Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 02:29 pm BST

PDB ID	:	2UW3
Title	:	Structure of PKA-PKB chimera complexed with 5-methyl-4-phenyl-1H-pyrazole
Authors	:	Davies, T.G.; Saxty, G.; Woodhead, S.J.; Berdini, V.; Verdonk, M.L.; Wyatt, P.G.; Boyle, R.G.; Barford, D.; Downham, R.; Garrett, M.D.; Carr, R.A.
Deposited on	:	2007-03-19
Resolution	:	2.19 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

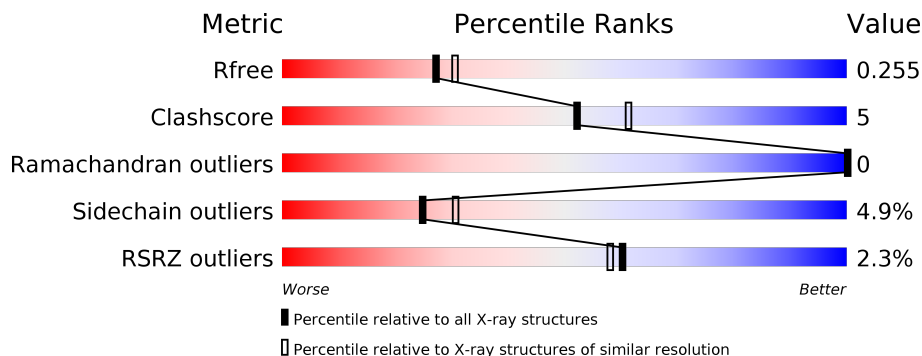|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.19 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		0.255
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		4.9%
RSRZ outliers		2.3%

■ 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. 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	351	2% / 81% / 13% · ·
2	I	20	10% / 90% / 5% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3200 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 CAMP-DEPENDENT PROTEIN KINASE, ALPHA-CATALYTIC SUBUNIT.

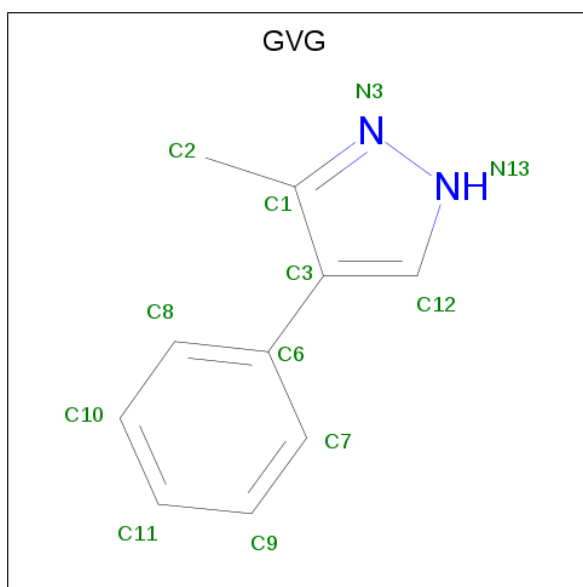| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	P	S	0	0	0
			2788	1803	467	505	3	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	THR	VAL	engineered mutation	UNP P00517
A	123	ALA	VAL	engineered mutation	UNP P00517
A	173	MET	LEU	engineered mutation	UNP P00517
A	181	LYS	GLN	engineered mutation	UNP P00517

- Molecule 2 is a protein called CAMP-DEPENDENT PROTEIN KINASE INHIBITOR AL-PHA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

- Molecule 3 is 3-METHYL-4-PHENYL-1H-PYRAZOLE (three-letter code: GVG) (formula: $C_{10}H_{10}N_2$).

GVG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 12	C 10	N 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total 215	O 215	0	0
4	I	28	Total 28	O 28	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 the various outlier classes 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: CAMP-DEPENDENT PROTEIN KINASE, ALPHA-CATALYTIC SUBUNIT
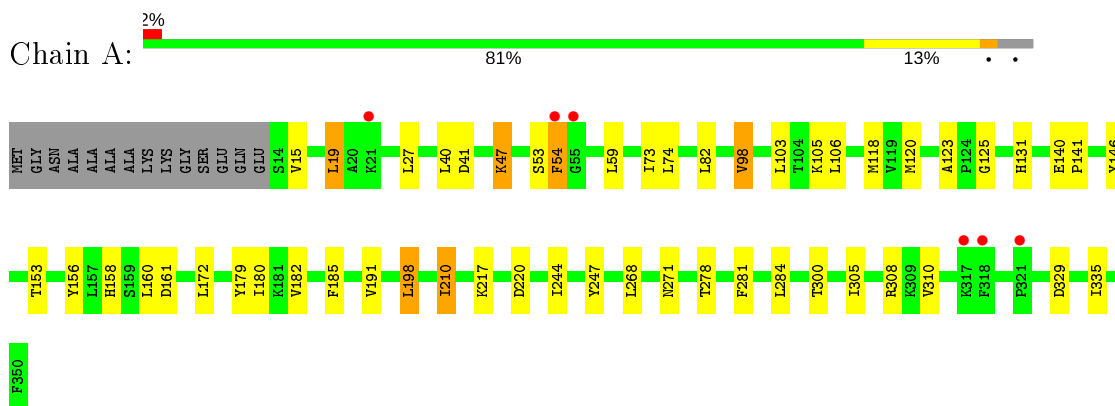
● Molecule 2: CAMP-DEPENDENT PROTEIN KINASE INHIBITOR ALPHA
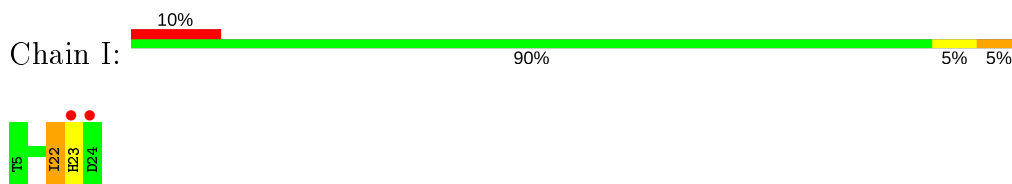
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.79Å 74.49Å 79.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.59 – 2.19 43.59 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.59-2.19) 98.4 (43.59-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.05 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019G	Depositor
R, R_{free}	0.187 , 0.252 0.196 , 0.255	Depositor DCC
R_{free} test set	1133 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.0	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3200	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: TPO, GVG, SEP

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	0.62	0/2827	0.69	0/3804
2	I	0.61	0/159	0.66	0/212
All	All	0.62	0/2986	0.69	0/4016

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	2788	0	2762	31	0
2	I	157	0	146	2	0
3	A	12	0	10	1	0
4	A	215	0	0	2	0
4	I	28	0	0	0	0
All	All	3200	0	2918	32	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 (32) 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:A:73:ILE:HD13	1:A:335:ILE:HD11	1.52	0.89
1:A:123:ALA:H	3:A:1351:GVG:H13	1.22	0.87
1:A:210:ILE:HD13	1:A:247:TYR:HB3	1.56	0.87
1:A:156:TYR:O	1:A:160:LEU:HD13	1.80	0.81
1:A:54:PHE:CD1	1:A:82:LEU:HD13	2.32	0.64
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.69	0.57
1:A:98:VAL:HG22	1:A:156:TYR:HE2	1.69	0.57
1:A:54:PHE:CD1	1:A:54:PHE:N	2.76	0.54
1:A:103:LEU:HD21	1:A:153:THR:CG2	2.41	0.51
1:A:300:THR:HG23	1:A:305:ILE:CD1	2.42	0.49
1:A:54:PHE:HD1	1:A:82:LEU:HD13	1.73	0.49
1:A:105:LYS:HA	4:A:2073:HOH:O	2.11	0.49
1:A:98:VAL:HG22	1:A:156:TYR:CE2	2.47	0.48
1:A:278:THR:O	1:A:284:LEU:HD22	2.13	0.47
1:A:305:ILE:HG13	1:A:310:VAL:HG21	1.95	0.47
1:A:15:VAL:HG12	1:A:19:LEU:HD22	1.95	0.47
1:A:125:GLY:O	1:A:131:HIS:CE1	2.68	0.47
2:I:22:ILE:HG12	2:I:23:HIS:N	2.30	0.46
1:A:271:ASN:HB3	1:A:281:PHE:CD1	2.52	0.45
1:A:198:LEU:HD22	2:I:22:ILE:HD11	1.98	0.45
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.99	0.44
1:A:73:ILE:HD13	1:A:335:ILE:CD1	2.37	0.44
1:A:106:LEU:HD11	1:A:118:MET:HB3	1.99	0.43
1:A:161:ASP:HA	1:A:217:LYS:HE2	2.00	0.43
1:A:103:LEU:HD21	1:A:153:THR:HG23	2.00	0.43
1:A:172:LEU:CD2	1:A:182:VAL:HG22	2.49	0.43
1:A:140:GLU:N	1:A:141:PRO:CD	2.82	0.42
1:A:146:TYR:HB3	1:A:180:ILE:HD11	2.01	0.42
1:A:47:LYS:NZ	1:A:329:ASP:OD1	2.52	0.41
1:A:179:TYR:CZ	1:A:308:ARG:HA	2.55	0.41
1:A:105:LYS:O	1:A:120:MET:HA	2.20	0.41
1:A:244:ILE:HG23	4:A:2155:HOH:O	2.21	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	332/351 (95%)	327 (98%)	5 (2%)	0	100	100
2	I	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
All	All	350/371 (94%)	344 (98%)	6 (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	294/302 (97%)	280 (95%)	14 (5%)	25	32
2	I	15/15 (100%)	14 (93%)	1 (7%)	16	18
All	All	309/317 (98%)	294 (95%)	15 (5%)	25	31

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

Mol	Chain	Res	Type
1	A	19	LEU
1	A	27	LEU
1	A	40	LEU
1	A	41	ASP
1	A	47	LYS
1	A	53	SER
1	A	54	PHE
1	A	59	LEU
1	A	74	LEU
1	A	98	VAL
1	A	191	VAL
1	A	198	LEU
1	A	210	ILE
1	A	268	LEU
2	I	22	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	158	HIS
1	A	307	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	TPO	A	197	1	8,10,11	1.17	0	10,14,16	1.46	2 (20%)
1	SEP	A	139	1	8,9,10	1.72	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	A	338	1	8,9,10	1.46	1 (12%)	8,12,14	1.67	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	197	1	-	1/9/11/13	-
1	SEP	A	139	1	-	0/5/8/10	-
1	SEP	A	338	1	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	SEP	P-O1P	3.55	1.62	1.50
1	A	338	SEP	P-O1P	2.90	1.59	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	SEP	OG-CB-CA	3.87	111.92	108.14
1	A	338	SEP	OG-CB-CA	3.44	111.50	108.14
1	A	197	TPO	CG2-CB-CA	-2.87	107.50	113.16
1	A	197	TPO	P-OG1-CB	-2.51	115.63	123.21
1	A	338	SEP	OG-P-O1P	2.31	112.95	106.47
1	A	139	SEP	P-OG-CB	-2.00	112.78	118.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	CB-OG-P-O2P
1	A	338	SEP	N-CA-CB-OG
1	A	197	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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
3	GVG	A	1351	-	12,13,13	0.88	0	10,17,17	0.49	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
3	GVG	A	1351	-	-	0/4/4/4	0/2/2/2

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1351	GVG	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 (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	334/351 (95%)	0.11	6 (1%)	68	66	19, 32, 56, 76	0
2	I	20/20 (100%)	0.45	2 (10%)	7	6	23, 27, 71, 79	0
All	All	354/371 (95%)	0.13	8 (2%)	60	58	19, 32, 56, 79	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	5.8
1	A	54	PHE	5.3
1	A	321	PRO	4.5
2	I	24	ASP	2.9
2	I	23	HIS	2.8
1	A	317	LYS	2.5
1	A	55	GLY	2.3
1	A	21	LYS	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. 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	B-factors(Å^2)	Q<0.9
1	SEP	A	139	10/11	0.88	0.20	33,40,65,67	0
1	SEP	A	338	10/11	0.97	0.15	36,40,44,45	0
1	TPO	A	197	11/12	0.99	0.13	21,25,27,28	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. 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	B-factors(Å^2)	Q<0.9
3	GVG	A	1351	12/12	0.96	0.09	18,24,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.