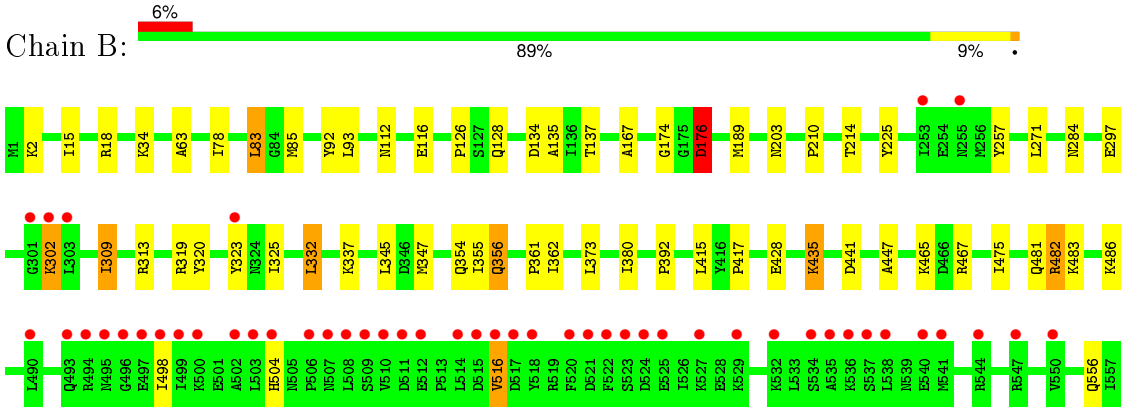
- Molecule 1: DNA polymerase

Chain A:



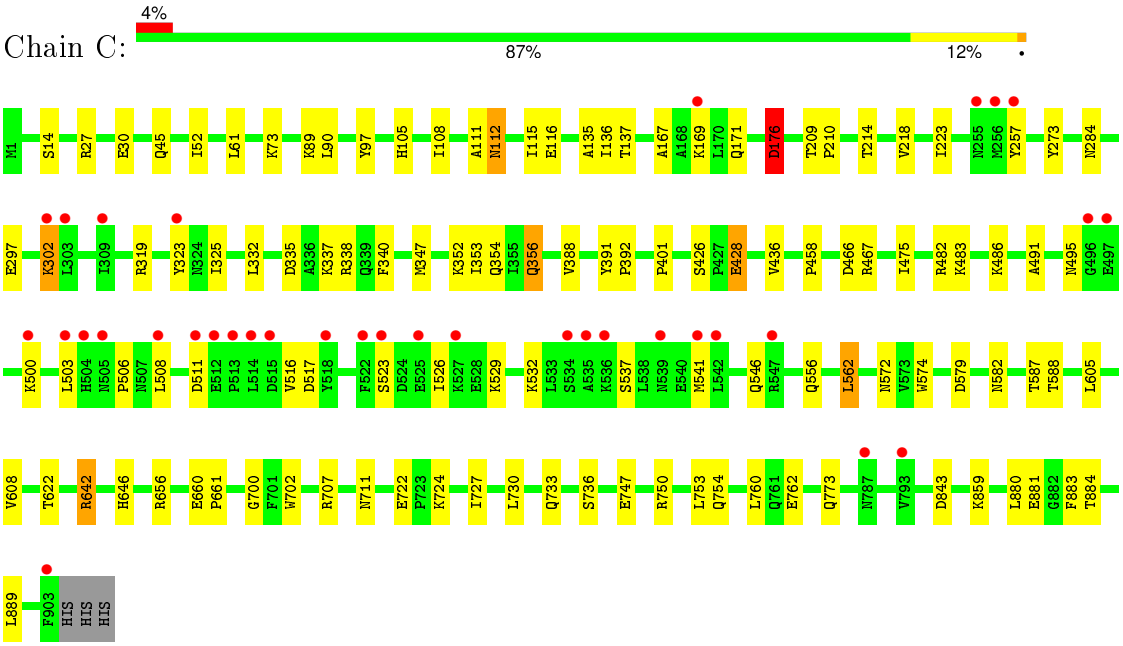
- Molecule 1: DNA polymerase

Chain B:



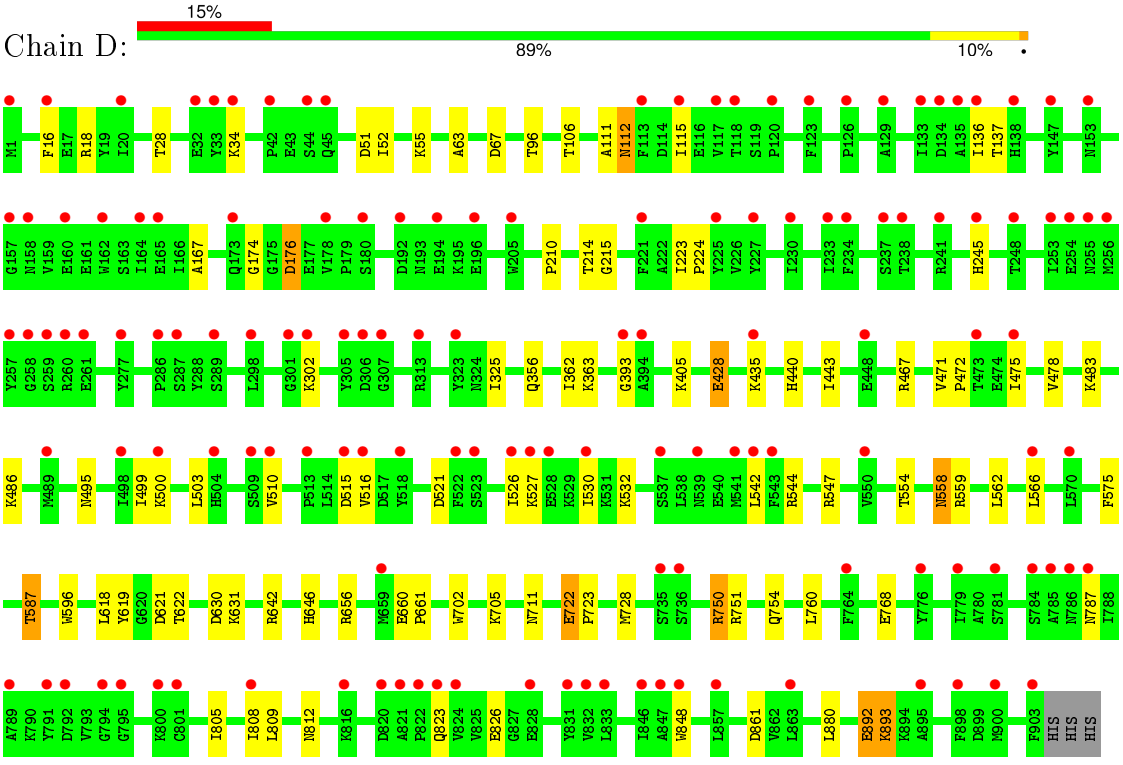
• Molecule 1: DNA polymerase

Chain C:



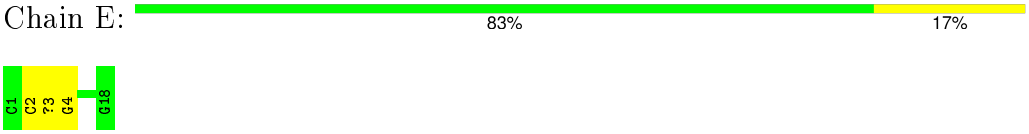
• Molecule 1: DNA polymerase

Chain D:



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

Chain E:

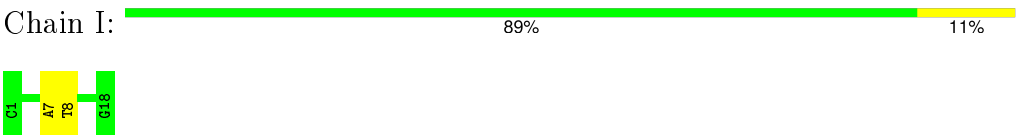


• Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:

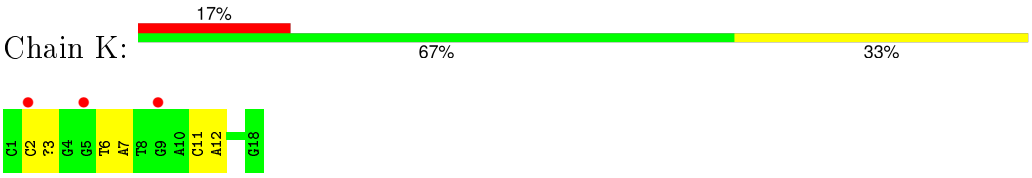
• Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:



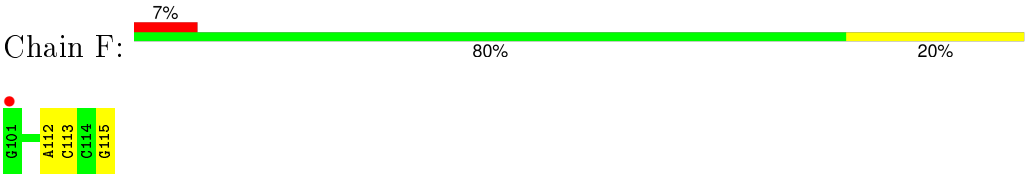
• Molecule 2: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:



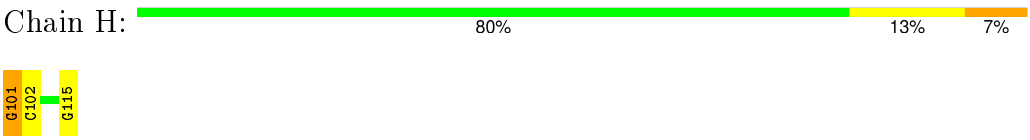
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain F:



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

Chain H:

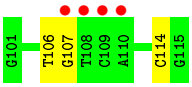


• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*G)-3')

Chain J:

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

Chain L:



4 Data and refinement statistics (i)

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 49.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.80) 100.0 (49.48-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.232 , 0.281 0.220 , 0.266	Depositor DCC
R_{free} test set	12694 reflections (10.67%)	DCC
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 , 39.8	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 131746 reflections	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.*

[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	A	0.41	2/7566 (0.0%)	0.48	0/10224
1	B	0.41	1/7566 (0.0%)	0.50	0/10224
1	C	0.41	1/7555 (0.0%)	0.49	0/10209
1	D	0.41	3/7555 (0.0%)	0.46	0/10209
2	E	0.22	0/387	0.75	0/593
2	G	0.54	1/391 (0.3%)	0.77	0/597
2	I	0.23	0/387	0.78	0/593
2	K	0.21	0/387	0.78	0/593
3	F	0.21	0/340	0.77	0/523
3	H	0.24	0/340	0.83	1/523 (0.2%)
3	J	0.28	0/340	0.82	1/523 (0.2%)
3	L	0.20	0/340	0.83	0/523
All	All	0.40	8/33154 (0.0%)	0.52	2/45334 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	DC	OP3-P	-9.49	1.49	1.61
1	C	702	TRP	CD2-CE2	5.15	1.47	1.41
1	B	848	TRP	CD2-CE2	5.07	1.47	1.41
1	A	702	TRP	CD2-CE2	5.07	1.47	1.41
1	D	596	TRP	CD2-CE2	5.04	1.47	1.41
1	D	702	TRP	CD2-CE2	5.03	1.47	1.41
1	A	865	TRP	CD2-CE2	5.01	1.47	1.41
1	D	848	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	101	DG	P-O3'-C3'	5.70	126.54	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	101	DG	P-O3'-C3'	5.23	125.97	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	59	0
1	B	7384	0	7274	50	0
1	C	7374	0	7267	46	0
1	D	7374	0	7267	39	0
2	E	366	0	201	3	0
2	G	370	0	200	6	0
2	I	366	0	201	2	0
2	K	366	0	201	4	0
3	F	304	0	170	3	0
3	H	304	0	170	2	0
3	J	304	0	170	2	0
3	L	304	0	170	3	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
4	K	5	0	0	0	0
5	A	25	0	0	4	0
5	B	71	0	0	0	0
5	C	39	0	0	0	0
5	D	10	0	0	1	0
5	E	1	0	0	0	0
5	G	6	0	0	0	0
5	H	6	0	0	0	0
5	I	4	0	0	0	0
5	K	1	0	0	0	0
All	All	32383	0	30565	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HG22	1:C:136:ILE:HG12	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:B:486:LYS:HG2	1:B:556:GLN:HG3	1.89	0.54
1:A:711:ASN:HD21	1:A:754:GLN:HE21	1.55	0.54
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.89	0.53
1:C:572:ASN:ND2	1:C:574:TRP:H	2.06	0.53
1:A:738:PRO:O	1:A:742:GLN:HB2	2.08	0.53
1:D:554:THR:O	1:D:558:ASN:HB2	2.09	0.53
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.90	0.53
1:D:111:ALA:HB3	1:D:210:PRO:HB3	1.91	0.53
2:G:15:DC:H2'	2:G:16:DG:C8	2.44	0.53
1:B:112:ASN:HB3	1:B:214:THR:CG2	2.35	0.53
1:D:440:HIS:HA	1:D:443:ILE:HD12	1.91	0.53
1:C:112:ASN:HB3	1:C:214:THR:CG2	2.40	0.52
1:B:660:GLU:HB2	1:B:661:PRO:HD3	1.92	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:C:302:LYS:H	1:C:302:LYS:HD2	1.75	0.51
1:B:167:ALA:HA	1:B:176:ASP:HB2	1.92	0.51
3:J:102:DC:H2"	3:J:103:DG:C8	2.45	0.51
1:C:391:TYR:HB2	1:C:392:PRO:HD2	1.94	0.50
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.94	0.50
1:D:214:THR:OG1	1:D:215:GLY:N	2.45	0.50
1:B:126:PRO:HA	1:B:225:TYR:CD2	2.46	0.50
2:I:7:DA:H2'	2:I:8:DT:H71	1.93	0.50
1:A:655:ALA:HA	1:A:659:MET:HB2	1.94	0.49
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.94	0.49
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.13	0.49
1:B:83:LEU:HD23	1:B:83:LEU:H	1.78	0.49
1:C:503:LEU:HA	1:C:506:PRO:HG3	1.93	0.49
1:A:101:ILE:HD12	1:A:352:LYS:HG2	1.95	0.49
1:A:660:GLU:HB2	1:A:661:PRO:HD3	1.95	0.49
1:B:354:GLN:HB3	1:B:356:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ASN:ND2	1:B:754:GLN:HE21	2.11	0.48
1:D:478:VAL:HG13	1:D:559:ARG:HD3	1.94	0.48
1:A:814:ALA:HB1	1:A:858:ILE:HG21	1.94	0.48
1:C:605:LEU:HA	1:C:608:VAL:HG22	1.94	0.48
1:D:728:MET:HG3	3:L:114:DC:H5"	1.95	0.48
1:B:126:PRO:HA	1:B:225:TYR:HD2	1.78	0.48
1:C:529:LYS:HD3	1:C:532:LYS:HD2	1.95	0.48
1:D:500:LYS:HA	1:D:503:LEU:HB2	1.95	0.48
1:B:34:LYS:HE3	1:B:63:ALA:HA	1.96	0.48
1:A:157:GLY:O	1:A:313:ARG:NH2	2.46	0.48
1:B:297:GLU:O	1:B:337:LYS:HE2	2.12	0.48
1:A:368:ILE:HD13	1:A:562:LEU:HD21	1.96	0.48
1:A:355:ILE:HD12	1:A:355:ILE:H	1.78	0.48
3:H:101:DG:H2"	3:H:102:DC:OP2	2.13	0.47
1:D:115:ILE:HG22	1:D:136:ILE:HG12	1.96	0.47
1:D:711:ASN:ND2	1:D:754:GLN:HE21	2.11	0.47
1:B:116:GLU:HB3	1:B:320:TYR:OH	2.15	0.47
1:A:202:LEU:O	1:A:206:GLN:HG2	2.14	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:D:660:GLU:HB2	1:D:661:PRO:HD3	1.97	0.47
1:C:727:ILE:HG23	1:C:730:LEU:HD12	1.96	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: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
1:B:18:ARG:NH2	1:B:210:PRO:O	2.47	0.45
1:B:15:ILE:HD11	1:B:92:TYR:CZ	2.51	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:B:362:ILE:HG12	2:G:2:DC:OP2	2.17	0.45
2:G:7:DA:H2"	2:G:8:DT:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:TYR:OH	1:C:335:ASP:HA	2.17	0.45
1:A:868:TYR:O	1:A:872:LEU:N	2.46	0.45
1:D:16:PHE:HB3	1:D:245:HIS:CE1	2.52	0.45
2:E:3:5OC:O2	3:F:115:DG:N2	2.41	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:HG2	1:A:642:ARG:H	1.59	0.44
1:C:711:ASN:ND2	1:C:754:GLN:HE21	2.15	0.44
1:C:579:ASP:HB3	1:C:582:ASN:HB2	1.99	0.44
1:B:134:ASP:HB2	1:B:313:ARG:NH1	2.32	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:D:393:GLY:HA2	1:D:587:THR:HG21	1.99	0.44
1:C:218:VAL:HG22	1:C:223:ILE:HG13	2.00	0.44
1:B:15:ILE:C	1:B:15:ILE:HD12	2.38	0.44
1:B:309:ILE:H	1:B:309:ILE:HG13	1.56	0.44
1:C:747:GLU:OE2	1:C:750:ARG:NH1	2.51	0.44
1:C:642:ARG:HH11	1:C:646:HIS:CE1	2.36	0.44
1:D:362:ILE:HG23	1:D:575:PHE:HD1	1.83	0.44
1:A:711:ASN:ND2	1:A:754:GLN:HE21	2.16	0.44
1:A:482:ARG:HH11	1:A:556:GLN:HG2	1.83	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: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:B:572:ASN:ND2	1:B:574:TRP:H	2.15	0.43
1:D:52:ILE:HD12	1:D:428:GLU:HG3	2.00	0.43
1:A:449:ARG:HA	1:A:450:PRO:HD3	1.89	0.43
1:C:354:GLN:HB3	1:C:356:GLN:OE1	2.19	0.43
1:A:52:ILE:HB	1:A:428:GLU:HG2	2.00	0.43
1:A:736:SER:OG	3:F:112:DA:H5"	2.19	0.43
1:D:642:ARG:HH21	1:D:646:HIS:CE1	2.37	0.43
1:D:495:ASN:O	1:D:499:ILE:HG12	2.19	0.43
1:A:313:ARG:HD2	5:A:930:HOH:O	2.19	0.43
1:A:599:ARG:HH12	1:A:600:LYS:HE2	1.84	0.43
2:E:2:DC:H2'	2:E:3:5OC:H6	2.01	0.42
1:B:137:THR:HG21	1:B:325:ILE:HA	2.01	0.42
1:D:805:ILE:HA	1:D:808:ILE:HD12	2.01	0.42
1:B:784:SER:HA	1:B:829:LYS:HA	2.01	0.42
1:A:441:ASP:HB3	1:A:447:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ALA:HB3	1:C:210:PRO:HB3	2.00	0.42
1:A:276:LEU:HG	1:A:340:PHE: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:747:GLU:OE2	1:A:750:ARG:NH1	2.53	0.42
1:A:303:LEU:HG	1:A:323:TYR:CZ	2.55	0.42
1:C:105:HIS:HA	1:C:108:ILE:HD12	2.02	0.41
1:B:373:LEU:HD12	1:B:380:ILE:HG22	2.02	0.41
1:B:271:LEU:HD11	1:B:355:ILE:CG2	2.51	0.41
2:K:6:DT:H2"	2:K:7:DA:H8	1.84	0.41
1:C:176:ASP:OD1	1:C:319:ARG:HD3	2.20	0.41
2:G:7:DA:H2'	2:G:8:DT:C6	2.55	0.41
1:B:85:MET:HA	1:B:380:ILE:HD11	2.01	0.41
1:D:527:LYS:O	1:D:530:ILE:HG22	2.19	0.41
1:C:537:SER:O	1:C:541:MET:HG2	2.20	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:D:619:TYR:CE2	1:D:621:ASP:HB2	2.56	0.41
1:A:302:LYS:HD2	1:A:302:LYS:H	1.85	0.41
1:C:736:SER:HB3	3:J:112:DA:H5"	2.03	0.41
1:C:209:THR:HA	1:C:210:PRO:HD3	1.86	0.41
1:C:700:GLY:HA2	1:C:753:LEU:HD22	2.03	0.41
1:C:523:SER:HB3	1:C:526:ILE:HG12	2.03	0.41
1:A:862:VAL:C	1:A:864:HIS:H	2.22	0.41
1:A:345:LEU:HD23	1:A:355:ILE:HG12	2.03	0.41
1:B:112:ASN:HD21	1:B:332:LEU:CD1	2.34	0.41
2:E:3:5OC:H2'	2:E:4:DG:C8	2.56	0.41
1:B:347:MET:CE	1:B:558:ASN:HD22	2.32	0.41
1:D:51:ASP:HB2	5:D:910:HOH:O	2.21	0.41
1:D:223:ILE:N	1:D:224:PRO:HD2	2.36	0.41
1:A:482:ARG:HD2	1:A:556:GLN:HG2	2.02	0.41
1:A:663:ILE:HG21	1:A:683:MET:HB3	2.01	0.41
1:C:587:THR:HG22	1:C:588:THR:N	2.35	0.41
1:B:112:ASN:HD21	1:B:332:LEU:HD11	1.85	0.40
1:D:728:MET:HG3	3:L:114:DC:OP1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3:5OC:O2	3:H:115:DG:N2	2.45	0.40
1:B:465:LYS:HE2	1:B:677:LYS:HA	2.03	0.40
1:A:137:THR:HG21	1:A:325:ILE:HA	2.04	0.40
1:A:16:PHE:HB3	1:A:245:HIS:CE1	2.57	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%)	46	79
1	B	902/906 (100%)	859 (95%)	39 (4%)	4 (0%)	39	74
1	C	901/906 (99%)	864 (96%)	32 (4%)	5 (1%)	30	65
1	D	901/906 (99%)	855 (95%)	41 (5%)	5 (1%)	30	65
All	All	3606/3624 (100%)	3436 (95%)	153 (4%)	17 (0%)	34	69

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	893	LYS
1	B	176	ASP
1	C	622	THR
1	D	622	THR
1	B	893	LYS
1	C	176	ASP
1	D	892	GLU
1	A	176	ASP
1	C	466	ASP
1	A	622	THR

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Mol	Chain	Res	Type
1	A	893	LYS
1	B	174	GLY
1	C	401	PRO
1	D	176	ASP
1	B	516	VAL
1	D	174	GLY
1	C	458	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	801/803 (100%)	763 (95%)	38 (5%)	32 67
1	B	801/803 (100%)	773 (96%)	28 (4%)	43 77
1	C	800/803 (100%)	760 (95%)	40 (5%)	30 64
1	D	800/803 (100%)	767 (96%)	33 (4%)	37 72
All	All	3202/3212 (100%)	3063 (96%)	139 (4%)	35 70

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	55	LYS
1	A	93	LEU
1	A	98	ASN
1	A	106	THR
1	A	203	ASN
1	A	257	TYR
1	A	273	TYR
1	A	302	LYS
1	A	314	GLU
1	A	332	LEU
1	A	346	ASP
1	A	356	GLN
1	A	389	GLN

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Mol	Chain	Res	Type
1	A	426	SER
1	A	428	GLU
1	A	439	LEU
1	A	479	PHE
1	A	494	ARG
1	A	516	VAL
1	A	580	LEU
1	A	599	ARG
1	A	618	LEU
1	A	642	ARG
1	A	724	LYS
1	A	728	MET
1	A	750	ARG
1	A	755	GLU
1	A	758	GLU
1	A	760	LEU
1	A	770	GLU
1	A	820	ASP
1	A	835	LEU
1	A	844	LYS
1	A	861	ASP
1	A	878	LYS
1	A	880	LEU
1	A	902	ASP
1	B	2	LYS
1	B	83	LEU
1	B	93	LEU
1	B	128	GLN
1	B	176	ASP
1	B	203	ASN
1	B	257	TYR
1	B	284	ASN
1	B	302	LYS
1	B	309	ILE
1	B	332	LEU
1	B	356	GLN
1	B	428	GLU
1	B	435	LYS
1	B	467	ARG
1	B	482	ARG
1	B	483	LYS
1	B	498	ILE

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Mol	Chain	Res	Type
1	B	504	HIS
1	B	516	VAL
1	B	580	LEU
1	B	587	THR
1	B	642	ARG
1	B	668	ARG
1	B	760	LEU
1	B	843	ASP
1	B	880	LEU
1	B	900	MET
1	C	27	ARG
1	C	45	GLN
1	C	61	LEU
1	C	73	LYS
1	C	89	LYS
1	C	112	ASN
1	C	169	LYS
1	C	176	ASP
1	C	257	TYR
1	C	284	ASN
1	C	302	LYS
1	C	332	LEU
1	C	356	GLN
1	C	388	VAL
1	C	426	SER
1	C	428	GLU
1	C	436	VAL
1	C	467	ARG
1	C	475	ILE
1	C	483	LYS
1	C	486	LYS
1	C	500	LYS
1	C	508	LEU
1	C	511	ASP
1	C	516	VAL
1	C	517	ASP
1	C	546	GLN
1	C	562	LEU
1	C	642	ARG
1	C	722	GLU
1	C	724	LYS
1	C	733	GLN

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Mol	Chain	Res	Type
1	C	760	LEU
1	C	762	GLU
1	C	773	GLN
1	C	843	ASP
1	C	859	LYS
1	C	880	LEU
1	C	881	GLU
1	C	883	PHE
1	D	55	LYS
1	D	67	ASP
1	D	96	THR
1	D	106	THR
1	D	112	ASN
1	D	302	LYS
1	D	356	GLN
1	D	363	LYS
1	D	405	LYS
1	D	428	GLU
1	D	435	LYS
1	D	467	ARG
1	D	483	LYS
1	D	486	LYS
1	D	510	VAL
1	D	515	ASP
1	D	521	ASP
1	D	532	LYS
1	D	558	ASN
1	D	562	LEU
1	D	587	THR
1	D	618	LEU
1	D	630	ASP
1	D	631	LYS
1	D	722	GLU
1	D	750	ARG
1	D	760	LEU
1	D	768	GLU
1	D	787	ASN
1	D	823	GLN
1	D	826	GLU
1	D	861	ASP
1	D	880	LEU

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

sidechains are listed below:

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

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

5.3.3 RNA

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	E	3	2	12,21,22	1.29	1 (8%)	12,30,33	0.40	0
2	5OC	G	3	2	12,21,22	1.30	1 (8%)	12,30,33	0.41	0
2	5OC	I	3	2	12,21,22	1.32	1 (8%)	12,30,33	0.41	0
2	5OC	K	3	2	12,21,22	1.32	1 (8%)	12,30,33	0.33	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
2	5OC	E	3	2	-	0/3/21/22	0/2/2/2
2	5OC	G	3	2	-	0/3/21/22	0/2/2/2
2	5OC	I	3	2	-	0/3/21/22	0/2/2/2
2	5OC	K	3	2	-	0/3/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	5OC	C6-C5	-3.83	1.34	1.39
2	K	3	5OC	C6-C5	-3.76	1.34	1.39
2	G	3	5OC	C6-C5	-3.72	1.34	1.39
2	E	3	5OC	C6-C5	-3.72	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.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	E	19	-	4,4,4	0.40	0	6,6,6	0.12	0
4	SO4	G	19	-	4,4,4	0.42	0	6,6,6	0.11	0
4	SO4	I	19	-	4,4,4	0.40	0	6,6,6	0.09	0
4	SO4	K	19	-	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	E	19	-	-	0/0/0/0	0/0/0/0
4	SO4	G	19	-	-	0/0/0/0	0/0/0/0
4	SO4	I	19	-	-	0/0/0/0	0/0/0/0
4	SO4	K	19	-	-	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 (i)

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	A	904/906 (99%)	0.55	75 (8%) 14 7	48, 84, 166, 266	0
1	B	904/906 (99%)	0.34	51 (5%) 28 18	35, 63, 156, 343	0
1	C	903/906 (99%)	0.29	35 (3%) 43 31	38, 68, 137, 233	0
1	D	903/906 (99%)	0.91	137 (15%) 3 1	69, 115, 201, 249	0
2	E	17/18 (94%)	0.02	0 100 100	69, 88, 133, 141	0
2	G	17/18 (94%)	-0.39	0 100 100	37, 52, 71, 72	0
2	I	17/18 (94%)	-0.26	0 100 100	50, 57, 78, 81	0
2	K	17/18 (94%)	1.28	3 (17%) 2 1	87, 123, 145, 148	0
3	F	15/15 (100%)	0.15	1 (6%) 21 12	65, 97, 160, 162	0
3	H	15/15 (100%)	-0.41	0 100 100	40, 53, 77, 82	0
3	J	15/15 (100%)	-0.27	0 100 100	45, 66, 99, 100	0
3	L	15/15 (100%)	1.86	4 (26%) 1 0	104, 145, 162, 163	0
All	All	3742/3756 (99%)	0.51	306 (8%) 14 7	35, 82, 181, 343	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	MET	13.3
1	D	135	ALA	12.2
1	B	510	VAL	10.3
1	D	847	ALA	9.4
1	D	789	ALA	9.2
1	B	499	ILE	8.6
1	A	256	MET	8.1
1	D	257	TYR	7.4
1	B	302	LYS	7.3
1	A	257	TYR	7.3
1	A	770	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	511	ASP	6.7
1	B	508	LEU	6.6
1	C	512	GLU	6.6
1	A	507	ASN	6.2
1	C	503	LEU	5.9
1	B	509	SER	5.8
1	B	895	ALA	5.7
1	A	500	LYS	5.7
1	D	254	GLU	5.7
1	B	502	ALA	5.7
1	A	799	PRO	5.6
1	A	523	SER	5.6
1	A	847	ALA	5.6
1	B	516	VAL	5.5
1	D	253	ILE	5.5
1	D	823	GLN	5.5
3	L	108	DT	5.4
1	C	500	LYS	5.4
1	A	528	GLU	5.4
1	D	165	GLU	5.2
1	D	786	ASN	5.1
1	A	504	HIS	5.1
1	B	498	ILE	5.0
1	B	534	SER	5.0
1	A	862	VAL	4.9
1	C	303	LEU	4.9
1	D	787	ASN	4.9
1	D	117	VAL	4.8
1	D	192	ASP	4.8
1	A	537	SER	4.8
1	A	508	LEU	4.7
1	D	779	ILE	4.7
1	A	800	LYS	4.7
1	D	543	PHE	4.7
1	B	522	PHE	4.6
1	D	831	TYR	4.6
1	B	517	ASP	4.6
1	D	306	ASP	4.6
1	A	858	ILE	4.6
1	B	497	GLU	4.6
1	D	301	GLY	4.5
1	D	134	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	828	GLU	4.5
1	A	863	LEU	4.5
1	A	530	ILE	4.5
1	D	530	ILE	4.5
1	D	800	LYS	4.5
1	D	277	TYR	4.4
1	A	543	PHE	4.4
1	A	532	LYS	4.4
1	D	286	PRO	4.3
1	A	531	LYS	4.3
1	D	261	GLU	4.3
1	D	305	TYR	4.3
1	A	805	ILE	4.3
1	D	801	CYS	4.2
1	B	535	ALA	4.2
1	A	542	LEU	4.2
1	A	514	LEU	4.2
1	D	513	PRO	4.2
1	B	537	SER	4.2
1	D	900	MET	4.2
1	A	37	LEU	4.1
1	D	515	ASP	4.1
1	D	255	ASN	4.1
1	A	301	GLY	4.1
1	C	535	ALA	4.1
1	B	511	ASP	4.1
1	A	501	GLU	4.1
1	B	536	LYS	4.0
3	L	109	DC	4.0
1	D	795	GLY	4.0
1	D	821	ALA	4.0
1	C	525	GLU	4.0
1	C	508	LEU	4.0
1	D	158	ASN	3.9
1	C	522	PHE	3.9
1	C	302	LYS	3.9
1	A	823	GLN	3.9
1	D	848	TRP	3.8
1	A	253	ILE	3.8
1	D	857	LEU	3.8
1	D	164	ILE	3.8
1	C	513	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	178	VAL	3.8
1	D	785	ALA	3.7
1	A	254	GLU	3.7
1	D	162	TRP	3.7
1	B	495	ASN	3.7
1	C	515	ASP	3.6
1	A	302	LYS	3.6
1	A	533	LEU	3.6
1	D	115	ILE	3.6
1	B	518	TYR	3.6
1	B	503	LEU	3.5
1	B	521	ASP	3.5
1	D	129	ALA	3.5
1	D	160	GLU	3.5
1	D	194	GLU	3.5
3	L	110	DA	3.5
1	A	496	GLY	3.5
1	D	509	SER	3.5
1	A	498	ILE	3.5
1	D	500	LYS	3.5
1	D	138	HIS	3.4
1	A	511	ASP	3.4
1	B	500	LYS	3.4
1	D	824	VAL	3.4
1	D	393	GLY	3.3
1	C	536	LYS	3.3
1	B	527	LYS	3.3
1	D	820	ASP	3.3
1	D	298	LEU	3.3
2	K	2	DC	3.3
1	D	259	SER	3.3
1	A	535	ALA	3.3
1	B	538	LEU	3.3
1	D	550	VAL	3.2
1	D	118	THR	3.2
1	D	526	ILE	3.2
1	D	173	GLN	3.2
1	D	233	ILE	3.2
1	D	784	SER	3.2
1	C	514	LEU	3.2
1	A	57	CYS	3.2
1	C	541	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	524	ASP	3.2
1	A	491	ALA	3.1
1	D	120	PRO	3.1
1	D	736	SER	3.1
1	D	153	ASN	3.1
1	C	169	LYS	3.1
1	D	33	TYR	3.0
1	A	787	ASN	3.0
1	B	504	HIS	3.0
1	C	256	MET	3.0
1	C	527	LYS	3.0
1	D	44	SER	3.0
1	D	504	HIS	3.0
1	B	512	GLU	3.0
1	C	518	TYR	3.0
1	D	473	THR	2.9
1	D	225	TYR	2.9
1	C	523	SER	2.9
1	B	541	MET	2.9
1	D	808	ILE	2.9
1	A	495	ASN	2.9
1	C	505	ASN	2.9
1	D	258	GLY	2.9
1	D	45	GLN	2.9
1	C	903	PHE	2.9
1	D	230	ILE	2.9
1	A	503	LEU	2.8
1	A	506	PRO	2.8
1	D	16	PHE	2.8
1	D	113	PHE	2.8
1	B	524	ASP	2.8
1	D	302	LYS	2.8
1	C	323	TYR	2.8
1	B	520	PHE	2.8
1	B	529	LYS	2.8
1	D	816	LYS	2.8
1	C	496	GLY	2.8
1	D	539	ASN	2.8
1	C	534	SER	2.8
1	D	498	ILE	2.8
1	A	252	VAL	2.8
1	B	496	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	819	ILE	2.7
1	D	791	TYR	2.7
1	C	497	GLU	2.7
2	K	5	DG	2.7
1	D	32	GLU	2.7
1	D	241	ARG	2.7
1	A	774	LEU	2.7
1	A	525	GLU	2.7
1	A	846	ILE	2.7
1	D	528	GLU	2.7
1	A	518	TYR	2.7
1	D	776	TYR	2.7
1	A	541	MET	2.7
1	A	49	TYR	2.7
1	A	82	ALA	2.7
1	D	542	LEU	2.6
1	A	255	ASN	2.6
1	C	257	TYR	2.6
1	D	42	PRO	2.6
1	D	903	PHE	2.6
1	D	566	LEU	2.6
1	D	147	TYR	2.6
1	D	245	HIS	2.6
1	B	532	LYS	2.6
1	D	898	PHE	2.6
1	D	20	ILE	2.6
1	A	536	LYS	2.5
1	A	785	ALA	2.5
1	D	123	PHE	2.5
1	D	659	MET	2.5
1	A	832	VAL	2.5
1	D	196	GLU	2.5
1	D	133	ILE	2.5
1	D	516	VAL	2.5
1	C	504	HIS	2.5
3	L	107	DG	2.5
1	C	255	ASN	2.5
1	C	542	LEU	2.5
1	D	234	PHE	2.5
1	A	497	GLU	2.5
1	D	523	SER	2.5
1	A	77	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	793	VAL	2.5
1	D	260	ARG	2.4
1	A	534	SER	2.4
1	D	792	ASP	2.4
1	B	506	PRO	2.4
1	B	255	ASN	2.4
1	D	136	ILE	2.4
1	B	515	ASP	2.4
1	B	514	LEU	2.4
1	D	833	LEU	2.4
1	C	787	ASN	2.4
1	D	527	LYS	2.4
1	D	846	ILE	2.4
1	D	735	SER	2.4
1	D	781	SER	2.4
1	D	764	PHE	2.4
1	B	544	ARG	2.4
1	C	539	ASN	2.4
1	A	516	VAL	2.4
1	D	1	MET	2.4
1	D	541	MET	2.4
1	D	522	PHE	2.4
1	B	323	TYR	2.4
1	D	34	LYS	2.4
2	K	9	DG	2.4
1	A	512	GLU	2.3
1	A	98	ASN	2.3
1	B	523	SER	2.3
1	B	253	ILE	2.3
1	D	238	THR	2.3
1	A	261	GLU	2.3
1	D	489	MET	2.3
1	D	435	LYS	2.3
1	D	822	PRO	2.3
1	B	301	GLY	2.3
3	F	101	DG	2.3
1	A	786	ASN	2.3
1	B	525	GLU	2.3
1	D	248	THR	2.2
1	D	227	TYR	2.2
1	B	490	LEU	2.2
1	D	237	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	323	TYR	2.2
1	D	570	LEU	2.2
1	D	895	ALA	2.2
1	D	832	VAL	2.2
1	A	804	HIS	2.2
1	D	180	SER	2.2
1	D	475	ILE	2.2
1	D	287	SER	2.2
1	D	126	PRO	2.2
1	A	505	ASN	2.2
1	D	313	ARG	2.2
1	A	62	PHE	2.2
1	A	258	GLY	2.2
1	A	833	LEU	2.2
1	B	547	ARG	2.2
1	D	205	TRP	2.2
1	D	518	TYR	2.2
1	A	492	ALA	2.2
1	D	537	SER	2.1
1	D	221	PHE	2.1
1	B	494	ARG	2.1
1	D	510	VAL	2.1
1	D	863	LEU	2.1
1	A	808	ILE	2.1
1	B	303	LEU	2.1
1	C	547	ARG	2.1
1	D	448	GLU	2.1
1	B	507	ASN	2.1
1	A	651	LEU	2.1
1	A	52	ILE	2.1
1	B	540	GLU	2.1
1	B	550	VAL	2.1
1	D	157	GLY	2.1
1	D	307	GLY	2.1
1	A	815	ILE	2.1
1	B	788	ILE	2.1
1	D	794	GLY	2.0
1	B	493	GLN	2.0
1	D	394	ALA	2.0
1	A	408	MET	2.0
1	D	289	SER	2.0
1	A	515	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	309	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. 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
2	5OC	G	3	20/21	0.97	0.18	-	38,40,43,44	0
2	5OC	E	3	20/21	0.92	0.17	-	69,76,81,82	0
2	5OC	K	3	20/21	0.82	0.47	-	112,114,118,119	0
2	5OC	I	3	20/21	0.95	0.15	-	56,60,62,64	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	G	19	5/5	0.92	0.18	-0.11	77,78,81,85	0
4	SO4	K	19	5/5	0.89	0.15	-	126,126,126,128	0
4	SO4	E	19	5/5	0.87	0.21	-	99,101,101,104	0
4	SO4	I	19	5/5	0.97	0.13	-	84,86,87,90	0

6.5 Other polymers (i)

There are no such residues in this entry.