Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:43 PM GMT

PDB ID	:	1Q9Y
Title	:	CRYSTAL STRUCTURE OF ENTEROBACTERIA PHAGE RB69 GP43 DNA POLYMERASE COMPLEXED WITH 8-OXOGUANOSINE CONTAINING DNA
Authors	:	Freisinger, E.; Grollman, A.P.; Miller, H.; Kisker, C.
Deposited on	:	2003-08-26
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:

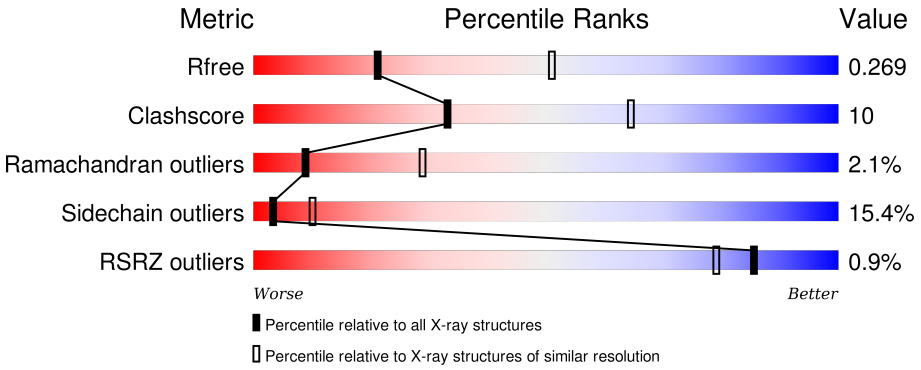
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	T	18	6% 72% 22%
2	P	14	64% 36%
3	A	906	% 68% 24% 6% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8123 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 5'-AC(8-OXOGUANOSINE)GGTAAGCAGTCCGCG-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	18	Total	C	N	O	P	0	0	0
			371	175	74	105	17			

- Molecule 2 is a DNA chain called 5'-GCGGACTGCTTAC(DIDEOXYCYTIDINE)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	14	Total	C	N	O	P	0	0	0
			281	135	51	82	13			

- Molecule 3 is a protein called DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	902	Total	C	N	O	S	0	0	0
			7356	4721	1227	1376	32			

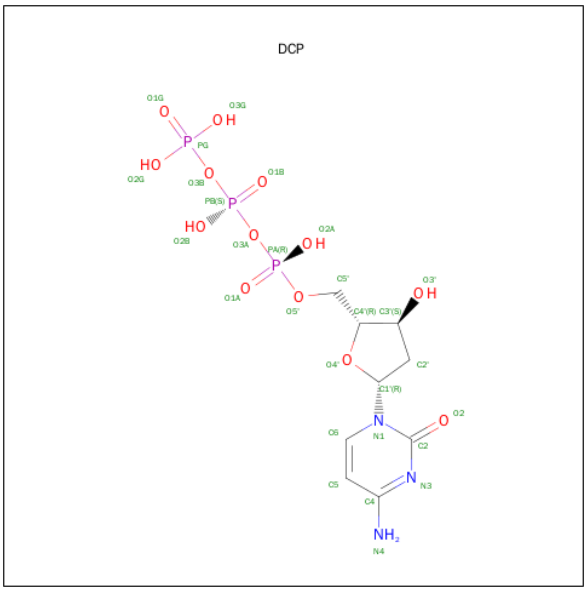
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	CLONING ARTIFACT	UNP Q38087
A	2	GLY	-	CLONING ARTIFACT	UNP Q38087
A	3	SER	-	CLONING ARTIFACT	UNP Q38087
A	225	ALA	ASP	ENGINEERED	UNP Q38087
A	330	ALA	ASP	ENGINEERED	UNP Q38087

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	P	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O	0	0
			77	77		
6	P	2	Total	O	0	0
			2	2		
6	T	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

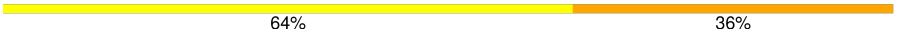
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

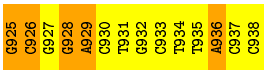
- Molecule 1: 5'-AC(8-OXOGUANOSINE)GGTAAGCAGTCCGCG-3'

Chain T:

- Molecule 2: 5'-GCGGACTGCTTAC(DIDEOXYCYTIDINE)-3'

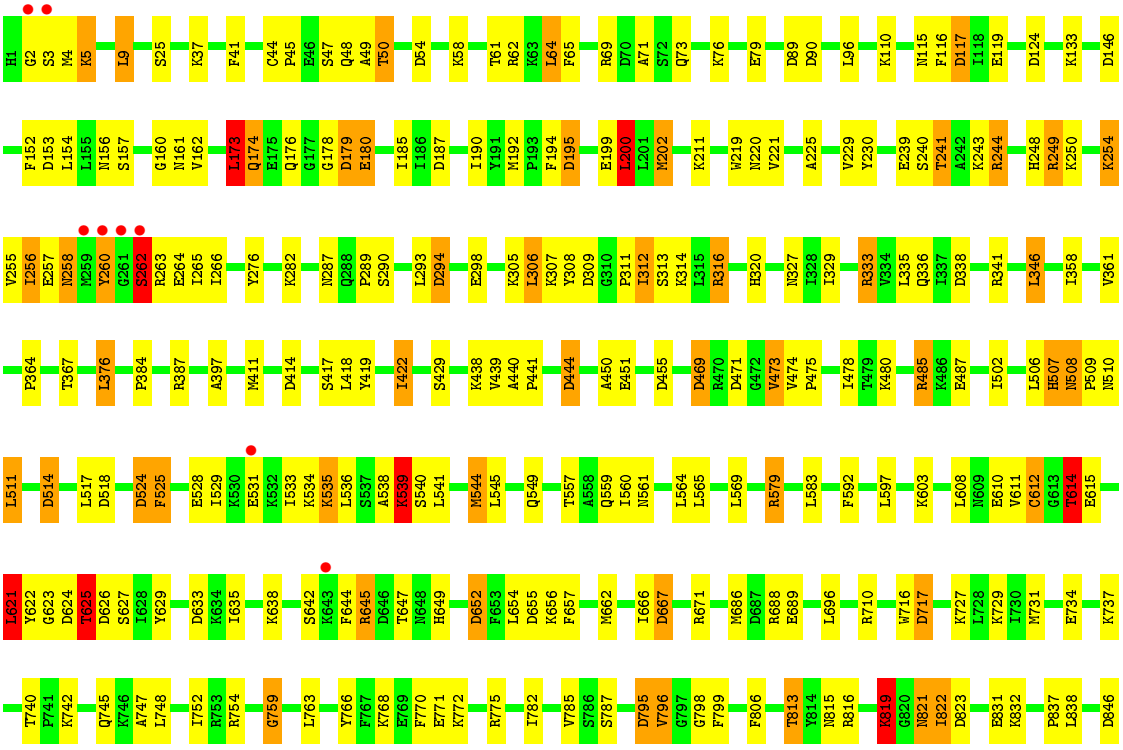
Chain P:





- Molecule 3: DNA POLYMERASE

Chain A:




K847
W851
E856
T857
T858
D859
L860
I861
K862
D863
D864
V865
M869
L874
L875
E876
K877
K881
P882
L883
D893
Y894
E895
K896
K897
A898
S899
D902
MET
PHE
ASP
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.82Å 118.56Å 127.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.06 – 2.80 46.06 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.06-2.80) 91.0 (46.06-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.271 0.203 , 0.269	Depositor DCC
R_{free} test set	1422 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 31088 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8123	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: 8OG, CA, DCP, DOC

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	T	1.40	0/390	2.49	35/598 (5.9%)
2	P	1.38	1/294 (0.3%)	2.61	27/452 (6.0%)
3	A	0.75	0/7536	0.97	31/10184 (0.3%)
All	All	0.82	1/8220 (0.0%)	1.21	93/11234 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	933	DC	C3'-O3'	-5.57	1.36	1.44

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	931	DT	O4'-C1'-N1	11.90	116.33	108.00
2	P	928	DG	O4'-C1'-N9	11.50	116.05	108.00
3	A	469	ASP	CB-CG-OD2	10.44	127.69	118.30
2	P	936	DA	O5'-P-OP2	-10.27	96.46	105.70
1	T	921	DC	O4'-C4'-C3'	-9.00	100.60	106.00
1	T	916	DC	P-O3'-C3'	8.65	130.08	119.70
2	P	925	DG	P-O3'-C3'	8.50	129.91	119.70
1	T	908	DC	O4'-C1'-N1	8.35	113.84	108.00
3	A	187	ASP	CB-CG-OD2	8.13	125.62	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	933	DC	O5'-P-OP2	-8.06	98.44	105.70
1	T	916	DC	O4'-C1'-N1	7.98	113.58	108.00
1	T	914	DA	N1-C6-N6	-7.83	113.90	118.60
2	P	932	DG	C8-N9-C4	-7.71	103.32	106.40
2	P	933	DC	O4'-C4'-C3'	-7.71	101.37	106.00
3	A	864	ASP	CB-CG-OD2	7.68	125.21	118.30
3	A	90	ASP	CB-CG-OD2	7.61	125.14	118.30
1	T	918	DG	O4'-C1'-N9	-7.60	102.68	108.00
1	T	919	DT	O4'-C1'-N1	-7.40	102.82	108.00
1	T	913	DA	N1-C2-N3	-7.34	125.63	129.30
2	P	932	DG	N7-C8-N9	7.21	116.71	113.10
3	A	717	ASP	CB-CG-OD2	7.16	124.75	118.30
1	T	910	DG	C2-N3-C4	-7.08	108.36	111.90
1	T	915	DG	O4'-C1'-N9	7.07	112.95	108.00
3	A	652	ASP	CB-CG-OD2	6.99	124.59	118.30
3	A	902	ASP	CB-CG-OD2	6.95	124.56	118.30
3	A	89	ASP	CB-CG-OD2	6.91	124.52	118.30
3	A	518	ASP	CB-CG-OD2	6.62	124.26	118.30
1	T	922	DG	O4'-C1'-N9	6.61	112.63	108.00
3	A	859	ASP	CB-CG-OD2	6.61	124.25	118.30
2	P	935	DT	O4'-C1'-N1	6.60	112.62	108.00
2	P	935	DT	C1'-O4'-C4'	-6.58	103.52	110.10
3	A	514	ASP	CB-CG-OD2	6.56	124.21	118.30
1	T	911	DG	O4'-C1'-N9	6.54	112.58	108.00
1	T	915	DG	C8-N9-C4	-6.54	103.79	106.40
1	T	912	DT	N3-C4-O4	6.48	123.79	119.90
1	T	923	DC	O4'-C1'-C2'	-6.37	100.80	105.90
2	P	926	DC	P-O3'-C3'	6.32	127.28	119.70
3	A	294	ASP	CB-CG-OD2	6.28	123.96	118.30
2	P	930	DC	OP1-P-OP2	6.24	128.96	119.60
1	T	908	DC	O4'-C4'-C3'	6.22	109.73	106.00
1	T	917	DA	O4'-C1'-N9	-6.16	103.69	108.00
2	P	934	DT	N3-C2-O2	-6.11	118.63	122.30
3	A	444	ASP	CB-CG-OD2	6.11	123.80	118.30
3	A	524	ASP	CB-CG-OD2	6.10	123.79	118.30
2	P	933	DC	O4'-C1'-C2'	-6.02	101.09	105.90
2	P	930	DC	O4'-C1'-C2'	-6.01	101.09	105.90
2	P	937	DC	O5'-P-OP2	-5.99	100.31	105.70
3	A	316	ARG	NE-CZ-NH2	-5.98	117.31	120.30
3	A	54	ASP	CB-CG-OD2	5.98	123.69	118.30
2	P	929	DA	O4'-C4'-C3'	-5.95	102.12	104.50
1	T	913	DA	C1'-O4'-C4'	-5.95	104.15	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	471	ASP	CB-CG-OD2	5.94	123.64	118.30
3	A	195	ASP	CB-CG-OD2	5.93	123.64	118.30
2	P	932	DG	O4'-C1'-N9	5.92	112.14	108.00
3	A	316	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	T	913	DA	P-O3'-C3'	5.78	126.63	119.70
1	T	913	DA	C4-C5-C6	-5.73	114.14	117.00
1	T	916	DC	C5-C4-N4	5.71	124.20	120.20
3	A	633	ASP	CB-CG-OD2	5.71	123.44	118.30
1	T	920	DC	N3-C4-N4	-5.60	114.08	118.00
3	A	863	ASP	CB-CG-OD2	5.53	123.27	118.30
1	T	923	DC	O4'-C1'-N1	5.47	111.83	108.00
2	P	932	DG	P-O5'-C5'	5.46	129.64	120.90
3	A	153	ASP	CB-CG-OD2	5.46	123.21	118.30
2	P	933	DC	P-O3'-C3'	5.44	126.23	119.70
3	A	200	LEU	CA-CB-CG	5.43	127.79	115.30
3	A	173	LEU	CA-CB-CG	5.41	127.75	115.30
3	A	759	GLY	N-CA-C	5.37	126.52	113.10
1	T	914	DA	O4'-C1'-N9	5.36	111.75	108.00
2	P	928	DG	O4'-C4'-C3'	5.36	109.22	106.00
1	T	910	DG	O5'-P-OP2	-5.36	100.88	105.70
3	A	179	ASP	CB-CG-OD2	5.33	123.10	118.30
1	T	916	DC	C2-N3-C4	5.33	122.56	119.90
2	P	932	DG	C5-N7-C8	-5.29	101.66	104.30
1	T	910	DG	O4'-C1'-N9	-5.28	104.30	108.00
2	P	935	DT	O4'-C4'-C3'	5.28	109.17	106.00
3	A	9	LEU	CA-CB-CG	5.24	127.36	115.30
2	P	937	DC	C6-N1-C2	5.23	122.39	120.30
1	T	910	DG	O4'-C1'-C2'	5.21	110.07	105.90
2	P	934	DT	O4'-C1'-C2'	-5.21	101.73	105.90
3	A	893	ASP	CB-CG-OD2	5.20	122.98	118.30
1	T	922	DG	N3-C2-N2	-5.17	116.28	119.90
2	P	931	DT	OP2-P-O3'	5.15	116.54	105.20
1	T	920	DC	P-O5'-C5'	5.15	129.14	120.90
1	T	917	DA	OP1-P-OP2	5.15	127.32	119.60
1	T	913	DA	O4'-C1'-N9	5.12	111.59	108.00
1	T	915	DG	N7-C8-N9	5.11	115.65	113.10
3	A	309	ASP	CB-CG-OD2	5.10	122.89	118.30
3	A	621	LEU	CA-CB-CG	5.06	126.94	115.30
3	A	200	LEU	CB-CG-CD1	5.06	119.59	111.00
1	T	923	DC	N1-C2-O2	5.04	121.92	118.90
1	T	915	DG	OP1-P-OP2	5.03	127.14	119.60
2	P	931	DT	C4-C5-C7	5.01	122.01	119.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	3	SER	Peptide

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	T	371	0	202	5	0
2	P	281	0	159	7	0
3	A	7356	0	7251	153	0
4	A	3	0	0	0	0
5	P	28	0	12	1	0
6	A	77	0	0	10	0
6	P	2	0	0	0	0
6	T	5	0	0	0	0
All	All	8123	0	7624	161	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 10.

All (161) 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)
3:A:202:MET:SD	3:A:202:MET:CE	2.01	1.48
3:A:174:GLN:HA	3:A:174:GLN:HE21	1.30	0.97
3:A:897:LYS:NZ	3:A:897:LYS:HA	1.91	0.86
3:A:508:ASN:O	3:A:508:ASN:CG	2.19	0.80
3:A:173:LEU:H	3:A:173:LEU:HD22	1.47	0.79
3:A:644:PHE:HA	3:A:649:HIS:HD2	1.47	0.78
3:A:5:LYS:NZ	3:A:5:LYS:HB3	1.99	0.78
3:A:2:GLY:HA2	6:A:997:HOH:O	1.83	0.77
3:A:49:ALA:O	3:A:50:THR:HG23	1.85	0.77
3:A:119:GLU:HG2	3:A:327:ASN:ND2	1.99	0.77
3:A:256:ILE:O	3:A:263:ARG:O	2.05	0.75
3:A:897:LYS:HA	3:A:897:LYS:HZ3	1.50	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:174:GLN:HE21	3:A:174:GLN:CA	2.01	0.72
2:P:928:DG:H4'	2:P:929:DA:OP1	1.89	0.72
3:A:44:CYS:HB2	3:A:45:PRO:HD2	1.71	0.71
3:A:667:ASP:O	3:A:671:ARG:HG3	1.90	0.71
3:A:644:PHE:HB2	6:A:952:HOH:O	1.93	0.69
3:A:174:GLN:NE2	3:A:178:GLY:O	2.26	0.68
3:A:119:GLU:HG2	3:A:327:ASN:HD22	1.58	0.68
3:A:64:LEU:HB3	6:A:973:HOH:O	1.92	0.68
3:A:644:PHE:HA	3:A:649:HIS:CD2	2.29	0.68
3:A:795:ASP:O	3:A:799:PHE:O	2.13	0.66
3:A:174:GLN:HA	3:A:174:GLN:NE2	2.09	0.65
3:A:49:ALA:O	3:A:50:THR:CG2	2.45	0.64
3:A:257:GLU:O	3:A:258:ASN:O	2.16	0.64
3:A:545:LEU:O	3:A:549:GLN:HG3	1.98	0.63
3:A:256:ILE:HA	6:A:990:HOH:O	1.98	0.63
3:A:857:ILE:HD12	3:A:862:LYS:HA	1.80	0.63
1:T:907:DA:H2"	1:T:908:DC:O5'	1.99	0.62
3:A:688:ARG:NH2	3:A:717:ASP:OD1	2.33	0.61
3:A:508:ASN:ND2	3:A:534:LYS:O	2.33	0.61
3:A:305:LYS:O	3:A:306:LEU:CB	2.48	0.61
3:A:508:ASN:ND2	3:A:510:ASN:HD21	1.99	0.61
3:A:782:ILE:HD11	3:A:869:MET:CE	2.31	0.60
3:A:173:LEU:H	3:A:173:LEU:CD2	2.13	0.60
3:A:257:GLU:HG3	3:A:262:SER:HA	1.84	0.59
3:A:329:ILE:HG22	3:A:333:ARG:HD3	1.85	0.59
3:A:418:LEU:HD22	3:A:626:ASP:HB3	1.85	0.58
3:A:737:LYS:O	3:A:745:GLN:NE2	2.36	0.57
3:A:747:ALA:HB2	3:A:770:PHE:CE2	2.39	0.57
2:P:925:DG:H1'	2:P:926:DC:H5'	1.86	0.57
3:A:225:ALA:O	3:A:229:VAL:HG13	2.04	0.57
3:A:748:LEU:O	3:A:752:ILE:HG13	2.05	0.57
3:A:644:PHE:HD2	3:A:649:HIS:CD2	2.22	0.56
3:A:289:PRO:HB3	3:A:785:VAL:HG21	1.86	0.56
3:A:782:ILE:HD11	3:A:869:MET:HE1	1.87	0.56
3:A:782:ILE:O	3:A:874:LEU:HD11	2.06	0.55
3:A:230:TYR:CD2	3:A:266:ILE:HD13	2.42	0.55
3:A:647:THR:HG21	3:A:716:TRP:CH2	2.42	0.55
3:A:174:GLN:HE22	3:A:179:ASP:HA	1.71	0.55
3:A:162:VAL:HG21	3:A:320:HIS:CD2	2.42	0.54
3:A:666:ILE:HG21	3:A:686:MET:HB3	1.88	0.54
3:A:508:ASN:N	3:A:509:PRO:CD	2.71	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:422:ILE:HD13	3:A:592:PHE:HD1	1.73	0.53
3:A:333:ARG:HA	3:A:336:GLN:HE21	1.73	0.53
3:A:422:ILE:HD13	3:A:592:PHE:CD1	2.43	0.53
3:A:856:GLU:OE1	3:A:862:LYS:NZ	2.20	0.53
3:A:821:ASN:OD1	3:A:823:ASP:HB3	2.10	0.53
3:A:614:THR:HG23	3:A:615:GLU:N	2.24	0.52
3:A:444:ASP:HB3	3:A:450:ALA:HB2	1.92	0.52
3:A:816:ARG:O	3:A:819:LYS:HB2	2.09	0.52
3:A:510:ASN:HB2	3:A:535:LYS:O	2.10	0.51
3:A:173:LEU:HD23	3:A:176:GLN:CB	2.40	0.51
3:A:858:THR:HG21	3:A:860:LEU:HD12	1.93	0.51
3:A:173:LEU:HD23	3:A:176:GLN:HB2	1.92	0.51
3:A:49:ALA:C	3:A:50:THR:HG23	2.31	0.50
3:A:146:ASP:OD2	3:A:211:LYS:NZ	2.38	0.50
2:P:938:DOC:H3'2	3:A:625:THR:HG23	1.94	0.50
3:A:897:LYS:HZ2	3:A:897:LYS:HA	1.72	0.49
3:A:119:GLU:OE2	6:A:942:HOH:O	2.20	0.49
3:A:795:ASP:HB3	6:A:1000:HOH:O	2.12	0.49
2:P:928:DG:H2"	2:P:929:DA:C8	2.48	0.49
3:A:624:ASP:O	3:A:626:ASP:N	2.46	0.49
3:A:621:LEU:HD13	3:A:629:TYR:O	2.13	0.49
3:A:64:LEU:HB2	6:A:975:HOH:O	2.12	0.49
3:A:795:ASP:O	3:A:796:VAL:HB	2.13	0.49
3:A:419:TYR:HA	3:A:422:ILE:HG13	1.95	0.49
3:A:881:LYS:N	3:A:882:PRO:HD2	2.28	0.49
3:A:248:HIS:O	3:A:249:ARG:HB2	2.12	0.48
3:A:475:PRO:O	3:A:478:ILE:HG22	2.13	0.48
3:A:608:LEU:O	3:A:612:CYS:HB3	2.13	0.48
3:A:474:VAL:HB	3:A:475:PRO:HD3	1.94	0.48
3:A:710:ARG:NH2	3:A:734:GLU:OE2	2.47	0.47
3:A:384:PRO:O	3:A:579:ARG:HD3	2.14	0.47
3:A:899:SER:OG	3:A:902:ASP:OD1	2.21	0.47
3:A:254:LYS:HB3	3:A:265:ILE:CD1	2.44	0.47
3:A:174:GLN:HG2	3:A:180:GLU:OE2	2.15	0.47
3:A:37:LYS:CE	6:A:977:HOH:O	2.62	0.47
3:A:5:LYS:HB3	3:A:5:LYS:HZ3	1.77	0.47
3:A:65:PHE:CG	3:A:71:ALA:HB2	2.49	0.47
3:A:508:ASN:ND2	3:A:510:ASN:OD1	2.48	0.47
3:A:662:MET:O	3:A:666:ILE:HG12	2.16	0.46
3:A:411:MET:HE3	3:A:654:LEU:HB3	1.98	0.46
3:A:507:HIS:N	3:A:507:HIS:ND1	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:411:MET:CE	3:A:654:LEU:HB3	2.46	0.46
3:A:312:ILE:HD13	3:A:312:ILE:O	2.16	0.45
3:A:260:TYR:O	3:A:260:TYR:CD2	2.69	0.45
3:A:160:GLY:O	3:A:316:ARG:NH2	2.49	0.45
3:A:440:ALA:HB1	3:A:441:PRO:HD2	1.98	0.45
3:A:813:THR:HB	3:A:816:ARG:NH2	2.32	0.45
3:A:241:THR:O	3:A:244:ARG:HG3	2.16	0.45
3:A:346:LEU:HD11	3:A:561:ASN:CB	2.46	0.45
3:A:897:LYS:NZ	3:A:897:LYS:CA	2.74	0.45
3:A:729:LYS:HE2	3:A:731:MET:SD	2.57	0.45
3:A:851:TRP:CG	3:A:857:ILE:HG23	2.52	0.44
3:A:635:ILE:HD13	3:A:657:PHE:CE1	2.52	0.44
3:A:508:ASN:ND2	3:A:510:ASN:ND2	2.66	0.44
3:A:47:SER:O	3:A:49:ALA:N	2.50	0.44
3:A:96:LEU:HA	3:A:96:LEU:HD23	1.86	0.44
1:T:913:DA:C2	2:P:936:DA:C2	3.05	0.44
3:A:341:ARG:O	3:A:557:THR:HG21	2.16	0.44
3:A:117:ASP:OD2	3:A:327:ASN:ND2	2.51	0.44
3:A:154:LEU:HB2	3:A:200:LEU:HD23	1.98	0.44
1:T:907:DA:H5'	1:T:907:DA:N3	2.32	0.44
3:A:200:LEU:HD12	3:A:200:LEU:C	2.37	0.44
3:A:837:PRO:CG	3:A:874:LEU:HD23	2.48	0.43
3:A:645:ARG:HG3	3:A:645:ARG:H	1.59	0.43
3:A:615:GLU:HA	3:A:615:GLU:OE1	2.18	0.43
2:P:927:DG:H2"	2:P:928:DG:OP2	2.18	0.43
3:A:474:VAL:HG13	3:A:569:LEU:HD21	2.01	0.43
3:A:287:ASN:OD1	3:A:832:LYS:NZ	2.51	0.43
3:A:822:ILE:HD13	3:A:822:ILE:H	1.83	0.43
1:T:914:DA:H2'	1:T:915:DG:C8	2.53	0.43
3:A:655:ASP:OD1	3:A:688:ARG:NH1	2.50	0.43
3:A:858:THR:HG22	3:A:860:LEU:H	1.84	0.43
1:T:909:8OG:OP2	3:A:364:PRO:HD2	2.19	0.43
3:A:564:LEU:HD23	6:A:951:HOH:O	2.19	0.43
3:A:508:ASN:O	3:A:510:ASN:OD1	2.35	0.43
3:A:376:LEU:HD13	3:A:473:VAL:HG11	2.01	0.43
3:A:194:PHE:CD1	3:A:200:LEU:HB2	2.54	0.42
3:A:41:PHE:CD1	3:A:41:PHE:N	2.87	0.42
3:A:502:ILE:HD13	3:A:544:MET:HB2	2.02	0.42
3:A:622:TYR:CG	3:A:623:GLY:N	2.88	0.42
3:A:358:ILE:O	3:A:361:VAL:HG22	2.19	0.42
3:A:311:PRO:HG2	3:A:314:LYS:HG3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:511:LEU:HD22	3:A:511:LEU:HA	1.95	0.42
3:A:418:LEU:O	3:A:422:ILE:HG13	2.19	0.42
3:A:397:ALA:CB	3:A:625:THR:HB	2.50	0.42
3:A:367:THR:HG21	3:A:565:LEU:HD11	2.02	0.42
3:A:688:ARG:HG2	3:A:689:GLU:N	2.34	0.41
3:A:156:ASN:HA	3:A:161:ASN:HD22	1.85	0.41
3:A:5:LYS:NZ	3:A:5:LYS:CB	2.76	0.41
2:P:936:DA:H5'	3:A:737:LYS:HA	2.02	0.41
3:A:524:ASP:O	3:A:525:PHE:C	2.58	0.41
3:A:293:LEU:O	3:A:294:ASP:C	2.58	0.41
3:A:294:ASP:OD2	3:A:305:LYS:O	2.37	0.41
3:A:307:LYS:O	3:A:308:TYR:HB3	2.21	0.41
3:A:256:ILE:HG22	3:A:256:ILE:O	2.21	0.41
3:A:152:PHE:HB3	3:A:200:LEU:HD13	2.02	0.41
3:A:44:CYS:HB2	3:A:45:PRO:CD	2.46	0.41
3:A:506:LEU:HD23	3:A:541:LEU:HD12	2.02	0.41
3:A:754:ARG:CZ	3:A:766:TYR:HB2	2.50	0.41
5:P:939:DCP:O2G	3:A:485:ARG:NH2	2.54	0.41
3:A:37:LYS:HE2	6:A:977:HOH:O	2.20	0.41
3:A:538:ALA:O	3:A:539:LYS:C	2.59	0.41
3:A:305:LYS:O	3:A:306:LEU:HB2	2.18	0.40
3:A:614:THR:HG23	3:A:615:GLU:H	1.85	0.40
3:A:529:ILE:HG22	3:A:533:ILE:HD12	2.03	0.40
3:A:806:PHE:CZ	3:A:877:LYS:NZ	2.89	0.40
3:A:276:TYR:OH	3:A:338:ASP:HA	2.22	0.40
3:A:219:TRP:O	3:A:220:ASN:CB	2.68	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	900/906 (99%)	813 (90%)	68 (8%)	19 (2%)	9 29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	256	ILE
3	A	258	ASN
3	A	306	LEU
3	A	625	THR
3	A	759	GLY
3	A	795	ASP
3	A	798	GLY
3	A	195	ASP
3	A	525	PHE
3	A	614	THR
3	A	48	GLN
3	A	50	THR
3	A	642	SER
3	A	815	ASN
3	A	819	LYS
3	A	796	VAL
3	A	860	LEU
3	A	262	SER
3	A	539	LYS

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	798/802 (100%)	675 (85%)	123 (15%)	3 10

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4	MET
3	A	5	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	9	LEU
3	A	25	SER
3	A	58	LYS
3	A	61	THR
3	A	62	ARG
3	A	64	LEU
3	A	69	ARG
3	A	73	GLN
3	A	76	LYS
3	A	79	GLU
3	A	110	LYS
3	A	115	ASN
3	A	116	PHE
3	A	117	ASP
3	A	124	ASP
3	A	133	LYS
3	A	157	SER
3	A	173	LEU
3	A	174	GLN
3	A	180	GLU
3	A	185	ILE
3	A	190	ILE
3	A	192	MET
3	A	199	GLU
3	A	200	LEU
3	A	202	MET
3	A	221	VAL
3	A	239	GLU
3	A	240	SER
3	A	241	THR
3	A	243	LYS
3	A	244	ARG
3	A	249	ARG
3	A	250	LYS
3	A	254	LYS
3	A	255	VAL
3	A	260	TYR
3	A	262	SER
3	A	264	GLU
3	A	282	LYS
3	A	290	SER
3	A	298	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	312	ILE
3	A	313	SER
3	A	333	ARG
3	A	335	LEU
3	A	346	LEU
3	A	376	LEU
3	A	387	ARG
3	A	414	ASP
3	A	417	SER
3	A	422	ILE
3	A	429	SER
3	A	438	LYS
3	A	439	VAL
3	A	451	GLU
3	A	455	ASP
3	A	469	ASP
3	A	473	VAL
3	A	480	LYS
3	A	485	ARG
3	A	487	GLU
3	A	507	HIS
3	A	508	ASN
3	A	511	LEU
3	A	514	ASP
3	A	517	LEU
3	A	528	GLU
3	A	531	GLU
3	A	535	LYS
3	A	536	LEU
3	A	539	LYS
3	A	540	SER
3	A	544	MET
3	A	559	GLN
3	A	560	ILE
3	A	579	ARG
3	A	583	LEU
3	A	597	LEU
3	A	603	LYS
3	A	610	GLU
3	A	611	VAL
3	A	612	CYS
3	A	614	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	621	LEU
3	A	625	THR
3	A	627	SER
3	A	638	LYS
3	A	645	ARG
3	A	652	ASP
3	A	656	LYS
3	A	667	ASP
3	A	696	LEU
3	A	727	LYS
3	A	740	THR
3	A	742	LYS
3	A	763	LEU
3	A	768	LYS
3	A	771	GLU
3	A	772	LYS
3	A	775	ARG
3	A	787	SER
3	A	813	THR
3	A	819	LYS
3	A	821	ASN
3	A	822	ILE
3	A	831	GLU
3	A	838	LEU
3	A	846	ASP
3	A	847	LYS
3	A	857	ILE
3	A	865	VAL
3	A	874	LEU
3	A	875	LEU
3	A	876	GLU
3	A	877	LYS
3	A	881	LYS
3	A	883	LEU
3	A	895	GLU
3	A	896	LYS
3	A	897	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	174	GLN
3	A	206	ASN
3	A	327	ASN
3	A	336	GLN
3	A	379	GLN
3	A	508	ASN
3	A	567	ASN
3	A	649	HIS
3	A	764	GLN
3	A	789	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

2 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	DOC	P	938	1,2	11,19,20	1.42	2 (18%)	14,26,29	1.23	1 (7%)
1	8OG	T	909	1	16,25,26	2.00	2 (12%)	21,37,40	4.31	6 (28%)

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	DOC	P	938	1,2	-	0/3/18/19	0/2/2/2
1	8OG	T	909	1	-	0/3/21/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	909	8OG	C8-N7	-6.45	1.27	1.34
2	P	938	DOC	C4-N3	-3.12	1.29	1.35
2	P	938	DOC	C6-C5	-2.99	1.31	1.38
1	T	909	8OG	C6-N1	3.97	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	909	8OG	C5-C6-N1	-10.48	109.27	123.59
1	T	909	8OG	C2'-C1'-N9	-8.92	106.88	115.83
1	T	909	8OG	N3-C2-N1	-2.43	123.74	127.44
1	T	909	8OG	C1'-N9-C4	2.68	131.54	127.37
2	P	938	DOC	C2-N3-C4	3.57	120.64	115.61
1	T	909	8OG	C6-N1-C2	7.25	126.00	115.94
1	T	909	8OG	O4'-C1'-N9	11.27	117.75	108.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	938	DOC	1	0
1	T	909	8OG	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\|>2$
5	DCP	P	939	4	21,29,29	1.01	0	33,45,45	1.59	5 (15%)

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
5	DCP	P	939	4	-	0/18/34/34	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	939	DCP	C2'-C1'-N1	-2.85	107.22	114.16
5	P	939	DCP	PB-O3A-PA	-2.79	124.91	132.73
5	P	939	DCP	C2-N3-C4	2.36	118.94	115.61
5	P	939	DCP	C5-C4-N4	2.57	125.25	121.31
5	P	939	DCP	O4'-C1'-N1	3.91	114.48	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	939	DCP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	T	17/18 (94%)	-0.45	0	100	100	17, 32, 51, 60	0
2	P	13/14 (92%)	-0.31	0	100	100	20, 33, 51, 56	0
3	A	902/906 (99%)	-0.35	8 (0%)	85	79	14, 35, 64, 90	0
All	All	932/938 (99%)	-0.35	8 (0%)	85	79	14, 35, 64, 90	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	260	TYR	4.4
3	A	3	SER	3.1
3	A	262	SER	2.7
3	A	261	GLY	2.6
3	A	2	GLY	2.4
3	A	643	LYS	2.3
3	A	531	GLU	2.2
3	A	259	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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	DOC	P	938	18/19	0.95	0.19	-	12,21,33,36	0
1	8OG	T	909	23/24	0.99	0.15	-	9,14,18,22	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
5	DCP	P	939	28/28	0.98	0.17	0.04	1,19,25,31	0
4	CA	A	939	1/1	0.98	0.11	-2.23	30,30,30,30	0
4	CA	A	940	1/1	0.70	0.29	-	55,55,55,55	0
4	CA	A	941	1/1	0.88	0.29	-	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.