



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:10 PM GMT

PDB ID : 4XV2
Title : B-Raf Kinase V600E oncogenic mutant in complex with Dabrafenib
Authors : zhang, Y.; zhang, c.
Deposited on : 2015-01-26
Resolution : 2.50 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

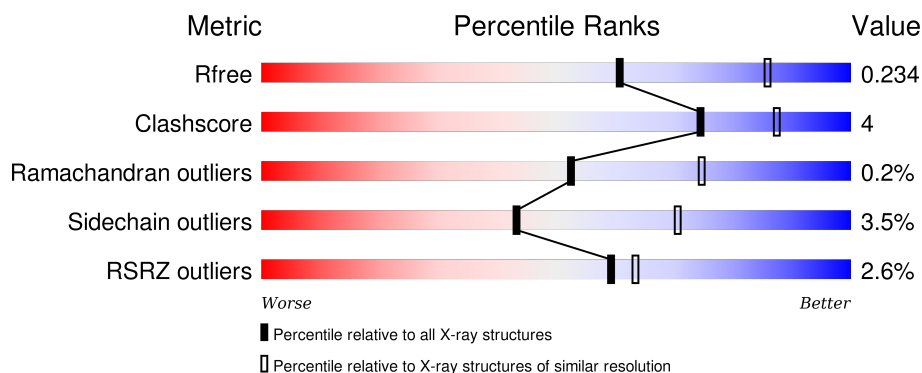
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	292	
1	B	292	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4094 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1979	1257	353	357	12			
1	B	249	Total	C	N	O	S	0	0	0
			1991	1262	355	362	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	MET	-	expression tag	UNP P15056
A	433	LYS	-	expression tag	UNP P15056
A	434	LYS	-	expression tag	UNP P15056
A	435	GLY	-	expression tag	UNP P15056
A	436	HIS	-	expression tag	UNP P15056
A	437	HIS	-	expression tag	UNP P15056
A	438	HIS	-	expression tag	UNP P15056
A	439	HIS	-	expression tag	UNP P15056
A	440	HIS	-	expression tag	UNP P15056
A	441	HIS	-	expression tag	UNP P15056
A	442	GLY	-	expression tag	UNP P15056
A	443	SER	-	expression tag	UNP P15056
A	446	ALA	SER	engineered mutation	UNP P15056
A	447	ALA	SER	engineered mutation	UNP P15056
A	543	ALA	ILE	engineered mutation	UNP P15056
A	544	SER	ILE	engineered mutation	UNP P15056
A	551	LYS	ILE	engineered mutation	UNP P15056
A	562	ARG	GLN	engineered mutation	UNP P15056
A	588	ASN	LEU	engineered mutation	UNP P15056
A	600	GLU	VAL	engineered mutation	UNP P15056
A	630	SER	LYS	engineered mutation	UNP P15056
A	667	GLU	PHE	engineered mutation	UNP P15056
A	673	SER	TYR	engineered mutation	UNP P15056
A	688	ARG	ALA	engineered mutation	UNP P15056
A	706	SER	-	expression tag	UNP P15056

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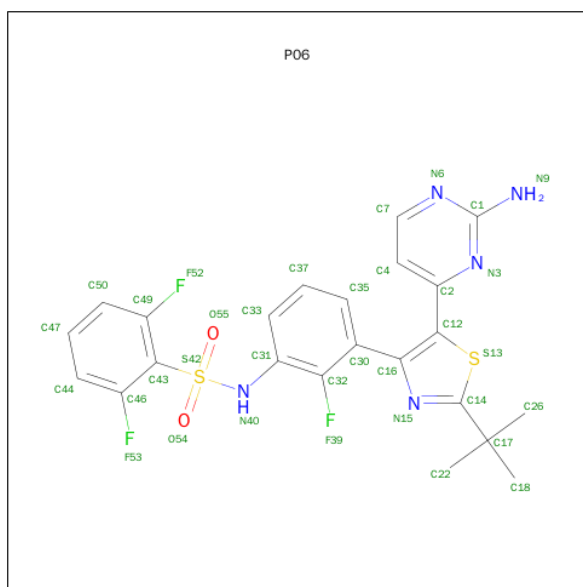
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	PHE	-	expression tag	UNP P15056
A	708	PRO	-	expression tag	UNP P15056
A	709	ARG	-	expression tag	UNP P15056
A	710	ILE	-	expression tag	UNP P15056
A	711	LEU	-	expression tag	UNP P15056
A	712	ALA	-	expression tag	UNP P15056
A	713	GLU	-	expression tag	UNP P15056
A	714	ILE	-	expression tag	UNP P15056
A	715	GLU	-	expression tag	UNP P15056
A	716	GLU	-	expression tag	UNP P15056
A	717	LEU	-	expression tag	UNP P15056
A	718	ALA	-	expression tag	UNP P15056
A	719	ARG	-	expression tag	UNP P15056
A	720	GLU	-	expression tag	UNP P15056
A	721	LEU	-	expression tag	UNP P15056
A	722	SER	-	expression tag	UNP P15056
A	723	GLY	-	expression tag	UNP P15056
B	432	MET	-	expression tag	UNP P15056
B	433	LYS	-	expression tag	UNP P15056
B	434	LYS	-	expression tag	UNP P15056
B	435	GLY	-	expression tag	UNP P15056
B	436	HIS	-	expression tag	UNP P15056
B	437	HIS	-	expression tag	UNP P15056
B	438	HIS	-	expression tag	UNP P15056
B	439	HIS	-	expression tag	UNP P15056
B	440	HIS	-	expression tag	UNP P15056
B	441	HIS	-	expression tag	UNP P15056
B	442	GLY	-	expression tag	UNP P15056
B	443	SER	-	expression tag	UNP P15056
B	446	ALA	SER	engineered mutation	UNP P15056
B	447	ALA	SER	engineered mutation	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	engineered mutation	UNP P15056
B	562	ARG	GLN	engineered mutation	UNP P15056
B	588	ASN	LEU	engineered mutation	UNP P15056
B	600	GLU	VAL	engineered mutation	UNP P15056
B	630	SER	LYS	engineered mutation	UNP P15056
B	667	GLU	PHE	engineered mutation	UNP P15056
B	673	SER	TYR	engineered mutation	UNP P15056
B	688	ARG	ALA	engineered mutation	UNP P15056
B	706	SER	-	expression tag	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
B	707	PHE	-	expression tag	UNP P15056
B	708	PRO	-	expression tag	UNP P15056
B	709	ARG	-	expression tag	UNP P15056
B	710	ILE	-	expression tag	UNP P15056
B	711	LEU	-	expression tag	UNP P15056
B	712	ALA	-	expression tag	UNP P15056
B	713	GLU	-	expression tag	UNP P15056
B	714	ILE	-	expression tag	UNP P15056
B	715	GLU	-	expression tag	UNP P15056
B	716	GLU	-	expression tag	UNP P15056
B	717	LEU	-	expression tag	UNP P15056
B	718	ALA	-	expression tag	UNP P15056
B	719	ARG	-	expression tag	UNP P15056
B	720	GLU	-	expression tag	UNP P15056
B	721	LEU	-	expression tag	UNP P15056
B	722	SER	-	expression tag	UNP P15056
B	723	GLY	-	expression tag	UNP P15056

- Molecule 2 is Dabrafenib (three-letter code: P06) (formula: $C_{23}H_{20}F_3N_5O_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		
2	B	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		

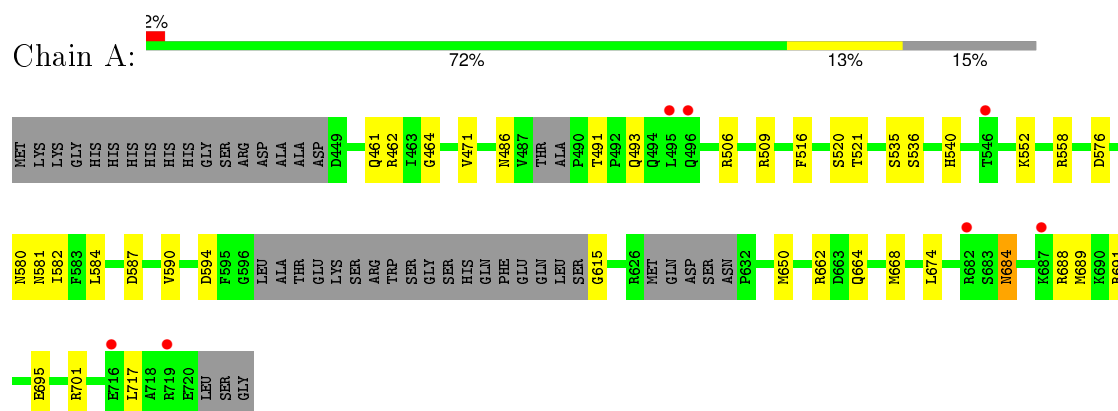
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	26	Total 26	O 26	0	0

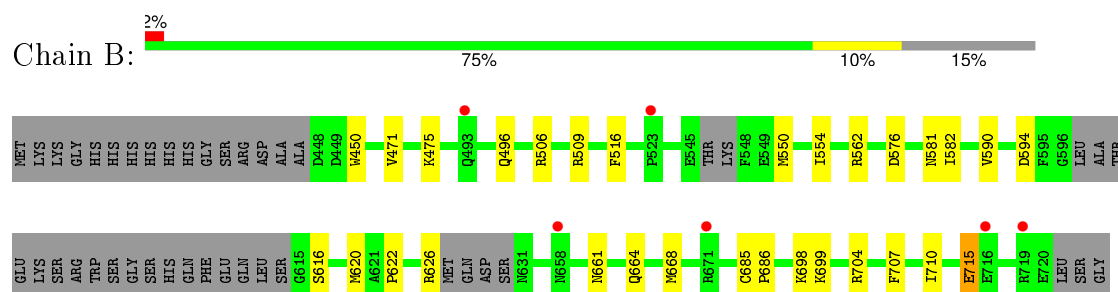
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein kinase B-raf



- Molecule 1: Serine/threonine-protein kinase B-raf



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.69Å 105.67Å 109.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.87 – 2.50 54.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.87-2.50) 99.9 (54.87-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.212 , 0.244 0.210 , 0.234	Depositor DCC
R_{free} test set	1128 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22268 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4094	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: P06

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	0.25	0/2019	0.42	0/2715
1	B	0.24	0/2031	0.42	0/2735
All	All	0.25	0/4050	0.42	0/5450

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	1979	0	1992	18	0
1	B	1991	0	1992	16	0
2	A	35	0	20	2	0
2	B	35	0	20	1	0
3	A	28	0	0	0	0
3	B	26	0	0	0	0
All	All	4094	0	4024	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 4.

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:594:ASP:H	2:A:801:P06:H17	1.15	0.92
1:B:594:ASP:H	2:B:801:P06:H17	1.19	0.88
1:A:576:ASP:O	1:A:581:ASN:ND2	2.28	0.67
1:B:576:ASP:O	1:B:581:ASN:ND2	2.31	0.64
1:A:688:ARG:HD2	1:A:717:LEU:HD13	1.80	0.64
1:A:491:THR:HG22	1:A:493:GLN:H	1.66	0.59
1:A:664:GLN:O	1:A:668:MET:HG3	2.06	0.56
1:B:661:ASN:HB3	1:B:664:GLN:HB2	1.93	0.50
1:A:684:ASN:OD1	1:A:684:ASN:N	2.32	0.49
1:B:698:LYS:HB2	1:B:704:ARG:HG2	1.94	0.49
1:A:650:MET:CE	1:A:689:MET:HG2	2.44	0.47
1:A:615:GLY:HA2	1:A:662:ARG:HH12	1.79	0.47
1:B:562:ARG:NH2	1:B:715:GLU:OE2	2.37	0.46
1:A:509:ARG:HD3	1:B:516:PHE:O	2.16	0.46
1:A:582:ILE:HG23	1:A:590:VAL:HG13	1.97	0.45
1:B:698:LYS:O	1:B:704:ARG:NH1	2.44	0.45
1:A:650:MET:HE3	1:A:689:MET:HG2	1.99	0.44
1:B:450:TRP:HE1	1:B:506:ARG:HH21	1.65	0.43
1:B:707:PHE:HA	1:B:710:ILE:HB	2.01	0.43
1:A:668:MET:CE	1:A:674:LEU:HD22	2.49	0.42
1:A:691:ARG:O	1:A:695:GLU:HG2	2.18	0.42
1:B:622:PRO:O	1:B:626:ARG:HG3	2.19	0.42
1:A:536:SER:HB2	1:A:580:ASN:HA	2.01	0.42
1:A:471:VAL:HG21	2:A:801:P06:N15	2.35	0.42
1:B:550:MET:O	1:B:554:ILE:HG12	2.20	0.41
1:A:540:HIS:CD2	1:A:584:LEU:HD12	2.56	0.41
1:A:462:ARG:NH1	1:A:464:GLY:HA2	2.36	0.41
1:B:685:CYS:HA	1:B:686:PRO:HD3	1.92	0.41
1:B:582:ILE:HG23	1:B:590:VAL:HG13	2.02	0.41
1:B:616:SER:O	1:B:620:MET:HG3	2.21	0.41
1:B:664:GLN:O	1:B:668:MET:HG3	2.22	0.40
1:A:516:PHE:O	1:B:509:ARG:HD3	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	239/292 (82%)	234 (98%)	4 (2%)	1 (0%)	39	61
1	B	241/292 (82%)	238 (99%)	3 (1%)	0	100	100
All	All	480/584 (82%)	472 (98%)	7 (2%)	1 (0%)	52	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	ASN

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	216/254 (85%)	206 (95%)	10 (5%)	33	57
1	B	217/254 (85%)	212 (98%)	5 (2%)	58	83
All	All	433/508 (85%)	418 (96%)	15 (4%)	43	70

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

Mol	Chain	Res	Type
1	A	461	GLN
1	A	506	ARG
1	A	520	SER
1	A	521	THR
1	A	535	SER

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Mol	Chain	Res	Type
1	A	552	LYS
1	A	558	ARG
1	A	587	ASP
1	A	684	ASN
1	A	701	ARG
1	B	471	VAL
1	B	475	LYS
1	B	496	GLN
1	B	699	LYS
1	B	715	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	P06	A	801	-	33,38,38	1.29	3 (9%)	39,58,58	1.26	5 (12%)
2	P06	B	801	-	33,38,38	1.32	3 (9%)	39,58,58	1.23	6 (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
2	P06	A	801	-	-	0/16/25/25	0/4/4/4
2	P06	B	801	-	-	0/16/25/25	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	P06	C30-C16	-3.75	1.45	1.49
2	A	801	P06	C30-C16	-3.72	1.45	1.49
2	A	801	P06	C1-N9	2.33	1.39	1.34
2	B	801	P06	C1-N9	2.36	1.39	1.34
2	A	801	P06	S42-N40	4.68	1.71	1.63
2	B	801	P06	S42-N40	4.80	1.72	1.63

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	P06	O55-S42-C43	-2.71	104.76	108.72
2	B	801	P06	N6-C1-N3	-2.34	123.47	125.86
2	A	801	P06	N6-C1-N3	-2.22	123.60	125.86
2	B	801	P06	O55-S42-C43	-2.16	105.56	108.72
2	A	801	P06	C4-C2-C12	2.03	123.19	120.63
2	B	801	P06	C4-C2-C12	2.09	123.27	120.63
2	B	801	P06	C35-C30-C16	2.22	122.99	119.58
2	A	801	P06	C2-N3-C1	2.91	117.73	116.32
2	B	801	P06	C2-N3-C1	2.94	117.75	116.32
2	B	801	P06	C46-C43-C49	3.36	119.02	116.62
2	A	801	P06	C46-C43-C49	3.52	119.13	116.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	P06	2	0
2	B	801	P06	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	247/292 (84%)	0.21	7 (2%) 56 61	32, 55, 102, 142	0
1	B	249/292 (85%)	0.29	6 (2%) 62 66	31, 63, 103, 116	0
All	All	496/584 (84%)	0.25	13 (2%) 59 63	31, 59, 103, 142	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	493	GLN	3.0
1	A	682	ARG	3.0
1	B	523	PRO	2.9
1	B	671	ARG	2.7
1	A	546	THR	2.6
1	B	658	ASN	2.6
1	A	719	ARG	2.5
1	B	716	GLU	2.5
1	B	719	ARG	2.4
1	A	496	GLN	2.3
1	A	495	LEU	2.3
1	A	687	LYS	2.1
1	A	716	GLU	2.1

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(\AA^2)	Q<0.9
2	P06	B	801	35/35	0.98	0.17	0.09	40,45,48,49	0
2	P06	A	801	35/35	0.98	0.16	-0.23	27,35,39,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.