Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:16 PM GMT

PDB ID	:	3TAG
Title	:	5-fluorocytosine paired with dAMP in RB69 gp43
Authors	:	Zahn, K.E.
Deposited on	:	2011-08-04
Resolution	:	2.95 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:

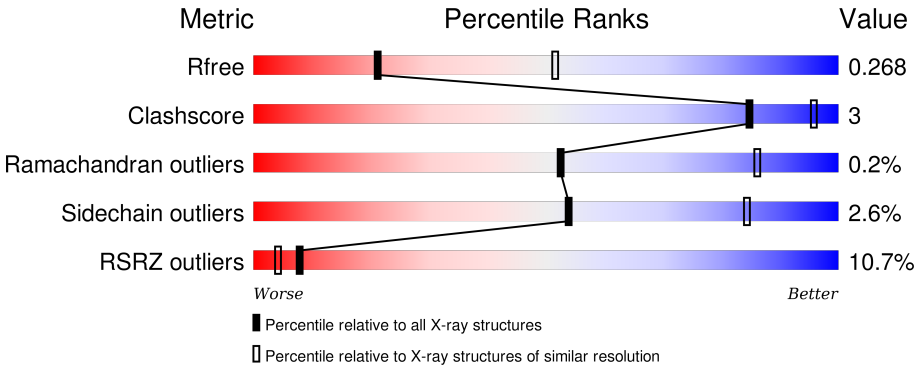
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	4% 90% 9% •
1	B	906	13% 90% 9% •
1	C	906	3% 90% 9% •
1	D	906	21% 92% 7% •
2	E	18	11% 61% 39%

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Mol	Chain	Length	Quality of chain
2	G	18	11% 50% 39% 6% 6%
2	I	18	67% 28% 6%
2	K	18	56% 83% 17%
3	F	15	7% 67% 27% 7%
3	H	15	33% 87% 13%
3	J	15	73% 27%
3	L	15	53% 33% 33% 7% 27%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31904 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	906	Total	C	N	O	S	0	0	0
			7404	4755	1235	1381	33			
1	B	901	Total	C	N	O	S	0	0	0
			7355	4724	1224	1374	33			
1	C	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			
1	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

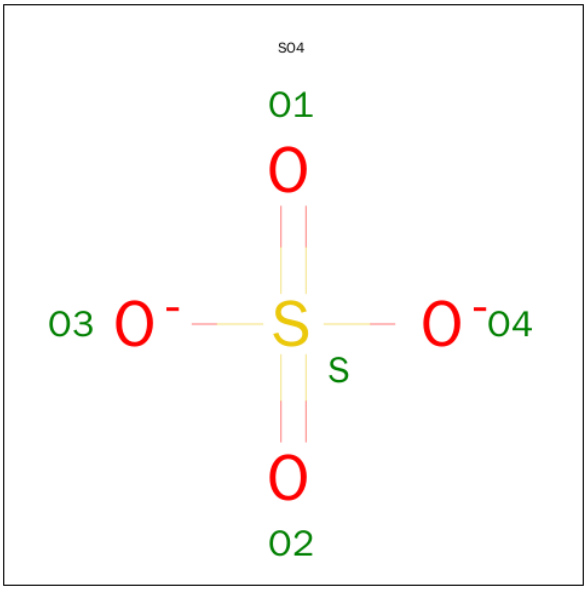
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	18	Total	C	F	N	O	P	0	0	0
			366	173	1	70	105	17			
2	I	17	Total	C	F	N	O	P	0	0	0
			350	164	1	67	101	17			
2	G	17	Total	C	N	O	P		0	0	1
			313	145	59	93	16				
2	K	15	Total	C	N	O	P		0	0	1
			271	125	52	80	14				

- Molecule 3 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
3	F	15	Total	C	N	O	P	0	0	0
			286	135	51	86	14			
3	J	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
3	H	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
3	L	11	Total	C	N	O	P	0	0	0
			223	107	40	66	10			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

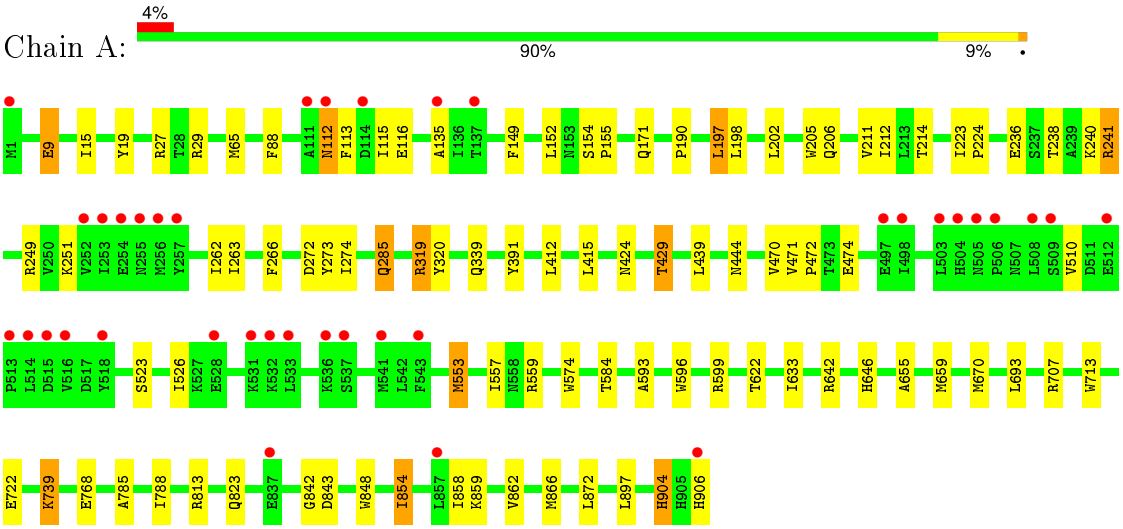
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	15	Total O 15 15	0	0
5	B	4	Total O 4 4	0	0
5	C	15	Total O 15 15	0	0
5	D	2	Total O 2 2	0	0
5	E	2	Total O 2 2	0	0
5	F	1	Total O 1 1	0	0
5	I	8	Total O 8 8	0	0
5	J	6	Total O 6 6	0	0
5	G	5	Total O 5 5	0	0
5	H	5	Total O 5 5	0	0

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.

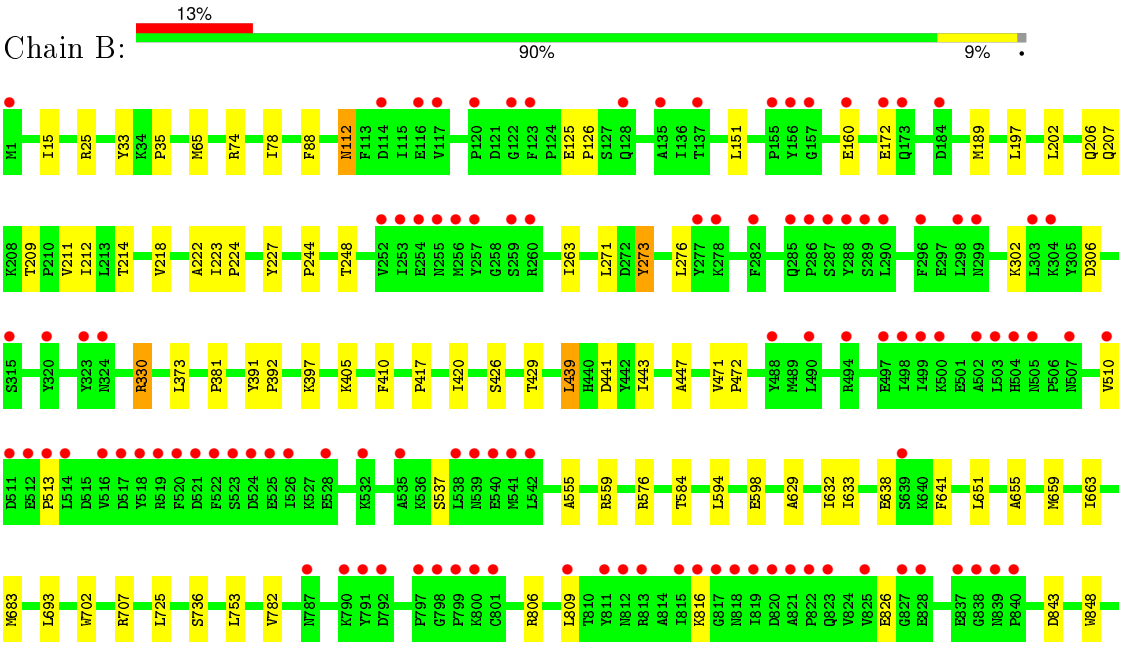
- Molecule 1: DNA polymerase

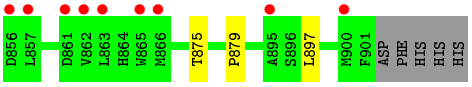
Chain A:



- Molecule 1: DNA polymerase

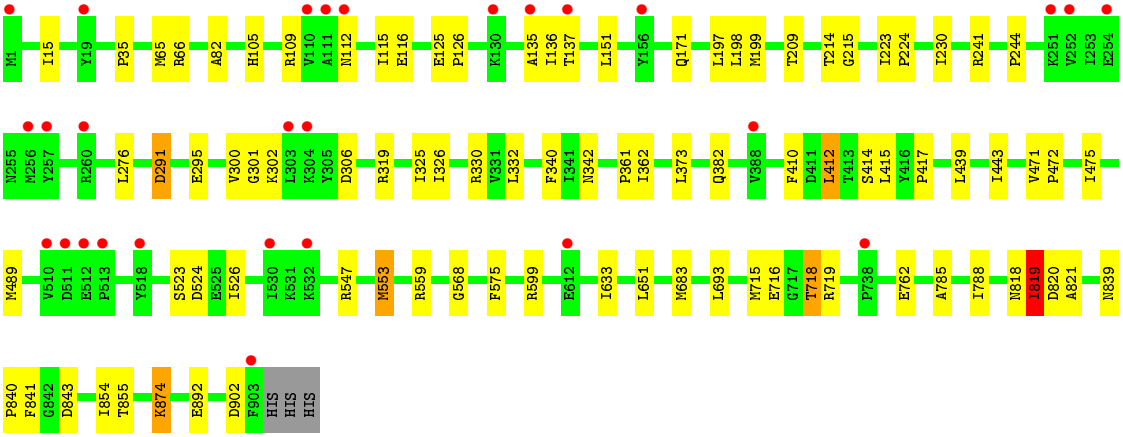
Chain B:





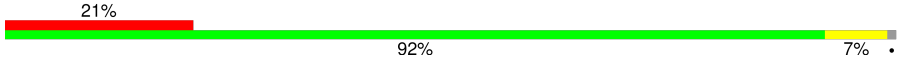
• Molecule 1: DNA polymerase

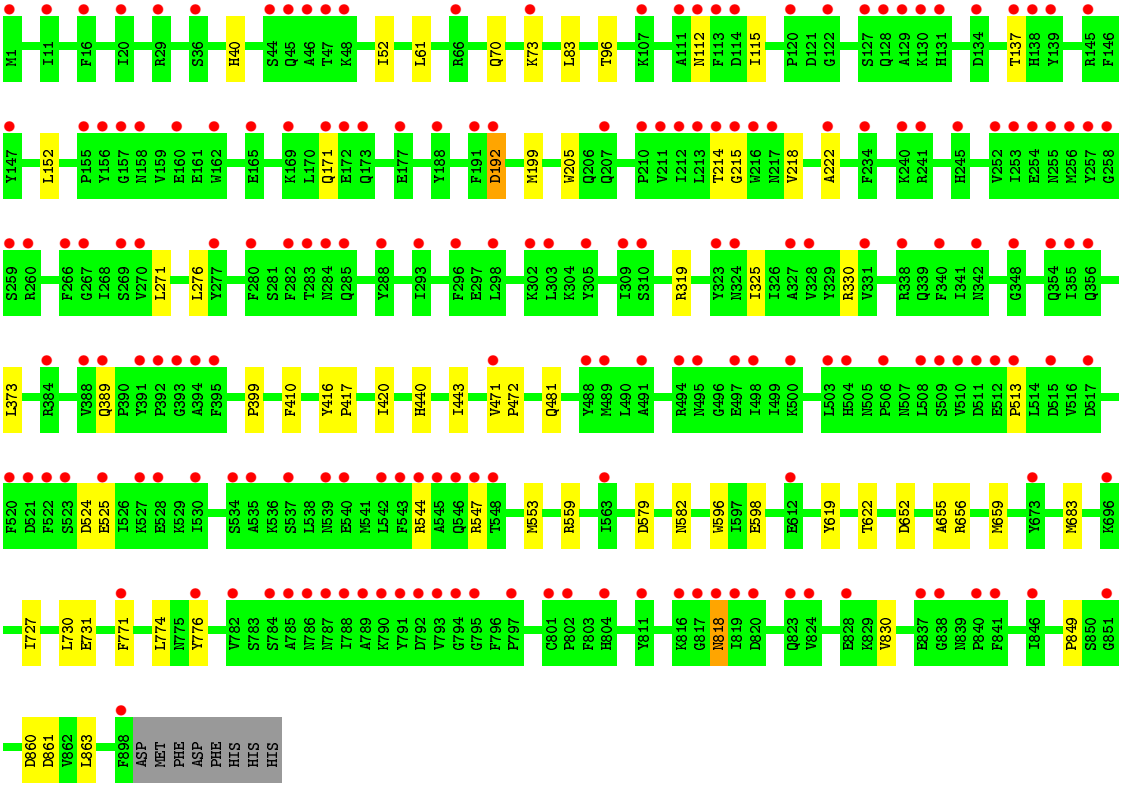
Chain C:



• Molecule 1: DNA polymerase

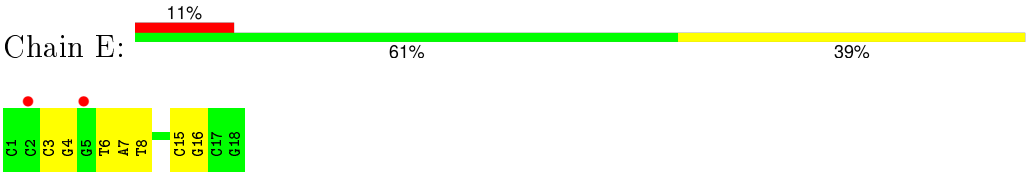
Chain D:





• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain E:

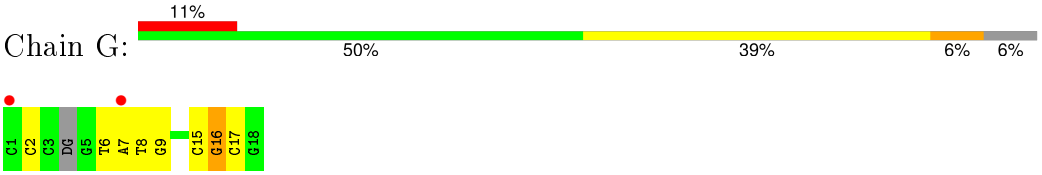


• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:

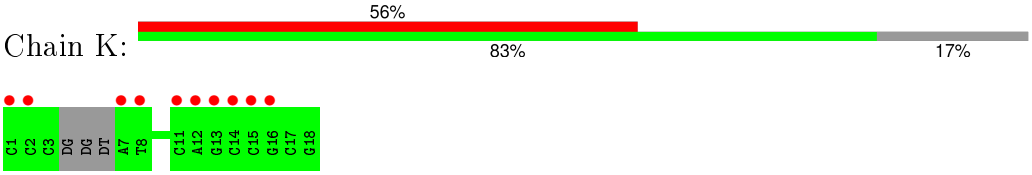
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:



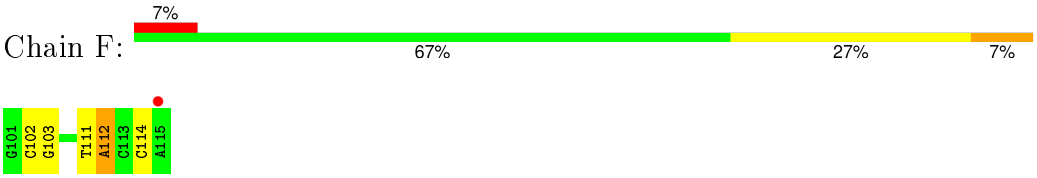
• Molecule 2: DNA (5'-D(*CP*CP*(C37)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:



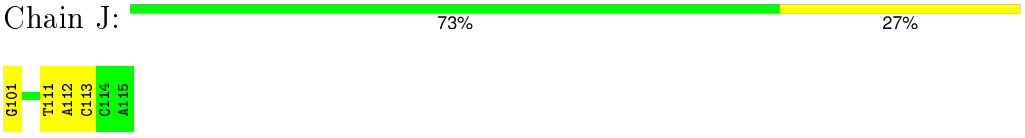
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

Chain F:



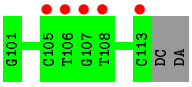
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

Chain J:



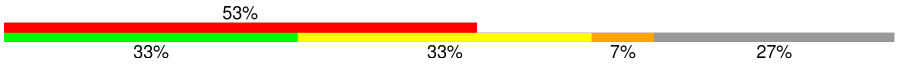
• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

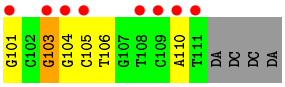
Chain H:



• Molecule 3: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-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	132.77Å 123.03Å 165.18Å 90.00° 96.39° 90.00°	Depositor
Resolution (Å)	29.95 – 2.95 29.95 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.95-2.95) 100.0 (29.95-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.239 , 0.284 0.224 , 0.268	Depositor DCC
R_{free} test set	10754 reflections (10.71%)	DCC
Wilson B-factor (Å^2)	73.8	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.7	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 111180 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31904	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: C37, 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	4/7588 (0.1%)	0.48	0/10254
1	B	0.40	2/7535 (0.0%)	0.46	0/10182
1	C	0.40	0/7555	0.48	0/10209
1	D	0.41	2/7507 (0.0%)	0.45	0/10145
2	E	0.20	0/387	0.78	0/593
2	G	0.22	0/345	0.78	1/529 (0.2%)
2	I	0.26	0/369	0.75	0/565
2	K	0.19	0/298	0.71	0/456
3	F	0.23	0/319	0.80	1/491 (0.2%)
3	H	0.22	0/294	0.75	0/452
3	J	0.25	0/339	0.80	1/521 (0.2%)
3	L	0.22	0/249	0.94	3/383 (0.8%)
All	All	0.39	8/32785 (0.0%)	0.51	6/44780 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	574	TRP	CD2-CE2	5.16	1.47	1.41
1	A	205	TRP	CD2-CE2	5.13	1.47	1.41
1	A	848	TRP	CD2-CE2	5.10	1.47	1.41
1	B	848	TRP	CD2-CE2	5.07	1.47	1.41
1	B	702	TRP	CD2-CE2	5.03	1.47	1.41
1	D	205	TRP	CD2-CE2	5.03	1.47	1.41
1	A	713	TRP	CD2-CE2	5.01	1.47	1.41
1	D	596	TRP	CD2-CE2	5.00	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	103	DG	P-O3'-C3'	8.12	129.44	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	101	DG	P-O3'-C3'	6.69	127.73	119.70
2	G	16	DG	P-O3'-C3'	6.39	127.37	119.70
3	L	110	DA	P-O3'-C3'	6.02	126.93	119.70
3	F	112	DA	P-O3'-C3'	5.17	125.90	119.70
3	J	101	DG	P-O3'-C3'	5.08	125.80	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	7404	0	7288	48	0
1	B	7355	0	7254	43	0
1	C	7374	0	7267	39	0
1	D	7328	0	7232	29	0
2	E	366	0	201	6	0
2	G	313	0	168	7	0
2	I	350	0	189	7	0
2	K	271	0	145	0	0
3	F	286	0	158	3	0
3	H	263	0	148	0	0
3	J	303	0	170	3	0
3	L	223	0	126	2	0
4	A	5	0	0	0	0
5	A	15	0	0	0	0
5	B	4	0	0	0	0
5	C	15	0	0	0	0
5	D	2	0	0	1	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
5	I	8	0	0	0	0
5	J	6	0	0	0	0
All	All	31904	0	30346	178	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 (178) 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	1.46	0.98
1:C:112:ASN:HB3	1:C:214:THR:HG23	1.53	0.90
2:E:6:DT:H2"	2:E:7:DA:H5"	1.63	0.79
1:A:112:ASN:HB3	1:A:214:THR:HG23	1.65	0.79
1:A:813:ARG:HH21	1:A:842:GLY:HA3	1.47	0.77
1:C:818:ASN:HD22	1:C:821:ALA:HB2	1.51	0.75
1:B:15:ILE:HD11	1:B:65:MET:HE3	1.71	0.72
1:B:112:ASN:HB3	1:B:214:THR:HG23	1.73	0.71
1:B:441:ASP:HB3	1:B:447:ALA:HB2	1.71	0.70
1:C:568:GLY:HA3	2:I:3:C37:O2	1.91	0.69
1:C:361:PRO:HD2	2:I:3:C37:O1P	1.92	0.69
1:B:271:LEU:HB3	1:B:276:LEU:HD11	1.76	0.67
1:A:65:MET:HE3	1:A:88:PHE:HB2	1.77	0.67
1:A:424:ASN:O	1:A:429:THR:HG21	1.96	0.65
1:D:776:TYR:HB3	1:D:863:LEU:HD21	1.79	0.64
2:G:6:DT:H2"	2:G:7:DA:H5"	1.80	0.64
2:I:2:DC:H2"	2:I:3:C37:O2P	1.97	0.64
1:B:391:TYR:HB2	1:B:584:THR:HG22	1.80	0.63
1:B:65:MET:HE2	1:B:88:PHE:HB3	1.80	0.63
1:A:707:ARG:HD2	2:E:8:DT:H4'	1.80	0.62
1:B:15:ILE:HD11	1:B:65:MET:CE	2.30	0.62
1:A:65:MET:CE	1:A:88:PHE:HB2	2.29	0.61
1:D:655:ALA:HA	1:D:659:MET:HB2	1.81	0.61
1:A:65:MET:HE3	1:A:88:PHE:CB	2.30	0.61
1:A:9:GLU:HG2	1:A:266:PHE:CD2	2.37	0.59
1:A:224:PRO:HA	1:A:263:ILE:HD12	1.84	0.59
1:C:410:PHE:HB3	1:C:683:MET:HG2	1.83	0.59
1:B:209:THR:HG21	1:B:244:PRO:HG3	1.84	0.59
1:C:489:MET:SD	1:C:553:MET:HG2	2.42	0.58
1:C:785:ALA:HB1	1:C:788:ILE:HD11	1.86	0.58
1:B:15:ILE:CD1	1:B:65:MET:HE3	2.33	0.58
2:I:2:DC:O4'	2:I:2:DC:O2	2.19	0.58
1:C:839:ASN:HB2	1:C:840:PRO:HD2	1.86	0.58
2:G:2:DC:O2	2:G:2:DC:H2'	2.05	0.57
1:B:65:MET:HE2	1:B:88:PHE:CB	2.34	0.57
1:A:211:VAL:HG12	1:A:212:ILE:HD12	1.86	0.57
1:A:596:TRP:HB3	1:A:670:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:DC:H2"	2:G:16:DG:C8	2.40	0.56
1:A:149:PHE:HB3	1:A:197:LEU:CD1	2.36	0.56
1:C:116:GLU:HB2	1:C:135:ALA:HB3	1.87	0.56
1:C:209:THR:HG21	1:C:244:PRO:HG3	1.87	0.55
1:C:443:ILE:O	1:C:599:ARG:NH1	2.40	0.55
3:J:112:DA:C2'	3:J:113:DC:H5"	2.37	0.54
2:G:16:DG:H2'	2:G:17:DC:O4'	2.07	0.54
1:A:593:ALA:HA	1:A:670:MET:HE1	1.90	0.54
1:C:414:SER:HB3	1:C:417:PRO:HG2	1.90	0.54
1:C:112:ASN:HD21	1:C:332:LEU:HG	1.72	0.54
1:A:739:LYS:HE3	1:A:739:LYS:HA	1.89	0.54
1:C:291:ASP:OD1	1:C:302:LYS:HD3	2.08	0.53
1:B:426:SER:HB3	1:B:429:THR:HG22	1.91	0.53
1:A:9:GLU:HG2	1:A:266:PHE:HD2	1.72	0.53
1:A:471:VAL:HB	1:A:472:PRO:HD3	1.89	0.53
1:A:202:LEU:O	1:A:206:GLN:HG2	2.09	0.53
3:J:112:DA:H2'	3:J:113:DC:H5"	1.91	0.53
1:D:271:LEU:HB3	1:D:276:LEU:HD11	1.90	0.52
1:A:470:VAL:O	1:A:474:GLU:HG2	2.09	0.52
1:C:35:PRO:HG3	1:C:65:MET:HG2	1.91	0.52
1:D:137:THR:HG21	1:D:325:ILE:HA	1.91	0.52
1:A:238:THR:O	1:A:241:ARG:HB2	2.10	0.51
1:C:223:ILE:HB	1:C:224:PRO:HD3	1.92	0.51
1:C:151:LEU:HB2	1:C:197:LEU:HD22	1.92	0.51
1:A:904:HIS:CD2	1:A:904:HIS:H	2.29	0.51
1:A:655:ALA:HA	1:A:659:MET:HB2	1.92	0.51
1:A:593:ALA:HA	1:A:670:MET:CE	2.41	0.50
1:C:326:ILE:O	1:C:330:ARG:HG2	2.11	0.50
1:A:116:GLU:HB2	1:A:135:ALA:HB3	1.93	0.50
1:B:224:PRO:HA	1:B:263:ILE:HD12	1.93	0.50
1:B:211:VAL:HG12	1:B:212:ILE:HD12	1.94	0.50
1:A:444:ASN:HD22	1:A:599:ARG:HD2	1.77	0.50
1:A:171:GLN:HE21	1:A:319:ARG:HH22	1.60	0.49
3:L:103:DG:H2"	3:L:104:DG:C8	2.47	0.49
1:C:471:VAL:HB	1:C:472:PRO:HD3	1.93	0.49
1:C:301:GLY:O	1:C:330:ARG:HD2	2.13	0.49
1:C:523:SER:H	1:C:526:ILE:HD12	1.77	0.49
1:D:152:LEU:HB2	1:D:192:ASP:HA	1.95	0.49
1:B:513:PRO:HG3	1:B:537:SER:HB2	1.95	0.48
3:F:111:DT:H2"	3:F:112:DA:H5"	1.95	0.48
3:F:102:DC:H2"	3:F:103:DG:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HB2	1:B:197:LEU:HD22	1.95	0.48
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.79	0.48
1:D:471:VAL:HB	1:D:472:PRO:HD3	1.95	0.48
1:D:70:GLN:HA	1:D:73:LYS:HG2	1.96	0.48
2:E:4:DG:H1	3:F:114:DC:H42	1.62	0.48
1:A:236:GLU:HG2	1:A:240:LYS:HE2	1.95	0.47
1:B:555:ALA:O	1:B:559:ARG:HG2	2.13	0.47
1:A:862:VAL:O	1:A:866:MET:HG3	2.14	0.47
1:D:727:ILE:HG23	1:D:730:LEU:HD12	1.96	0.47
1:B:410:PHE:HB3	1:B:683:MET:HG2	1.96	0.47
1:C:171:GLN:HE21	1:C:319:ARG:HH22	1.62	0.47
1:D:652:ASP:CG	1:D:656:ARG:HH12	2.17	0.47
1:D:440:HIS:HA	1:D:443:ILE:HD12	1.95	0.47
1:D:513:PRO:HB2	1:D:544:ARG:HH22	1.80	0.47
1:A:251:LYS:HB3	1:A:262:ILE:HG13	1.97	0.47
1:D:416:TYR:HB2	1:D:417:PRO:HD3	1.96	0.47
1:D:818:ASN:H	1:D:818:ASN:HD22	1.63	0.47
1:B:663:ILE:HG21	1:B:683:MET:HB3	1.96	0.47
1:A:642:ARG:HE	1:A:646:HIS:CE1	2.33	0.47
1:C:715:MET:O	1:C:718:THR:HG23	2.15	0.46
1:C:412:LEU:HG	1:C:415:LEU:HD13	1.96	0.46
1:A:272:ASP:OD1	1:A:274:ILE:HG22	2.14	0.46
1:A:412:LEU:HG	1:A:415:LEU:HD13	1.98	0.46
2:I:15:DC:H2"	2:I:16:DG:C8	2.51	0.46
1:A:391:TYR:HB2	1:A:584:THR:HG22	1.97	0.46
1:D:171:GLN:HE21	1:D:319:ARG:HH22	1.62	0.46
1:B:125:GLU:HA	1:B:126:PRO:HD3	1.83	0.46
1:B:202:LEU:O	1:B:206:GLN:HG2	2.16	0.46
1:B:218:VAL:HA	1:B:222:ALA:HB3	1.98	0.45
1:B:736:SER:HA	1:B:782:VAL:O	2.16	0.45
1:A:149:PHE:HB3	1:A:197:LEU:HD13	1.98	0.45
1:C:137:THR:HG21	1:C:325:ILE:HA	1.97	0.45
2:G:2:DC:C2'	2:G:2:DC:O2	2.62	0.45
1:B:655:ALA:HA	1:B:659:MET:HB2	1.99	0.45
1:B:806:ARG:HA	1:B:809:LEU:HD12	1.99	0.44
1:B:633:ILE:HD11	1:B:651:LEU:HD11	1.98	0.44
1:B:629:ALA:HA	1:B:632:ILE:HD12	1.97	0.44
1:C:115:ILE:HG13	1:C:136:ILE:HG12	2.00	0.44
1:C:125:GLU:HA	1:C:126:PRO:HD3	1.83	0.44
1:A:152:LEU:HD11	1:A:190:PRO:HB2	2.00	0.44
1:A:785:ALA:HB1	1:A:788:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TYR:HA	1:B:276:LEU:HB2	1.99	0.44
1:B:707:ARG:HD2	2:G:8:DT:H4'	1.99	0.44
1:A:523:SER:H	1:A:526:ILE:HD12	1.82	0.44
1:D:218:VAL:HA	1:D:222:ALA:HB3	1.99	0.44
1:A:553:MET:O	1:A:557:ILE:HG12	2.18	0.44
1:A:149:PHE:HB3	1:A:197:LEU:HD11	1.99	0.43
1:B:302:LYS:HA	1:B:330:ARG:HH11	1.83	0.43
1:A:19:TYR:CE1	1:A:29:ARG:HG3	2.52	0.43
1:C:874:LYS:HE2	2:I:11:DC:OP1	2.17	0.43
1:D:830:VAL:HG12	1:D:849:PRO:HA	1.99	0.43
1:B:381:PRO:HG2	1:B:576:ARG:HG2	1.99	0.43
1:B:875:THR:O	1:B:879:PRO:HG2	2.18	0.43
1:A:510:VAL:HG11	1:D:61:LEU:H	1.84	0.43
1:B:74:ARG:O	1:B:78:ILE:HG12	2.18	0.43
1:A:854:ILE:HD12	1:A:859:LYS:HA	2.01	0.43
1:B:391:TYR:HB2	1:B:392:PRO:HD2	2.00	0.42
1:C:719:ARG:HB3	1:D:525:GLU:HG2	2.01	0.42
1:A:223:ILE:HB	1:A:224:PRO:HD3	1.99	0.42
1:A:27:ARG:NH2	1:B:189:MET:HB2	2.34	0.42
1:C:109:ARG:HD2	1:C:209:THR:O	2.19	0.42
1:B:33:TYR:O	1:B:35:PRO:HD3	2.20	0.42
2:G:8:DT:H2"	2:G:9:DG:C8	2.55	0.42
1:B:439:LEU:HD13	1:B:443:ILE:HD11	2.02	0.42
3:J:111:DT:H2"	3:J:112:DA:H8	1.84	0.42
1:D:579:ASP:HB3	1:D:582:ASN:HB2	2.02	0.42
1:D:214:THR:OG1	1:D:215:GLY:N	2.53	0.42
1:C:633:ILE:HD11	1:C:651:LEU:HD11	2.02	0.42
1:C:362:ILE:HG23	1:C:575:PHE:HD1	1.85	0.42
1:A:154:SER:HB2	1:A:155:PRO:HD2	2.02	0.42
1:B:417:PRO:HA	1:B:420:ILE:HD12	2.02	0.42
1:C:839:ASN:HD22	1:C:841:PHE:H	1.67	0.41
1:B:223:ILE:HB	1:B:224:PRO:HD3	2.00	0.41
2:I:3:C37:H2'2	2:I:3:C37:H6	1.81	0.41
1:A:904:HIS:C	1:A:906:HIS:H	2.23	0.41
1:C:276:LEU:HG	1:C:340:PHE:HB3	2.02	0.41
1:B:471:VAL:HB	1:B:472:PRO:HD3	2.01	0.41
1:A:116:GLU:HB3	1:A:320:TYR:OH	2.20	0.41
1:D:399:PRO:HB3	1:D:619:TYR:HB2	2.02	0.41
1:B:397:LYS:NZ	1:B:598:GLU:OE2	2.53	0.41
1:D:40:HIS:CD2	1:D:83:LEU:HD11	2.56	0.41
1:D:52:ILE:HG12	5:D:908:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:THR:OG1	1:C:215:GLY:N	2.54	0.41
2:E:6:DT:H2"	2:E:7:DA:C5'	2.44	0.41
1:A:768:GLU:HG3	1:A:872:LEU:HD21	2.02	0.41
1:B:725:LEU:HD22	1:B:753:LEU:HD12	2.01	0.41
1:C:198:LEU:HD23	1:C:230:ILE:HG12	2.02	0.41
2:E:3:C37:H2'1	2:E:4:DG:C8	2.56	0.41
1:C:82:ALA:H	1:C:382:GLN:NE2	2.19	0.41
1:B:227:TYR:CE1	1:B:248:THR:HG21	2.56	0.41
1:D:417:PRO:HA	1:D:420:ILE:HD12	2.04	0.40
1:D:481:GLN:HB3	1:D:559:ARG:HD3	2.02	0.40
1:D:771:PHE:HA	1:D:774:LEU:HD12	2.03	0.40
1:B:638:GLU:HA	1:B:641:PHE:HD2	1.86	0.40
3:L:105:DC:H2"	3:L:106:DT:H5'	2.03	0.40
1:D:330:ARG:H	1:D:330:ARG:HG2	1.69	0.40
1:C:819:ILE:HB	1:C:820:ASP:H	1.61	0.40
1:C:105:HIS:CE1	1:C:547:ARG:HH21	2.40	0.40
1:D:410:PHE:HB3	1:D:683:MET:HG2	2.03	0.40
2:E:15:DC:H2"	2:E:16:DG:C8	2.56	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	904/906 (100%)	869 (96%)	32 (4%)	3 (0%)	46	81
1	B	899/906 (99%)	858 (95%)	40 (4%)	1 (0%)	56	89
1	C	901/906 (99%)	870 (97%)	30 (3%)	1 (0%)	56	89
1	D	896/906 (99%)	850 (95%)	44 (5%)	2 (0%)	52	86
All	All	3600/3624 (99%)	3447 (96%)	146 (4%)	7 (0%)	52	86

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	819	ILE
1	A	904	HIS
1	D	192	ASP
1	D	622	THR
1	A	858	ILE
1	B	405	LYS
1	A	622	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	803/803 (100%)	778 (97%)	25 (3%)	47 81
1	B	798/803 (99%)	781 (98%)	17 (2%)	61 88
1	C	800/803 (100%)	773 (97%)	27 (3%)	44 79
1	D	795/803 (99%)	782 (98%)	13 (2%)	70 90
All	All	3196/3212 (100%)	3114 (97%)	82 (3%)	54 84

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	15	ILE
1	A	112	ASN
1	A	113	PHE
1	A	115	ILE
1	A	197	LEU
1	A	198	LEU
1	A	241	ARG
1	A	249	ARG
1	A	273	TYR
1	A	285	GLN
1	A	319	ARG
1	A	339	GLN
1	A	429	THR
1	A	439	LEU

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Mol	Chain	Res	Type
1	A	553	MET
1	A	559	ARG
1	A	633	ILE
1	A	693	LEU
1	A	722	GLU
1	A	739	LYS
1	A	823	GLN
1	A	843	ASP
1	A	854	ILE
1	A	897	LEU
1	B	25	ARG
1	B	112	ASN
1	B	160	GLU
1	B	172	GLU
1	B	207	GLN
1	B	273	TYR
1	B	306	ASP
1	B	330	ARG
1	B	373	LEU
1	B	439	LEU
1	B	510	VAL
1	B	594	LEU
1	B	693	LEU
1	B	816	LYS
1	B	826	GLU
1	B	843	ASP
1	B	897	LEU
1	C	15	ILE
1	C	66	ARG
1	C	199	MET
1	C	241	ARG
1	C	291	ASP
1	C	295	GLU
1	C	300	VAL
1	C	306	ASP
1	C	342	ASN
1	C	373	LEU
1	C	412	LEU
1	C	439	LEU
1	C	475	ILE
1	C	524	ASP
1	C	553	MET

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Mol	Chain	Res	Type
1	C	559	ARG
1	C	693	LEU
1	C	716	GLU
1	C	718	THR
1	C	762	GLU
1	C	819	ILE
1	C	843	ASP
1	C	854	ILE
1	C	855	THR
1	C	874	LYS
1	C	892	GLU
1	C	902	ASP
1	D	96	THR
1	D	115	ILE
1	D	199	MET
1	D	373	LEU
1	D	389	GLN
1	D	524	ASP
1	D	547	ARG
1	D	553	MET
1	D	598	GLU
1	D	731	GLU
1	D	818	ASN
1	D	860	ASP
1	D	861	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	112	ASN
1	A	171	GLN
1	A	193	ASN
1	A	284	ASN
1	A	285	GLN
1	A	444	ASN
1	A	646	HIS
1	A	839	ASN
1	B	70	GLN
1	B	285	GLN
1	B	342	ASN
1	B	382	GLN

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Mol	Chain	Res	Type
1	B	389	GLN
1	B	481	GLN
1	B	507	ASN
1	B	646	HIS
1	B	818	ASN
1	B	823	GLN
1	C	193	ASN
1	C	284	ASN
1	C	285	GLN
1	C	382	GLN
1	C	444	ASN
1	C	480	ASN
1	C	775	ASN
1	C	818	ASN
1	C	839	ASN
1	D	105	HIS
1	D	171	GLN
1	D	193	ASN
1	D	389	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	$\#\|Z\| > 2$
2	C37	E	3	2	13,21,22	1.00	2 (15%)	17,30,33	1.87	4 (23%)
2	C37	G	3	2	0,3,22	0.00	-	0,3,33	0.00	-
2	C37	I	3	2	13,21,22	1.04	2 (15%)	17,30,33	1.87	4 (23%)
2	C37	K	3	2	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
2	C37	E	3	2	-	0/3/21/22	0/2/2/2
2	C37	G	3	2	-	0/0/0/22	0/0/0/2
2	C37	I	3	2	-	0/3/21/22	0/2/2/2
2	C37	K	3	2	-	0/0/0/22	0/0/0/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	C37	C6-C5	-2.10	1.34	1.38
2	E	3	C37	C6-C5	-2.08	1.34	1.38
2	E	3	C37	C4-C5	2.11	1.43	1.40
2	I	3	C37	C4-C5	2.21	1.43	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	C37	C6-C5-C4	-4.04	117.44	121.48
2	E	3	C37	C5-C4-N4	-4.01	120.13	122.63
2	I	3	C37	C6-C5-C4	-4.00	117.48	121.48
2	I	3	C37	C5-C4-N4	-3.96	120.16	122.63
2	I	3	C37	C5-C4-N3	3.39	121.91	118.51
2	E	3	C37	C5-C4-N3	3.43	121.96	118.51
2	I	3	C37	F-C5-C4	3.59	122.49	119.70
2	E	3	C37	F-C5-C4	3.69	122.56	119.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	C37	1	0
2	I	3	C37	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	A	907	-	4,4,4	0.37	0	6,6,6	0.11	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	A	907	-	-	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	906/906 (100%)	0.16	37 (4%) 41 24	35, 57, 143, 252	0
1	B	901/906 (99%)	0.73	118 (13%) 5 2	41, 86, 239, 299	0
1	C	903/906 (99%)	0.21	28 (3%) 52 33	32, 65, 131, 181	0
1	D	898/906 (99%)	1.13	187 (20%) 1 1	72, 128, 220, 255	0
2	E	17/18 (94%)	0.60	2 (11%) 6 3	61, 83, 146, 164	0
2	G	16/18 (88%)	1.19	2 (12%) 5 2	61, 106, 121, 138	0
2	I	16/18 (88%)	-0.09	0 100 100	39, 53, 76, 113	0
2	K	14/18 (77%)	2.79	10 (71%) 0 0	59, 166, 217, 220	0
3	F	15/15 (100%)	0.88	1 (6%) 21 11	75, 91, 147, 158	0
3	H	13/15 (86%)	1.77	5 (38%) 0 0	96, 108, 132, 139	0
3	J	15/15 (100%)	-0.21	0 100 100	38, 63, 92, 98	0
3	L	11/15 (73%)	2.69	8 (72%) 0 0	160, 183, 214, 215	0
All	All	3725/3756 (99%)	0.57	398 (10%) 8 4	32, 79, 210, 299	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	819	ILE	10.7
1	D	257	TYR	10.4
1	D	510	VAL	9.8
1	B	857	LEU	9.1
1	D	528	GLU	8.0
1	D	789	ALA	7.9
1	B	538	LEU	7.5
1	A	256	MET	7.4
1	D	395	PHE	7.3
1	B	528	GLU	7.2
1	D	256	MET	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	820	ASP	7.1
1	B	821	ALA	7.0
1	D	522	PHE	6.9
1	D	111	ALA	6.8
1	D	305	TYR	6.7
1	B	865	TRP	6.7
1	D	394	ALA	6.7
1	D	523	SER	6.7
1	B	256	MET	6.6
1	D	137	THR	6.6
1	B	277	TYR	6.5
1	D	114	ASP	6.4
1	D	788	ILE	6.3
1	D	157	GLY	6.2
1	D	214	THR	6.2
1	D	792	ASP	5.9
1	D	509	SER	5.8
1	D	215	GLY	5.7
1	D	269	SER	5.7
1	D	504	HIS	5.7
1	B	818	ASN	5.7
1	B	827	GLY	5.7
1	D	160	GLU	5.7
1	A	532	LYS	5.6
1	D	130	LYS	5.6
2	K	14	DC	5.6
1	A	505	ASN	5.6
1	B	510	VAL	5.6
1	C	903	PHE	5.5
1	D	253	ILE	5.5
1	B	298	LEU	5.5
1	D	282	PHE	5.4
1	D	503	LEU	5.4
1	B	505	ASN	5.2
1	B	817	GLY	5.2
1	D	506	PRO	5.1
1	B	540	GLU	5.1
1	D	787	ASN	5.1
1	D	303	LEU	5.0
1	A	253	ILE	5.0
1	B	516	VAL	5.0
1	D	277	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	514	LEU	4.9
1	D	823	GLN	4.9
1	B	315	SER	4.9
1	D	511	ASP	4.9
1	B	539	ASN	4.9
1	B	813	ARG	4.9
1	B	856	ASP	4.9
1	D	254	GLU	4.9
1	D	548	THR	4.9
1	D	785	ALA	4.8
1	B	502	ALA	4.8
1	B	512	GLU	4.8
1	D	131	HIS	4.8
1	D	288	TYR	4.8
1	D	46	ALA	4.8
1	A	506	PRO	4.7
1	D	508	LEU	4.6
1	B	862	VAL	4.6
1	C	1	MET	4.6
1	B	499	ILE	4.6
1	B	507	ASN	4.6
1	B	257	TYR	4.5
1	D	786	ASN	4.5
1	D	547	ARG	4.5
1	B	518	TYR	4.5
3	L	103	DG	4.5
1	B	838	GLY	4.4
2	K	1	DC	4.4
2	K	13	DG	4.4
1	D	828	GLU	4.4
1	D	171	GLN	4.4
1	D	129	ALA	4.4
1	D	491	ALA	4.3
1	B	815	ILE	4.3
1	D	252	VAL	4.3
1	D	356	GLN	4.3
1	D	328	VAL	4.3
1	A	514	LEU	4.3
1	C	130	LYS	4.2
1	C	252	VAL	4.2
1	D	791	TYR	4.2
1	D	535	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	543	PHE	4.1
1	B	286	PRO	4.1
1	B	811	TYR	4.1
1	B	497	GLU	4.1
1	D	112	ASN	4.1
1	B	801	CYS	4.1
1	D	384	ARG	4.1
3	H	108	DT	4.0
1	D	851	GLY	4.0
1	B	866	MET	4.0
1	B	535	ALA	4.0
1	B	157	GLY	4.0
1	A	498	ILE	4.0
2	K	2	DC	4.0
1	B	840	PRO	3.9
1	D	1	MET	3.9
1	D	811	TYR	3.9
1	B	812	ASN	3.9
2	K	11	DC	3.9
1	D	820	ASP	3.9
1	B	822	PRO	3.9
1	D	270	VAL	3.9
1	D	207	GLN	3.8
1	D	284	ASN	3.8
1	D	534	SER	3.8
1	B	259	SER	3.8
2	K	12	DA	3.8
1	D	539	ASN	3.8
1	B	541	MET	3.8
1	D	537	SER	3.7
1	D	258	GLY	3.7
1	C	530	ILE	3.7
1	B	160	GLU	3.7
1	D	340	PHE	3.7
1	B	490	LEU	3.6
1	D	546	GLN	3.6
1	B	128	GLN	3.6
1	D	156	TYR	3.6
1	D	498	ILE	3.6
1	B	320	TYR	3.5
1	D	192	ASP	3.5
1	D	517	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	837	GLU	3.5
3	L	110	DA	3.5
1	D	793	VAL	3.5
1	A	541	MET	3.5
1	D	525	GLU	3.5
1	D	16	PHE	3.5
1	C	254	GLU	3.5
1	A	257	TYR	3.5
1	D	388	VAL	3.5
1	B	156	TYR	3.5
1	C	251	LYS	3.4
1	D	544	ARG	3.4
1	C	256	MET	3.4
3	L	108	DT	3.4
1	D	216	TRP	3.4
1	B	861	ASP	3.4
1	B	253	ILE	3.4
1	B	526	ILE	3.4
1	B	792	ASP	3.4
1	B	816	LYS	3.3
1	D	500	LYS	3.3
1	D	259	SER	3.3
1	B	296	PHE	3.3
1	B	289	SER	3.3
1	B	519	ARG	3.3
1	D	298	LEU	3.3
1	D	147	TYR	3.3
1	D	816	LYS	3.3
1	B	500	LYS	3.2
1	D	120	PRO	3.2
1	B	260	ARG	3.2
1	A	255	ASN	3.2
1	C	510	VAL	3.2
3	L	111	DT	3.2
1	A	857	LEU	3.2
1	A	537	SER	3.2
2	K	15	DC	3.2
1	B	521	ASP	3.2
1	B	303	LEU	3.2
1	A	504	HIS	3.2
1	D	107	LYS	3.2
1	D	520	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	323	TYR	3.2
1	B	517	ASP	3.2
3	H	105	DC	3.1
1	B	184	ASP	3.1
1	D	838	GLY	3.1
1	A	254	GLU	3.1
1	B	123	PHE	3.1
1	D	165	GLU	3.1
1	B	122	GLY	3.1
1	A	497	GLU	3.1
1	D	348	GLY	3.1
1	C	511	ASP	3.1
1	A	516	VAL	3.1
1	D	782	VAL	3.1
1	D	172	GLU	3.1
1	A	508	LEU	3.1
1	D	158	ASN	3.0
1	B	155	PRO	3.0
1	B	172	GLU	3.0
1	D	113	PHE	3.0
3	L	101	DG	3.0
1	D	217	ASN	3.0
1	D	494	ARG	3.0
1	B	117	VAL	3.0
1	A	112	ASN	3.0
1	D	29	ARG	3.0
1	D	696	LYS	3.0
1	D	128	GLN	2.9
1	D	393	GLY	2.9
1	D	127	SER	2.9
1	D	44	SER	2.9
1	D	255	ASN	2.9
1	B	825	VAL	2.9
1	B	513	PRO	2.9
1	D	355	ILE	2.9
1	D	489	MET	2.9
1	D	497	GLU	2.9
2	G	1	DC	2.9
1	D	169	LYS	2.9
1	B	542	LEU	2.9
1	D	527	LYS	2.9
1	D	801	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	809	LEU	2.9
1	D	513	PRO	2.9
1	A	1	MET	2.9
1	A	906	HIS	2.9
1	B	828	GLU	2.8
2	G	7	DA	2.8
1	D	837	GLU	2.8
1	B	288	TYR	2.8
1	D	122	GLY	2.8
1	D	138	HIS	2.8
1	C	513	PRO	2.8
1	D	327	ALA	2.8
1	D	293	ILE	2.8
1	D	338	ARG	2.8
1	D	302	LYS	2.8
1	B	255	ASN	2.8
1	B	498	ILE	2.8
1	A	518	TYR	2.8
1	A	509	SER	2.7
1	B	504	HIS	2.7
1	B	900	MET	2.7
1	D	797	PRO	2.7
1	B	287	SER	2.7
1	D	191	PHE	2.7
1	D	521	ASP	2.7
1	B	137	THR	2.7
1	C	137	THR	2.7
1	D	47	THR	2.7
1	A	543	PHE	2.7
1	C	303	LEU	2.7
1	D	818	ASN	2.7
3	L	109	DC	2.6
1	B	525	GLU	2.6
1	C	111	ALA	2.6
1	A	135	ALA	2.6
1	D	515	ASP	2.6
1	D	784	SER	2.6
1	D	266	PHE	2.6
1	B	299	ASN	2.6
1	D	210	PRO	2.6
1	D	280	PHE	2.6
1	D	795	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	252	VAL	2.6
1	D	211	VAL	2.6
1	D	73	LYS	2.6
2	K	8	DT	2.6
1	A	114	ASP	2.6
1	D	324	ASN	2.6
1	C	257	TYR	2.6
1	C	388	VAL	2.6
1	D	817	GLY	2.6
1	B	323	TYR	2.6
1	D	162	TRP	2.6
1	D	241	ARG	2.5
1	D	213	LEU	2.5
1	A	137	THR	2.5
1	D	283	THR	2.5
1	B	1	MET	2.5
1	D	488	TYR	2.5
1	B	494	ARG	2.5
1	B	503	LEU	2.5
1	B	798	GLY	2.5
1	B	254	GLU	2.5
1	D	841	PHE	2.5
1	D	245	HIS	2.5
1	D	389	GLN	2.5
1	A	837	GLU	2.5
1	B	116	GLU	2.5
1	B	511	ASP	2.5
1	B	520	PHE	2.5
3	H	107	DG	2.5
1	D	139	TYR	2.5
1	C	19	TYR	2.5
1	D	285	GLN	2.5
3	F	115	DA	2.5
1	D	134	ASP	2.5
1	B	839	ASN	2.4
1	B	285	GLN	2.4
1	C	156	TYR	2.4
1	D	188	TYR	2.4
1	B	863	LEU	2.4
2	K	7	DA	2.4
3	H	113	DC	2.4
1	D	354	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	522	PHE	2.4
1	B	523	SER	2.4
1	A	252	VAL	2.4
1	A	515	ASP	2.4
1	B	114	ASP	2.4
1	B	800	LYS	2.3
1	D	173	GLN	2.3
1	B	532	LYS	2.3
1	D	846	ILE	2.3
1	D	392	PRO	2.3
1	B	135	ALA	2.3
1	D	545	ALA	2.3
2	E	5	DG	2.3
1	B	524	ASP	2.3
1	C	112	ASN	2.3
1	D	542	LEU	2.3
2	E	2	DC	2.3
1	D	260	ARG	2.3
1	D	177	GLU	2.3
1	D	331	VAL	2.3
1	B	787	ASN	2.3
1	B	278	LYS	2.3
1	B	324	ASN	2.3
1	D	495	ASN	2.3
1	D	20	ILE	2.3
1	D	776	TYR	2.3
1	D	66	ARG	2.3
1	A	503	LEU	2.3
1	D	391	TYR	2.2
1	D	267	GLY	2.2
1	D	802	PRO	2.2
1	D	342	ASN	2.2
1	D	310	SER	2.2
1	B	173	GLN	2.2
1	D	804	HIS	2.2
1	C	260	ARG	2.2
1	D	296	PHE	2.2
1	D	824	VAL	2.2
1	D	145	ARG	2.2
1	B	282	PHE	2.2
1	D	540	GLU	2.2
3	L	104	DG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	895	ALA	2.2
1	C	532	LYS	2.1
1	D	234	PHE	2.1
1	C	512	GLU	2.1
1	D	212	ILE	2.1
1	A	111	ALA	2.1
1	B	790	LYS	2.1
1	D	790	LYS	2.1
1	D	673	TYR	2.1
1	B	304	LYS	2.1
1	C	612	GLU	2.1
1	B	791	TYR	2.1
1	A	531	LYS	2.1
1	B	639	SER	2.1
1	D	36	SER	2.1
1	D	530	ILE	2.1
1	B	797	PRO	2.1
1	D	563	ILE	2.1
1	A	513	PRO	2.1
1	D	45	GLN	2.1
1	D	771	PHE	2.1
1	D	794	GLY	2.1
1	A	512	GLU	2.1
1	D	840	PRO	2.1
2	K	16	DG	2.1
1	D	11	ILE	2.1
1	D	819	ILE	2.1
1	D	512	GLU	2.1
1	D	612	GLU	2.1
1	A	528	GLU	2.1
1	D	309	ILE	2.1
1	B	290	LEU	2.1
1	C	135	ALA	2.1
1	C	304	LYS	2.0
1	D	48	LYS	2.0
1	C	518	TYR	2.0
1	B	823	GLN	2.0
1	A	533	LEU	2.0
1	D	222	ALA	2.0
1	A	536	LYS	2.0
3	H	106	DT	2.0
3	L	105	DC	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	488	TYR	2.0
1	C	110	VAL	2.0
1	D	240	LYS	2.0
1	C	738	PRO	2.0
1	D	155	PRO	2.0
1	D	898	PHE	2.0
1	D	471	VAL	2.0
1	B	120	PRO	2.0
1	B	799	PRO	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	C37	G	3	4/21	0.94	0.12	-	93,97,98,98	0
2	C37	I	3	20/21	0.93	0.22	-	83,91,95,95	0
2	C37	K	3	4/21	0.69	0.27	-	118,129,134,135	0
2	C37	E	3	20/21	0.71	0.35	-	168,175,178,180	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	A	907	5/5	0.81	0.29	-	92,97,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.