Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:29 PM GMT

PDB ID	:	4TKG
Title	:	Crystal Structure of human Tankyrase 2 in complex with AZD2281.
Authors	:	Qiu, W.; Lam, R.; Romanov, V.; Gordon, R.; Gebremeskel, S.; Vodsedalek, J.; Thompson, C.; Beletskaya, I.; Battaile, K.P.; Pai, E.F.; Chirgadze, N.Y.
Deposited on	:	2014-05-26
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references (i)) 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 1.95 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.2%
RSRZ outliers		14.0%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
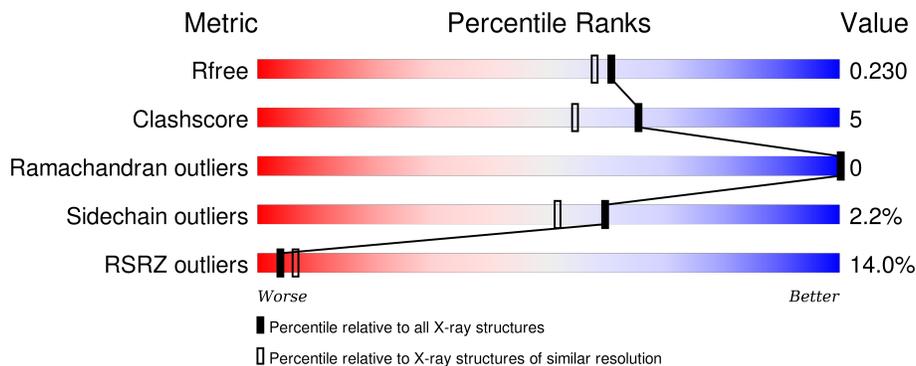
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	227	14% / 79% / 8% · 12%
1	B	227	10% / 81% / 9% 10%
1	C	227	7% / 83% / 8% 8%
1	D	227	19% / 76% / 10% · 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	1203	-	-	-	X
4	GOL	B	1204	-	-	-	X
4	GOL	C	1203	-	-	-	X

2   Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7201 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1603	1010	297	285	11			
1	B	205	Total	C	N	O	S	0	0	0
			1639	1030	303	295	11			
1	C	208	Total	C	N	O	S	0	1	0
			1679	1056	310	302	11			
1	D	196	Total	C	N	O	S	0	2	0
			1578	994	295	278	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	938	MET	-	initiating methionine	UNP Q9H2K2
A	939	GLY	-	expression tag	UNP Q9H2K2
A	940	SER	-	expression tag	UNP Q9H2K2
A	941	SER	-	expression tag	UNP Q9H2K2
A	942	HIS	-	expression tag	UNP Q9H2K2
A	943	HIS	-	expression tag	UNP Q9H2K2
A	944	HIS	-	expression tag	UNP Q9H2K2
A	945	HIS	-	expression tag	UNP Q9H2K2
A	946	HIS	-	expression tag	UNP Q9H2K2
A	947	HIS	-	expression tag	UNP Q9H2K2
A	948	SER	-	expression tag	UNP Q9H2K2
A	949	SER	-	expression tag	UNP Q9H2K2
A	950	GLY	-	expression tag	UNP Q9H2K2
A	951	ARG	-	expression tag	UNP Q9H2K2
A	952	GLU	-	expression tag	UNP Q9H2K2
A	953	ASN	-	expression tag	UNP Q9H2K2
A	954	LEU	-	expression tag	UNP Q9H2K2
A	955	TYR	-	expression tag	UNP Q9H2K2
A	956	PHE	-	expression tag	UNP Q9H2K2
A	957	GLN	-	expression tag	UNP Q9H2K2
A	958	GLY	-	expression tag	UNP Q9H2K2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	938	MET	-	initiating methionine	UNP Q9H2K2
B	939	GLY	-	expression tag	UNP Q9H2K2
B	940	SER	-	expression tag	UNP Q9H2K2
B	941	SER	-	expression tag	UNP Q9H2K2
B	942	HIS	-	expression tag	UNP Q9H2K2
B	943	HIS	-	expression tag	UNP Q9H2K2
B	944	HIS	-	expression tag	UNP Q9H2K2
B	945	HIS	-	expression tag	UNP Q9H2K2
B	946	HIS	-	expression tag	UNP Q9H2K2
B	947	HIS	-	expression tag	UNP Q9H2K2
B	948	SER	-	expression tag	UNP Q9H2K2
B	949	SER	-	expression tag	UNP Q9H2K2
B	950	GLY	-	expression tag	UNP Q9H2K2
B	951	ARG	-	expression tag	UNP Q9H2K2
B	952	GLU	-	expression tag	UNP Q9H2K2
B	953	ASN	-	expression tag	UNP Q9H2K2
B	954	LEU	-	expression tag	UNP Q9H2K2
B	955	TYR	-	expression tag	UNP Q9H2K2
B	956	PHE	-	expression tag	UNP Q9H2K2
B	957	GLN	-	expression tag	UNP Q9H2K2
B	958	GLY	-	expression tag	UNP Q9H2K2
C	938	MET	-	initiating methionine	UNP Q9H2K2
C	939	GLY	-	expression tag	UNP Q9H2K2
C	940	SER	-	expression tag	UNP Q9H2K2
C	941	SER	-	expression tag	UNP Q9H2K2
C	942	HIS	-	expression tag	UNP Q9H2K2
C	943	HIS	-	expression tag	UNP Q9H2K2
C	944	HIS	-	expression tag	UNP Q9H2K2
C	945	HIS	-	expression tag	UNP Q9H2K2
C	946	HIS	-	expression tag	UNP Q9H2K2
C	947	HIS	-	expression tag	UNP Q9H2K2
C	948	SER	-	expression tag	UNP Q9H2K2
C	949	SER	-	expression tag	UNP Q9H2K2
C	950	GLY	-	expression tag	UNP Q9H2K2
C	951	ARG	-	expression tag	UNP Q9H2K2
C	952	GLU	-	expression tag	UNP Q9H2K2
C	953	ASN	-	expression tag	UNP Q9H2K2
C	954	LEU	-	expression tag	UNP Q9H2K2
C	955	TYR	-	expression tag	UNP Q9H2K2
C	956	PHE	-	expression tag	UNP Q9H2K2
C	957	GLN	-	expression tag	UNP Q9H2K2
C	958	GLY	-	expression tag	UNP Q9H2K2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	HIS	-	expression tag	UNP Q9H2K2
D	944	HIS	-	expression tag	UNP Q9H2K2
D	945	HIS	-	expression tag	UNP Q9H2K2
D	946	HIS	-	expression tag	UNP Q9H2K2
D	947	HIS	-	expression tag	UNP Q9H2K2
D	948	SER	-	expression tag	UNP Q9H2K2
D	949	SER	-	expression tag	UNP Q9H2K2
D	950	GLY	-	expression tag	UNP Q9H2K2
D	951	ARG	-	expression tag	UNP Q9H2K2
D	952	GLU	-	expression tag	UNP Q9H2K2
D	953	ASN	-	expression tag	UNP Q9H2K2
D	954	LEU	-	expression tag	UNP Q9H2K2
D	955	TYR	-	expression tag	UNP Q9H2K2
D	956	PHE	-	expression tag	UNP Q9H2K2
D	957	GLN	-	expression tag	UNP Q9H2K2
D	958	GLY	-	expression tag	UNP Q9H2K2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0

- Molecule 3 is 4-(3-{[4-(cyclopropylcarbonyl)piperazin-1-yl]carbonyl}-4-fluorobenzyl)phthalazin-1(2H)-one (three-letter code: 09L) (formula: $C_{24}H_{23}FN_4O_3$).
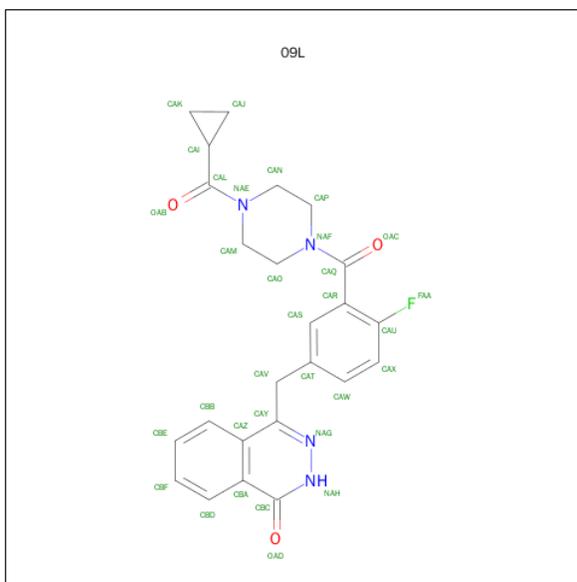
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			32	24	1	4	3		
3	B	1	Total	C	F	N	O	0	0
			32	24	1	4	3		
3	C	1	Total	C	F	N	O	0	0
			32	24	1	4	3		
3	D	1	Total	C	F	N	O	0	0
			32	24	1	4	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
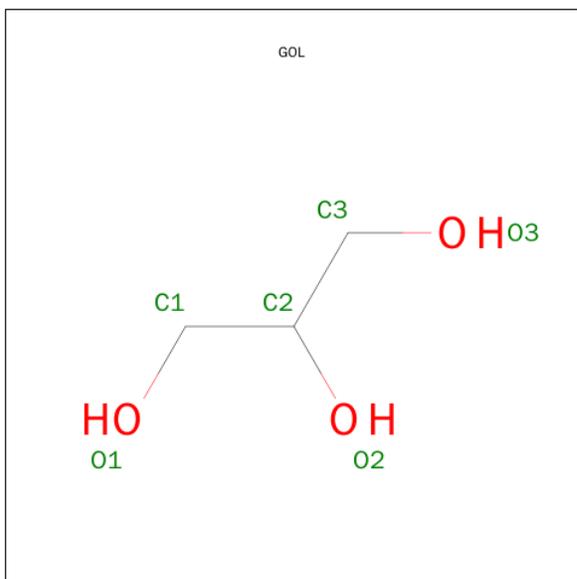
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total 145	O 145	0	0
5	B	140	Total 140	O 140	0	0
5	C	146	Total 146	O 146	0	0
5	D	109	Total 109	O 109	0	0

3 Residue-property plots ⓘ

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: Tankyrase-2
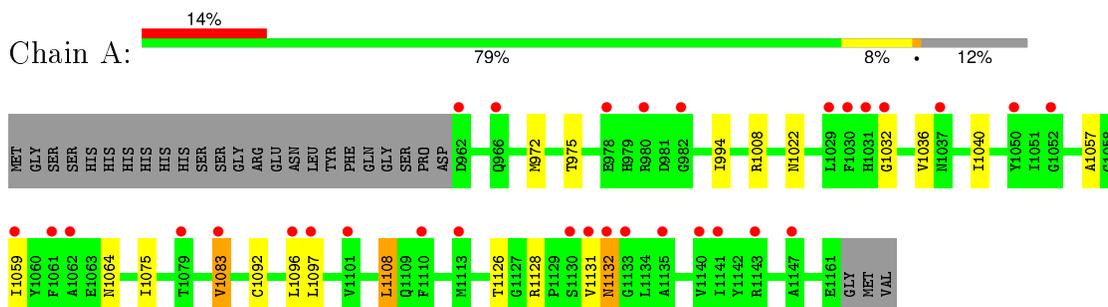

- Molecule 1: Tankyrase-2
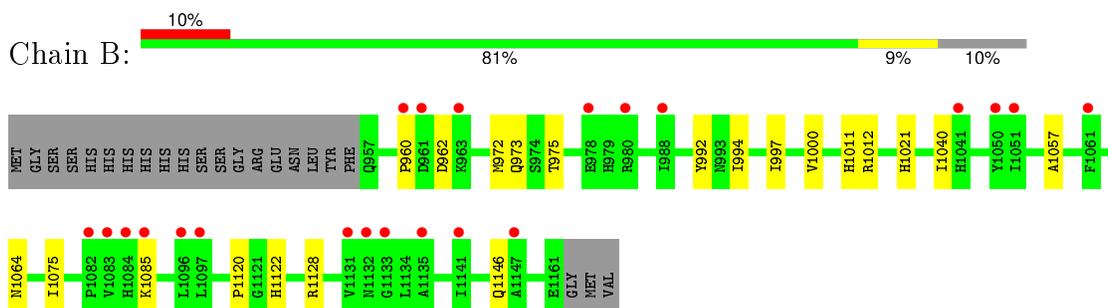
- Molecule 1: Tankyrase-2
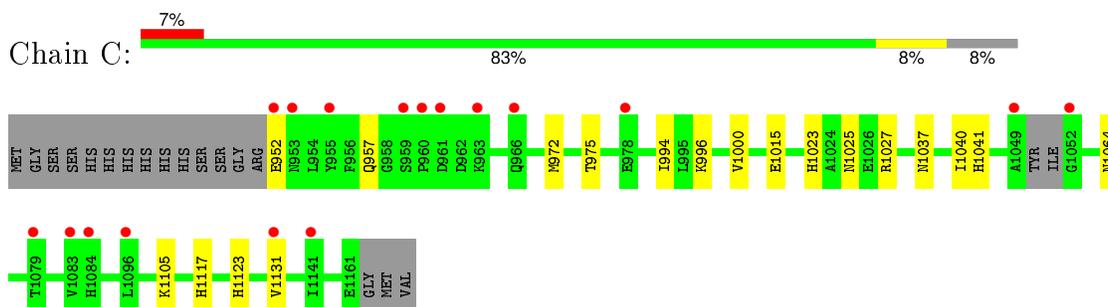
- Molecule 1: Tankyrase-2
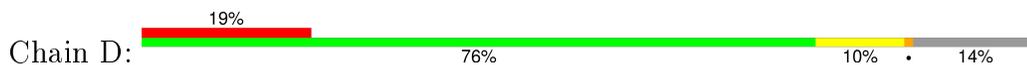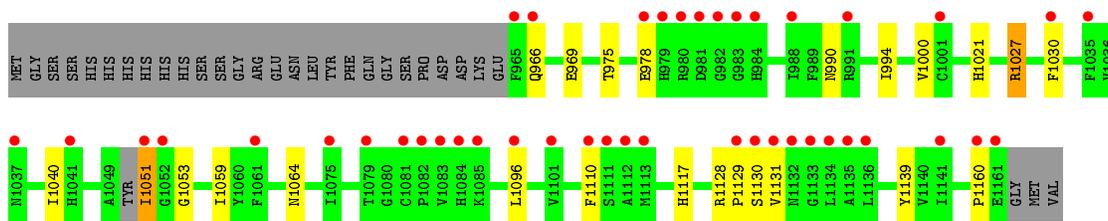
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.79Å 79.39Å 153.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.55 – 1.95 28.41 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.55-1.95) 100.0 (28.41-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.15 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.185 , 0.216 0.191 , 0.230	Depositor DCC
R_{free} test set	999 reflections (1.52%)	DCC
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	2 of 66638 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7201	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, 09L

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	0.52	0/1646	0.65	0/2214
1	B	0.52	0/1683	0.66	0/2263
1	C	0.51	0/1727	0.66	0/2321
1	D	0.51	0/1627	0.66	0/2189
All	All	0.51	0/6683	0.66	0/8987

There are no bond length outliers.

There are no bond angle outliers.

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	1603	0	1530	13	0
1	B	1639	0	1559	13	0
1	C	1679	0	1597	16	0
1	D	1578	0	1502	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	23	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	23	5	0
3	C	32	0	23	0	0
3	D	32	0	23	2	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	6	0	8	0	0
5	A	145	0	0	0	0
5	B	140	0	0	2	0
5	C	146	0	0	1	0
5	D	109	0	0	1	0
All	All	7201	0	6320	65	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 5.

All (65) 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:B:1000:VAL:HG21	1:B:1040:ILE:HD12	1.45	0.97
1:D:1000:VAL:HG21	1:D:1040:ILE:HD12	1.47	0.96
1:C:1000:VAL:HG21	1:C:1040:ILE:HD12	1.47	0.95
1:C:1105:LYS:H	1:C:1123:HIS:HD2	1.21	0.84
1:D:1110:PHE:HD2	1:D:1130:SER:HB3	1.51	0.74
1:D:1030:PHE:CD1	1:D:1096:LEU:HD21	2.22	0.74
1:C:1023[A]:HIS:HD2	1:C:1025:ASN:H	1.34	0.74
1:D:1051:ILE:HG23	1:D:1053:GLY:H	1.54	0.72
1:D:1000:VAL:HG21	1:D:1040:ILE:CD1	2.19	0.72
3:B:1202:09L:H12	3:B:1202:09L:FAA	1.81	0.71
1:C:1000:VAL:HG21	1:C:1040:ILE:CD1	2.20	0.71
1:B:1000:VAL:HG21	1:B:1040:ILE:CD1	2.19	0.70
1:D:1030:PHE:HD1	1:D:1096:LEU:HD21	1.56	0.69
1:C:957:GLN:HE22	1:C:996:LYS:HG2	1.56	0.69
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.80	0.64
1:A:1036:VAL:O	1:A:1040:ILE:HD12	1.98	0.64
1:A:1083:VAL:HG13	1:A:1092:CYS:SG	2.39	0.63
1:C:1023[A]:HIS:CD2	1:C:1025:ASN:H	2.16	0.62
1:B:1012:ARG:HE	1:B:1146:GLN:HE21	1.48	0.62
1:D:990:ASN:ND2	1:D:1160:PRO:HB3	2.14	0.62
3:A:1202:09L:H12	3:A:1202:09L:FAA	1.90	0.62
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.82	0.61
1:B:973:GLN:HE22	1:B:992:TYR:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1000:VAL:CG2	1:D:1040:ILE:HD12	2.29	0.59
3:B:1202:09L:CAP	3:B:1202:09L:FAA	2.41	0.59
1:C:1117:HIS:HD2	5:C:1333:HOH:O	1.85	0.58
1:C:1027:ARG:HD2	1:D:1021[B]:HIS:CE1	2.38	0.58
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.87	0.57
1:C:1000:VAL:CG2	1:C:1040:ILE:HD12	2.29	0.57
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.86	0.57
1:C:1105:LYS:H	1:C:1123:HIS:CD2	2.12	0.56
1:A:1040:ILE:HD11	1:A:1097:LEU:HD21	1.86	0.56
1:D:1051:ILE:HG21	3:D:1202:09L:H15	1.88	0.56
1:B:972:MET:HG2	1:B:994:ILE:HD11	1.89	0.55
1:B:1000:VAL:CG2	1:B:1040:ILE:HD12	2.28	0.54
3:B:1202:09L:CAU	3:B:1202:09L:H12	2.37	0.54
1:D:969:GLU:HG3	1:D:994:ILE:HD13	1.90	0.52
1:A:1059:ILE:HG23	3:A:1202:09L:H9	1.92	0.52
1:C:1037:ASN:O	1:C:1041:HIS:HD2	1.92	0.51
1:D:1128:ARG:HD3	1:D:1129:PRO:CD	2.41	0.51
1:A:1132:ASN:HD22	1:A:1132:ASN:H	1.59	0.51
1:D:1128:ARG:HD3	1:D:1129:PRO:HD2	1.92	0.50
3:A:1202:09L:CAU	3:A:1202:09L:H12	2.41	0.49
1:C:1023[A]:HIS:HD2	1:C:1025:ASN:N	2.08	0.48
1:B:1075:ILE:CD1	3:B:1202:09L:H16	2.43	0.47
1:A:1075:ILE:CD1	3:A:1202:09L:H16	2.43	0.47
1:D:1059:ILE:HG23	3:D:1202:09L:H8	1.95	0.47
1:D:1027:ARG:NH1	1:D:1139:TYR:OH	2.47	0.47
1:A:1032:GLY:HA2	1:A:1096:LEU:HD23	2.00	0.44
1:A:1008:ARG:HG2	1:C:1015:GLU:OE2	2.17	0.44
1:B:1011:HIS:HE1	5:B:1356:HOH:O	2.00	0.44
1:B:960:PRO:HD3	1:B:997:ILE:O	2.19	0.43
3:A:1202:09L:CAP	3:A:1202:09L:FAA	2.54	0.43
1:C:975:THR:HB	1:C:1064:ASN:HA	2.00	0.43
1:D:1117:HIS:HD2	5:D:1325:HOH:O	2.01	0.43
3:B:1202:09L:H5	3:B:1202:09L:H11	1.88	0.43
1:D:1128:ARG:CD	1:D:1129:PRO:HD2	2.49	0.42
1:A:1108:LEU:HD12	1:A:1126:THR:HB	2.02	0.41
1:D:978:GLU:CD	1:D:978:GLU:H	2.24	0.41
1:B:1021:HIS:HD2	5:B:1302:HOH:O	2.03	0.41
1:A:975:THR:HB	1:A:1064:ASN:HA	2.03	0.41
1:D:975:THR:HB	1:D:1064:ASN:HA	2.02	0.41
1:A:1075:ILE:HD12	3:A:1202:09L:H16	2.02	0.41
1:B:1120:PRO:O	1:B:1122:HIS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:THR:HB	1:B:1064:ASN:HA	2.03	0.41

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	198/227 (87%)	195 (98%)	3 (2%)	0	100	100
1	B	203/227 (89%)	199 (98%)	4 (2%)	0	100	100
1	C	205/227 (90%)	201 (98%)	4 (2%)	0	100	100
1	D	194/227 (86%)	189 (97%)	5 (3%)	0	100	100
All	All	800/908 (88%)	784 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	166/192 (86%)	160 (96%)	6 (4%)	42	28
1	B	170/192 (88%)	167 (98%)	3 (2%)	66	60
1	C	176/192 (92%)	174 (99%)	2 (1%)	80	77
1	D	164/192 (85%)	160 (98%)	4 (2%)	57	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	676/768 (88%)	661 (98%)	15 (2%)	60 51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1022	ASN
1	A	1083	VAL
1	A	1108	LEU
1	A	1128	ARG
1	A	1131	VAL
1	A	1132	ASN
1	B	962	ASP
1	B	1085	LYS
1	B	1128	ARG
1	C	952	GLU
1	C	1131	VAL
1	D	966	GLN
1	D	1027	ARG
1	D	1051	ILE
1	D	1131	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1132	ASN
1	A	1156	GLN
1	B	973	GLN
1	B	1011	HIS
1	B	1122	HIS
1	B	1146	GLN
1	B	1156	GLN
1	C	957	GLN
1	C	1037	ASN
1	C	1041	HIS
1	C	1095	GLN
1	C	1117	HIS
1	C	1123	HIS
1	C	1156	GLN
1	D	990	ASN
1	D	1025	ASN
1	D	1109	GLN

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Mol	Chain	Res	Type
1	D	1117	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#|Z| > 2$
3	09L	A	1202	-	36,36,36	2.56	13 (36%)	45,52,52	1.80	9 (20%)
4	GOL	A	1203	-	5,5,5	0.12	0	5,5,5	0.34	0
4	GOL	A	1204	-	5,5,5	0.12	0	5,5,5	0.19	0
3	09L	B	1202	-	36,36,36	2.50	12 (33%)	45,52,52	1.70	6 (13%)
4	GOL	B	1203	-	5,5,5	0.11	0	5,5,5	0.22	0
4	GOL	B	1204	-	5,5,5	0.12	0	5,5,5	0.17	0
3	09L	C	1202	-	36,36,36	2.67	13 (36%)	45,52,52	2.08	8 (17%)
4	GOL	C	1203	-	5,5,5	0.17	0	5,5,5	0.31	0
3	09L	D	1202	-	36,36,36	2.80	13 (36%)	45,52,52	2.18	9 (20%)

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
3	09L	A	1202	-	-	0/20/32/32	0/4/5/5
4	GOL	A	1203	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1204	-	-	0/4/4/4	0/0/0/0
3	09L	B	1202	-	-	0/20/32/32	0/4/5/5
4	GOL	B	1203	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1204	-	-	0/4/4/4	0/0/0/0
3	09L	C	1202	-	-	0/20/32/32	0/4/5/5
4	GOL	C	1203	-	-	0/4/4/4	0/0/0/0
3	09L	D	1202	-	-	0/20/32/32	0/4/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	09L	CBE-CBB	2.00	1.41	1.36
3	A	1202	09L	CAW-CAT	2.01	1.43	1.38
3	B	1202	09L	CAR-CAU	2.05	1.41	1.38
3	B	1202	09L	CBC-CBA	2.06	1.44	1.41
3	A	1202	09L	CBE-CBB	2.15	1.41	1.36
3	A	1202	09L	CAY-NAG	2.24	1.35	1.32
3	C	1202	09L	CAY-CAZ	2.30	1.45	1.43
3	C	1202	09L	CAW-CAT	2.35	1.43	1.38
3	C	1202	09L	CBC-CBA	2.38	1.45	1.41
3	D	1202	09L	CAY-CAZ	2.38	1.45	1.43
3	C	1202	09L	CBB-CAZ	2.57	1.47	1.42
3	B	1202	09L	OAB-CAL	2.69	1.27	1.22
3	D	1202	09L	CBE-CBB	2.70	1.42	1.36
3	A	1202	09L	CAR-CAU	2.72	1.42	1.38
3	C	1202	09L	NAH-NAG	2.72	1.41	1.34
3	D	1202	09L	CBC-CBA	2.79	1.46	1.41
3	A	1202	09L	CBB-CAZ	2.89	1.48	1.42
3	B	1202	09L	NAH-NAG	2.90	1.41	1.34
3	B	1202	09L	CBB-CAZ	2.91	1.48	1.42
3	B	1202	09L	CBF-CBD	2.91	1.43	1.36
3	A	1202	09L	NAH-NAG	2.96	1.41	1.34
3	A	1202	09L	CAV-CAY	2.97	1.54	1.51
3	D	1202	09L	NAH-NAG	3.02	1.41	1.34
3	D	1202	09L	CAS-CAR	3.02	1.44	1.39
3	D	1202	09L	OAB-CAL	3.03	1.28	1.22
3	D	1202	09L	CAY-NAG	3.04	1.36	1.32
3	C	1202	09L	CAS-CAR	3.08	1.44	1.39
3	A	1202	09L	OAB-CAL	3.09	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	09L	CBF-CBD	3.09	1.43	1.36
3	B	1202	09L	CAS-CAR	3.11	1.44	1.39
3	A	1202	09L	CAS-CAR	3.18	1.44	1.39
3	B	1202	09L	CAY-NAG	3.24	1.36	1.32
3	A	1202	09L	CBF-CBD	3.25	1.44	1.36
3	D	1202	09L	CBB-CAZ	3.27	1.48	1.42
3	D	1202	09L	CBF-CBD	3.34	1.44	1.36
3	C	1202	09L	OAB-CAL	3.64	1.29	1.22
3	C	1202	09L	CAV-CAY	4.41	1.55	1.51
3	B	1202	09L	CAV-CAY	4.47	1.55	1.51
3	C	1202	09L	CAI-CAL	4.99	1.59	1.51
3	A	1202	09L	CAI-CAL	5.23	1.59	1.51
3	D	1202	09L	CAV-CAY	5.33	1.56	1.51
3	B	1202	09L	CAI-CAL	5.34	1.59	1.51
3	A	1202	09L	CAQ-NAF	5.47	1.47	1.34
3	C	1202	09L	CAQ-NAF	5.50	1.47	1.34
3	D	1202	09L	CAQ-NAF	5.53	1.47	1.34
3	D	1202	09L	CAI-CAL	5.63	1.60	1.51
3	B	1202	09L	CAQ-NAF	5.73	1.48	1.34
3	B	1202	09L	CAL-NAE	7.91	1.46	1.34
3	A	1202	09L	CAL-NAE	8.47	1.47	1.34
3	D	1202	09L	CAL-NAE	9.22	1.48	1.34
3	C	1202	09L	CAL-NAE	9.27	1.48	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1202	09L	CAJ-CAI-CAL	-6.28	109.98	117.22
3	B	1202	09L	CAJ-CAI-CAL	-5.53	110.85	117.22
3	B	1202	09L	OAB-CAL-NAE	-4.64	115.87	121.66
3	A	1202	09L	OAB-CAL-NAE	-4.18	116.45	121.66
3	C	1202	09L	CAK-CAI-CAL	-4.01	112.60	117.22
3	D	1202	09L	OAC-CAQ-CAR	-3.53	112.96	120.14
3	D	1202	09L	OAC-CAQ-NAF	-3.48	116.89	122.42
3	C	1202	09L	OAC-CAQ-CAR	-3.40	113.20	120.14
3	D	1202	09L	OAB-CAL-NAE	-3.39	117.43	121.66
3	D	1202	09L	CAJ-CAI-CAL	-3.19	113.54	117.22
3	C	1202	09L	CAJ-CAI-CAL	-2.94	113.83	117.22
3	C	1202	09L	OAB-CAL-NAE	-2.91	118.03	121.66
3	C	1202	09L	OAC-CAQ-NAF	-2.89	117.82	122.42
3	A	1202	09L	CAX-CAU-CAR	-2.59	120.18	123.20
3	A	1202	09L	CAP-CAN-NAE	-2.52	104.75	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	09L	OAC-CAQ-CAR	-2.42	115.21	120.14
3	B	1202	09L	CAX-CAU-CAR	-2.34	120.47	123.20
3	A	1202	09L	OAC-CAQ-NAF	-2.23	118.87	122.42
3	D	1202	09L	CAK-CAI-CAL	-2.08	114.82	117.22
3	D	1202	09L	CBC-NAH-NAG	2.14	120.90	119.30
3	A	1202	09L	FAA-CAU-CAR	2.16	122.71	119.53
3	D	1202	09L	CAN-CAP-NAF	2.40	115.96	110.49
3	B	1202	09L	CAS-CAR-CAU	2.42	120.03	116.62
3	A	1202	09L	OAB-CAL-CAI	2.54	124.79	120.81
3	A	1202	09L	CAS-CAR-CAU	2.68	120.40	116.62
3	C	1202	09L	CAN-CAP-NAF	2.71	116.64	110.49
3	C	1202	09L	CAP-CAN-NAE	2.81	116.88	110.49
3	D	1202	09L	CAP-CAN-NAE	3.25	117.88	110.49
3	A	1202	09L	CAR-CAQ-NAF	5.03	123.93	118.29
3	B	1202	09L	CAR-CAQ-NAF	5.04	123.93	118.29
3	C	1202	09L	CAR-CAQ-NAF	9.53	128.97	118.29
3	D	1202	09L	CAR-CAQ-NAF	10.58	130.15	118.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	09L	6	0
3	B	1202	09L	5	0
3	D	1202	09L	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	200/227 (88%)	0.75	31 (15%)	3	4	25, 40, 64, 78	0
1	B	205/227 (90%)	0.51	22 (10%)	8	12	23, 39, 68, 85	0
1	C	208/227 (91%)	0.46	17 (8%)	14	23	24, 37, 71, 90	0
1	D	196/227 (86%)	1.06	43 (21%)	1	1	26, 43, 77, 98	0
All	All	809/908 (89%)	0.69	113 (13%)	4	6	23, 40, 71, 98	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1131	VAL	12.1
1	D	1083	VAL	6.9
1	B	961	ASP	6.3
1	D	1082	PRO	6.3
1	D	1132	ASN	5.9
1	D	1079	THR	5.9
1	A	1131	VAL	5.7
1	B	1131	VAL	5.7
1	D	1135	ALA	5.6
1	A	1132	ASN	5.5
1	D	988	ILE	5.4
1	C	953	ASN	5.3
1	D	1133	GLY	5.0
1	C	961	ASP	5.0
1	D	981	ASP	5.0
1	C	955	TYR	4.9
1	A	1133	GLY	4.9
1	B	1132	ASN	4.9
1	D	1110	PHE	4.6
1	D	982	GLY	4.4
1	D	980	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	1131	VAL	4.4
1	C	1083	VAL	4.3
1	D	965	PHE	4.2
1	A	1061	PHE	4.1
1	D	1129	PRO	4.1
1	B	1083	VAL	3.9
1	C	959	SER	3.9
1	D	1130	SER	3.8
1	A	1141	ILE	3.7
1	D	1085	LYS	3.7
1	D	978	GLU	3.7
1	C	952	GLU	3.6
1	B	960	PRO	3.5
1	D	1134	LEU	3.5
1	D	1081	CYS	3.5
1	A	1147	ALA	3.5
1	A	1052	GLY	3.5
1	D	1113	MET	3.4
1	D	1052	GLY	3.4
1	A	978	GLU	3.4
1	B	1085	LYS	3.4
1	D	1112	ALA	3.3
1	A	966	GLN	3.3
1	D	1051	ILE	3.3
1	B	980	ARG	3.3
1	C	1052	GLY	3.2
1	D	966	GLN	3.1
1	A	1096	LEU	3.1
1	A	1140	VAL	3.1
1	A	1059	ILE	3.0
1	A	1079	THR	3.0
1	B	1096	LEU	3.0
1	C	1049	ALA	3.0
1	D	1075	ILE	2.9
1	C	960	PRO	2.9
1	A	1050	TYR	2.9
1	A	962	ASP	2.9
1	A	1110	PHE	2.9
1	A	1135	ALA	2.9
1	A	982	GLY	2.9
1	D	1111	SER	2.8
1	D	1084	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1101	VAL	2.7
1	D	1096	LEU	2.7
1	B	1041	HIS	2.7
1	B	1133	GLY	2.7
1	A	1030	PHE	2.7
1	D	1041[A]	HIS	2.7
1	D	1037	ASN	2.6
1	C	963	LYS	2.6
1	D	1161	GLU	2.6
1	C	978	GLU	2.5
1	D	984	HIS	2.5
1	A	1083	VAL	2.5
1	A	980	ARG	2.5
1	A	1062	ALA	2.5
1	D	1035	PHE	2.5
1	A	1029	LEU	2.4
1	D	979	HIS	2.4
1	D	1141	ILE	2.4
1	D	991	ARG	2.4
1	B	1084	HIS	2.4
1	B	1141	ILE	2.4
1	B	1061	PHE	2.4
1	B	1050	TYR	2.3
1	B	1082	PRO	2.3
1	D	1061	PHE	2.3
1	B	978	GLU	2.3
1	D	1030	PHE	2.2
1	D	1001	CYS	2.2
1	A	1113	MET	2.2
1	A	1097	LEU	2.2
1	D	1101	VAL	2.2
1	C	1079	THR	2.2
1	C	966	GLN	2.2
1	D	983	GLY	2.2
1	B	963	LYS	2.2
1	A	1032	GLY	2.2
1	B	988	ILE	2.2
1	B	1051	ILE	2.2
1	B	1097	LEU	2.1
1	D	1136	LEU	2.1
1	A	1037	ASN	2.1
1	C	1141	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1084	HIS	2.1
1	A	1143	ARG	2.0
1	B	1147	ALA	2.0
1	A	1130	SER	2.0
1	C	1096	LEU	2.0
1	A	1031	HIS	2.0
1	B	1135	ALA	2.0
1	D	1160	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	B	1204	6/6	0.11	0.87	18.07	162,162,162,162	0
4	GOL	B	1203	6/6	0.61	0.42	7.13	94,95,96,98	0
4	GOL	C	1203	6/6	0.70	0.28	5.17	69,71,73,75	0
4	GOL	A	1203	6/6	0.79	0.21	0.91	48,56,60,64	0
3	09L	A	1202	32/32	0.87	0.21	0.87	26,38,51,52	0
3	09L	C	1202	32/32	0.91	0.16	0.66	26,42,64,65	0
3	09L	D	1202	32/32	0.88	0.17	0.41	27,49,67,68	0
3	09L	B	1202	32/32	0.89	0.15	0.40	26,38,49,50	0
2	ZN	C	1201	1/1	0.98	0.04	-1.39	45,45,45,45	0
2	ZN	D	1201	1/1	0.97	0.06	-1.62	64,64,64,64	0
2	ZN	A	1201	1/1	0.98	0.04	-1.68	44,44,44,44	0
2	ZN	B	1201	1/1	0.97	0.04	-1.79	57,57,57,57	0
4	GOL	A	1204	6/6	0.01	1.19	-	147,148,148,149	0

6.5 Other polymers (i)

There are no such residues in this entry.