Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:42 AM GMT

PDB ID	:	3MVH
Title	:	Crystal structure of Akt-1-inhibitor complexes
Authors	:	Pandit, J.
Deposited on	:	2010-05-04
Resolution	:	2.01 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:

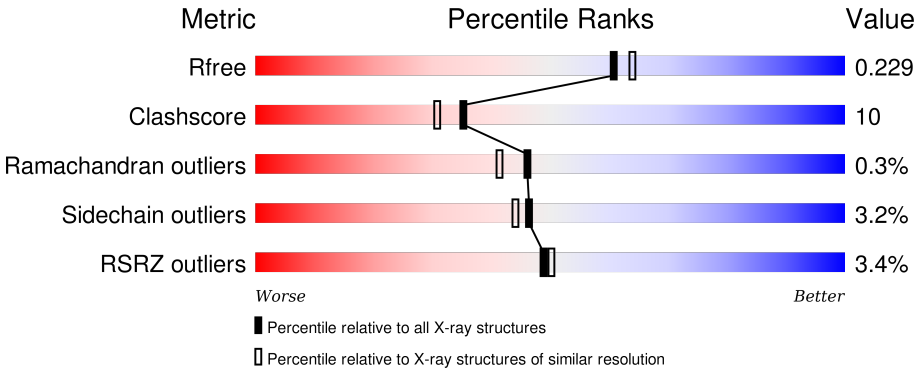
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.01 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	342	3%, 73%, 17%, •, 9%
2	B	10	90%, 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2962 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 v-akt murine thymoma viral oncogene homolog 1 (AKT1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	P	S	0	9	0
			2606	1674	435	480	1	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	GLY	-	EXPRESSION TAG	UNP B2RAM5
A	140	ALA	-	EXPRESSION TAG	UNP B2RAM5
A	141	MET	-	EXPRESSION TAG	UNP B2RAM5
A	142	ASP	-	EXPRESSION TAG	UNP B2RAM5
A	143	PRO	-	EXPRESSION TAG	UNP B2RAM5
A	473	ASP	SER	ENGINEERED	UNP B2RAM5

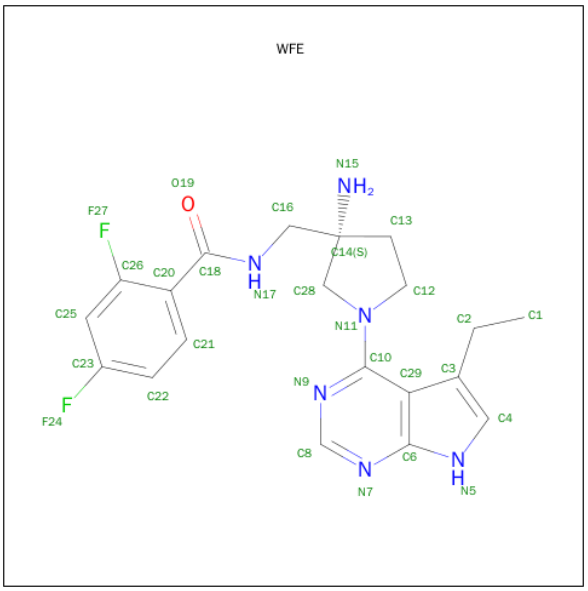
- Molecule 2 is a protein called GSK3-beta peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			79	47	16	16			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is N-{[(3S)-3-AMINO-1-(5-ETHYL-7H-PYRROLO[2,3-D]PYRIMIDIN-4-YL) PYRROLIDIN-3-YL]METHYL}-2,4-DIFLUOROBENZAMIDE (three-letter code: WFE) (formula: $C_{20}H_{22}F_2N_6O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			29	20	2	6	1		

- Molecule 5 is water.

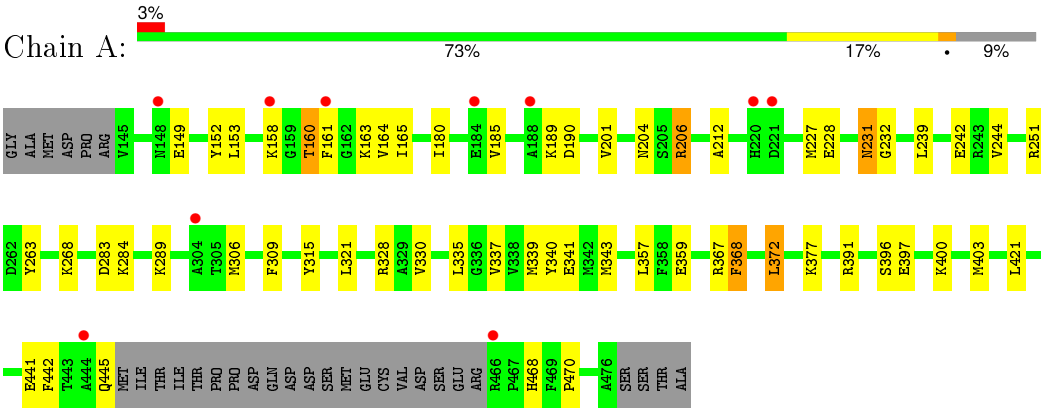
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total	O	0	0
			230	230		
5	B	17	Total	O	0	0
			17	17		

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.

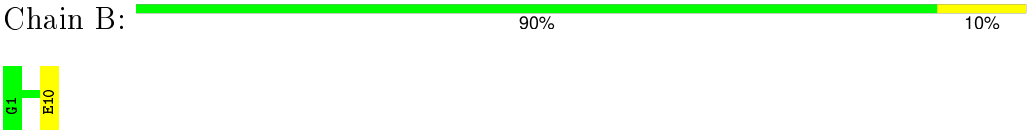
- Molecule 1: v-akt murine thymoma viral oncogene homolog 1 (AKT1)

Chain A:



- Molecule 2: GSK3-beta peptide

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.35Å 55.26Å 92.31Å 90.00° 102.64° 90.00°	Depositor
Resolution (Å)	50.00 – 2.01 34.91 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.01) 99.3 (34.91-2.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.07 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.230 0.176 , 0.229	Depositor DCC
R_{free} test set	1391 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.8	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 27814 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2962	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% 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: TPO, MN, WFE

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	1.35	12/2675 (0.4%)	1.07	10/3597 (0.3%)
2	B	1.43	0/80	1.09	0/105
All	All	1.35	12/2755 (0.4%)	1.07	10/3702 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	VAL	CB-CG1	7.14	1.67	1.52
1	A	397	GLU	CG-CD	6.38	1.61	1.51
1	A	330	VAL	CB-CG2	6.20	1.65	1.52
1	A	340	TYR	CE1-CZ	6.14	1.46	1.38
1	A	359	GLU	CG-CD	5.99	1.60	1.51
1	A	328	ARG	CG-CD	5.88	1.66	1.51
1	A	315	TYR	CD2-CE2	5.78	1.48	1.39
1	A	396	SER	CA-CB	5.67	1.61	1.52
1	A	256	GLU	CB-CG	5.44	1.62	1.52
1	A	201	VAL	CB-CG1	5.39	1.64	1.52
1	A	341	GLU	CG-CD	-5.26	1.44	1.51
1	A	368	PHE	CE1-CZ	5.17	1.47	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ASP	CB-CG-OD1	8.36	125.82	118.30
1	A	328	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	367	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	434	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	A	372	LEU	CA-CB-CG	6.27	129.72	115.30
1	A	328	ARG	CG-CD-NE	-5.92	99.36	111.80
1	A	261	LEU	CB-CG-CD1	-5.50	101.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	153	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	391	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2606	0	2564	50	0
2	B	79	0	77	3	0
3	A	1	0	0	0	0
4	A	29	0	22	6	0
5	A	230	0	0	15	0
5	B	17	0	0	1	0
All	All	2962	0	2663	53	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 (53) 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:289:LYS:HE2	5:A:1232:HOH:O	1.38	1.24
1:A:204:ASN:HB2	5:A:1221:HOH:O	1.40	1.20
1:A:244:VAL:HB	5:A:1239:HOH:O	1.51	1.08
1:A:431:SER:O	1:A:432:GLU:HB2	1.38	1.08
1:A:357:LEU:HD13	5:A:1234:HOH:O	1.70	0.91
1:A:231[A]:ASN:HD21	1:A:284:LYS:HA	1.35	0.89
1:A:400:LYS:HG3	1:A:403:MET:CE	2.05	0.87
1:A:431:SER:O	1:A:432:GLU:CB	2.20	0.87
1:A:400:LYS:HA	1:A:403:MET:HE2	1.57	0.85
4:A:999:WFE:H28A	4:A:999:WFE:H2	1.59	0.85
1:A:231[A]:ASN:ND2	1:A:284:LYS:HA	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HA	1:A:403:MET:CE	2.17	0.74
1:A:231[B]:ASN:HB2	5:A:1139:HOH:O	1.86	0.74
1:A:441:GLU:O	1:A:445:GLN:HG3	1.90	0.71
1:A:400:LYS:HG3	1:A:403:MET:HE2	1.73	0.70
1:A:204:ASN:CB	5:A:1221:HOH:O	2.13	0.68
1:A:158:LYS:HG3	1:A:158:LYS:O	1.92	0.68
2:B:10:GLU:OE1	5:B:1233:HOH:O	2.12	0.67
1:A:206:ARG:HD3	5:A:1142:HOH:O	1.95	0.65
1:A:357:LEU:HD22	5:A:1234:HOH:O	1.97	0.64
1:A:242:GLU:OE2	5:A:1220:HOH:O	2.15	0.63
1:A:165:ILE:HD12	1:A:180:ILE:HD12	1.81	0.63
1:A:164[A]:VAL:HG21	4:A:999:WFE:H28	1.82	0.62
1:A:227:MET:CE	4:A:999:WFE:H1B	2.31	0.60
4:A:999:WFE:C2	4:A:999:WFE:H28A	2.33	0.56
1:A:206:ARG:CD	5:A:1142:HOH:O	2.52	0.56
1:A:231[A]:ASN:HB3	5:A:1139:HOH:O	2.05	0.56
1:A:400:LYS:HG3	1:A:403:MET:HE1	1.85	0.55
1:A:227:MET:HE3	4:A:999:WFE:H1B	1.87	0.55
1:A:400:LYS:CA	1:A:403:MET:HE2	2.34	0.55
1:A:309:PHE:HD2	2:B:10:GLU:HG3	1.71	0.55
1:A:185:VAL:HG13	1:A:189:LYS:HE2	1.88	0.54
1:A:335:LEU:O	1:A:339[B]:MET:HG3	2.08	0.52
1:A:163:LYS:HE3	1:A:165:ILE:HD11	1.91	0.52
1:A:400:LYS:CG	1:A:403:MET:HE2	2.38	0.52
1:A:468:HIS:O	1:A:470:PRO:HD3	2.09	0.52
1:A:160:THR:HG23	1:A:189:LYS:HE3	1.92	0.51
1:A:263:TYR:OH	1:A:268:LYS:HE3	2.10	0.51
1:A:160:THR:HG22	1:A:161:PHE:CD2	2.46	0.51
1:A:158:LYS:HG2	1:A:442:PHE:CE1	2.48	0.48
1:A:239[B]:LEU:HD23	1:A:239[B]:LEU:HA	1.50	0.48
1:A:309:PHE:CD2	2:B:10:GLU:HG3	2.49	0.48
1:A:160:THR:N	5:A:1212:HOH:O	2.45	0.48
1:A:283:ASP:HB2	5:A:1167:HOH:O	2.14	0.46
1:A:421:LEU:HD22	5:A:1175:HOH:O	2.16	0.45
1:A:227:MET:HE1	4:A:999:WFE:H1B	1.98	0.45
1:A:212:ALA:HB3	1:A:228:GLU:HG3	2.00	0.43
1:A:368:PHE:CD1	1:A:377:LYS:HG3	2.55	0.41
1:A:152:TYR:CD2	1:A:152:TYR:N	2.87	0.41
1:A:231[A]:ASN:HD22	1:A:232:GLY:N	2.18	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.91	0.41
1:A:343:MET:C	5:A:1239:HOH:O	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231[A]:ASN:ND2	1:A:284:LYS:CA	2.77	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	316/342 (92%)	304 (96%)	11 (4%)	1 (0%)	46 41
2	B	8/10 (80%)	8 (100%)	0	0	100 100
All	All	324/352 (92%)	312 (96%)	11 (3%)	1 (0%)	46 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	GLU

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	281/299 (94%)	271 (96%)	10 (4%)	42 39
2	B	8/8 (100%)	8 (100%)	0	100 100
All	All	289/307 (94%)	279 (96%)	10 (4%)	46 40

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	GLU
1	A	160	THR
1	A	190	ASP
1	A	206	ARG
1	A	231[A]	ASN
1	A	231[B]	ASN
1	A	306	MET
1	A	372	LEU
1	A	431	SER
1	A	432	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	TPO	A	308	1	8,10,11	1.18	0	7,14,16	2.28	2 (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
1	TPO	A	308	1	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	TPO	OG1-P-O1P	-3.78	97.67	107.11
1	A	308	TPO	O3P-P-O1P	3.71	122.53	110.58

There are no chirality outliers.

There are no torsion outliers.

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)

Of 2 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
4	WFE	A	999	-	30,32,32	1.27	4 (13%)	27,47,47	3.63	11 (40%)

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	WFE	A	999	-	-	0/15/27/27	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	WFE	C13-C14	-3.86	1.49	1.54
4	A	999	WFE	C29-C6	-2.04	1.37	1.43
4	A	999	WFE	C12-N11	2.16	1.50	1.47
4	A	999	WFE	C3-C29	2.79	1.45	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	999	WFE	N7-C8-N9	-13.60	118.48	128.89
4	A	999	WFE	N9-C10-N11	-5.06	110.98	117.28
4	A	999	WFE	C3-C29-C6	-3.94	104.15	110.09
4	A	999	WFE	C2-C3-C4	-3.86	122.87	128.04
4	A	999	WFE	C26-C20-C18	-3.60	116.48	124.96
4	A	999	WFE	C25-C26-C20	-3.47	119.86	123.70
4	A	999	WFE	C26-C25-C23	2.25	118.98	116.63
4	A	999	WFE	C20-C18-N17	2.30	122.21	117.52
4	A	999	WFE	C29-C10-N11	3.36	129.74	121.44
4	A	999	WFE	C21-C20-C26	4.04	121.13	116.59
4	A	999	WFE	C8-N9-C10	5.71	123.58	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	WFE	6	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	A	311/342 (90%)	-0.27	11 (3%) 48 49	11, 24, 52, 61	0
2	B	10/10 (100%)	-0.27	0 100 100	17, 21, 38, 39	0
All	All	321/352 (91%)	-0.27	11 (3%) 49 50	11, 23, 51, 61	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	HIS	4.4
1	A	188	ALA	3.0
1	A	444	ALA	2.7
1	A	161	PHE	2.6
1	A	304	ALA	2.3
1	A	221	ASP	2.2
1	A	184	GLU	2.2
1	A	158	LYS	2.2
1	A	148	ASN	2.1
1	A	431	SER	2.1
1	A	466	ARG	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
1	TPO	A	308	11/12	0.98	0.07	-	18,22,27,34	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	WFE	A	999	29/29	0.92	0.15	0.18	25,30,55,56	0
3	MN	A	1	1/1	0.99	0.04	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.