



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 11:43 AM EDT

PDB ID : 3OG7
Title : B-Raf Kinase V600E oncogenic mutant in complex with PLX4032
Authors : Zhang, Y.; Zhang, K.Y.; Zhang, C.
Deposited on : unknown
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

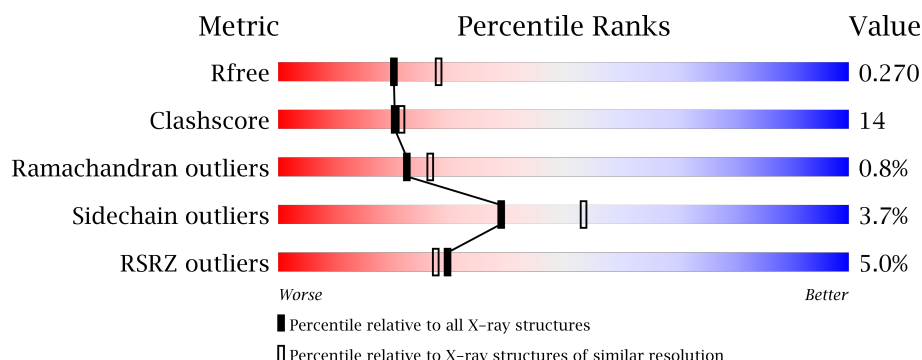
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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	289	<div> <div>6%</div> <div>59%</div> <div>25%</div> <div>•</div> <div>15%</div> </div>
1	B	289	<div> <div>3%</div> <div>56%</div> <div>29%</div> <div>•</div> <div>12%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4100 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 AKAP9-BRAF fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1974	1253	353	356	12			
1	B	254	Total	C	N	O	S	0	0	0
			2028	1286	361	369	12			

There are 66 discrepancies between the modelled and reference sequences:

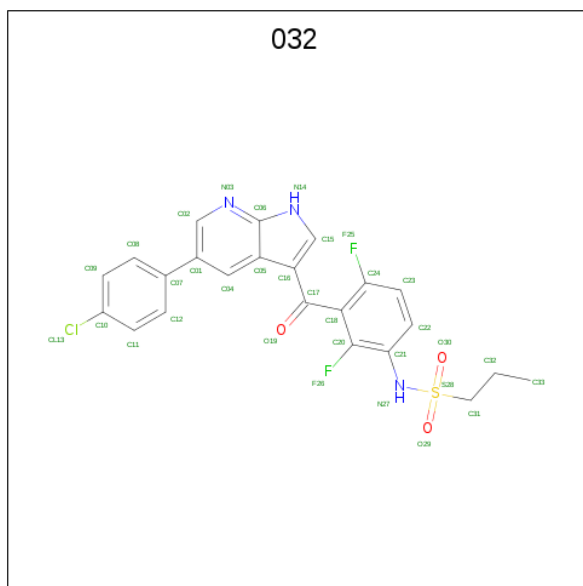
Chain	Residue	Modelled	Actual	Comment	Reference
A	432	MET	-	EXPRESSION TAG	UNP Q5IBP5
A	433	LYS	-	EXPRESSION TAG	UNP Q5IBP5
A	434	LYS	-	EXPRESSION TAG	UNP Q5IBP5
A	435	GLY	-	EXPRESSION TAG	UNP Q5IBP5
A	436	HIS	-	EXPRESSION TAG	UNP Q5IBP5
A	437	HIS	-	EXPRESSION TAG	UNP Q5IBP5
A	438	HIS	-	EXPRESSION TAG	UNP Q5IBP5
A	439	HIS	-	EXPRESSION TAG	UNP Q5IBP5
A	440	HIS	-	EXPRESSION TAG	UNP Q5IBP5
A	441	HIS	-	EXPRESSION TAG	UNP Q5IBP5
A	442	GLY	-	EXPRESSION TAG	UNP Q5IBP5
A	443	SER	-	EXPRESSION TAG	UNP Q5IBP5
A	444	ARG	-	EXPRESSION TAG	UNP Q5IBP5
A	445	ASP	-	EXPRESSION TAG	UNP Q5IBP5
A	446	ALA	-	EXPRESSION TAG	UNP Q5IBP5
A	447	ALA	-	EXPRESSION TAG	UNP Q5IBP5
A	448	ASP	-	EXPRESSION TAG	UNP Q5IBP5
A	522	ALA	LYS	ENGINEERED MUTATION	UNP Q5IBP5
A	543	ALA	ILE	ENGINEERED MUTATION	UNP Q5IBP5
A	544	SER	ILE	ENGINEERED MUTATION	UNP Q5IBP5
A	551	LYS	ILE	ENGINEERED MUTATION	UNP Q5IBP5
A	562	ARG	GLN	ENGINEERED MUTATION	UNP Q5IBP5
A	588	ASN	LEU	ENGINEERED MUTATION	UNP Q5IBP5
A	600	GLU	VAL	VARIANT	UNP Q5IBP5
A	630	SER	LYS	ENGINEERED MUTATION	UNP Q5IBP5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	667	GLU	PHE	ENGINEERED MUTATION	UNP Q5IBP5
A	673	SER	TYR	ENGINEERED MUTATION	UNP Q5IBP5
A	688	ARG	ALA	ENGINEERED MUTATION	UNP Q5IBP5
A	706	SER	LEU	ENGINEERED MUTATION	UNP Q5IBP5
A	709	ARG	GLN	ENGINEERED MUTATION	UNP Q5IBP5
A	713	GLU	SER	ENGINEERED MUTATION	UNP Q5IBP5
A	716	GLU	LEU	ENGINEERED MUTATION	UNP Q5IBP5
A	720	GLU	SER	ENGINEERED MUTATION	UNP Q5IBP5
B	432	MET	-	EXPRESSION TAG	UNP Q5IBP5
B	433	LYS	-	EXPRESSION TAG	UNP Q5IBP5
B	434	LYS	-	EXPRESSION TAG	UNP Q5IBP5
B	435	GLY	-	EXPRESSION TAG	UNP Q5IBP5
B	436	HIS	-	EXPRESSION TAG	UNP Q5IBP5
B	437	HIS	-	EXPRESSION TAG	UNP Q5IBP5
B	438	HIS	-	EXPRESSION TAG	UNP Q5IBP5
B	439	HIS	-	EXPRESSION TAG	UNP Q5IBP5
B	440	HIS	-	EXPRESSION TAG	UNP Q5IBP5
B	441	HIS	-	EXPRESSION TAG	UNP Q5IBP5
B	442	GLY	-	EXPRESSION TAG	UNP Q5IBP5
B	443	SER	-	EXPRESSION TAG	UNP Q5IBP5
B	444	ARG	-	EXPRESSION TAG	UNP Q5IBP5
B	445	ASP	-	EXPRESSION TAG	UNP Q5IBP5
B	446	ALA	-	EXPRESSION TAG	UNP Q5IBP5
B	447	ALA	-	EXPRESSION TAG	UNP Q5IBP5
B	448	ASP	-	EXPRESSION TAG	UNP Q5IBP5
B	522	ALA	LYS	ENGINEERED MUTATION	UNP Q5IBP5
B	543	ALA	ILE	ENGINEERED MUTATION	UNP Q5IBP5
B	544	SER	ILE	ENGINEERED MUTATION	UNP Q5IBP5
B	551	LYS	ILE	ENGINEERED MUTATION	UNP Q5IBP5
B	562	ARG	GLN	ENGINEERED MUTATION	UNP Q5IBP5
B	588	ASN	LEU	ENGINEERED MUTATION	UNP Q5IBP5
B	600	GLU	VAL	VARIANT	UNP Q5IBP5
B	630	SER	LYS	ENGINEERED MUTATION	UNP Q5IBP5
B	667	GLU	PHE	ENGINEERED MUTATION	UNP Q5IBP5
B	673	SER	TYR	ENGINEERED MUTATION	UNP Q5IBP5
B	688	ARG	ALA	ENGINEERED MUTATION	UNP Q5IBP5
B	706	SER	LEU	ENGINEERED MUTATION	UNP Q5IBP5
B	709	ARG	GLN	ENGINEERED MUTATION	UNP Q5IBP5
B	713	GLU	SER	ENGINEERED MUTATION	UNP Q5IBP5
B	716	GLU	LEU	ENGINEERED MUTATION	UNP Q5IBP5
B	720	GLU	SER	ENGINEERED MUTATION	UNP Q5IBP5

- Molecule 2 is N-(3-{[5-(4-chlorophenyl)-1H-pyrrolo[2,3-b]pyridin-3-yl]carbonyl}-2,4-difluoro

phenyl)propane-1-sulfonamide (three-letter code: 032) (formula: $\text{C}_{23}\text{H}_{18}\text{ClF}_2\text{N}_3\text{O}_3\text{S}$).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			33	23	1	2	3	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	24	Total O 24 24	0	0

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 ($\text{RSRZ} > 2$). 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.

Chain A:

6% 59% 25% 15%

Met Lys Lys Gly His His His His His Gly Ser Arg Asp Ala Asp D449 P450 E451 V459 R462 S465 G466 S467 W476 V480 M484 T488 A489 P490 L495 L505 R506 R509 N512 I513 L514 L515 F516 Y519 S520 T521 A522 P523 E533

H339 H540 L541 H542 A543 S544 G545 T546 T547 L548 T549 I554 H568 H574 R575 K578 S579 N580 N581 I582 F583 L584 H585 E586 S587 V590 D594 P595 G596 L597 A598 T599 T600 G601 L602 P603 L604 P605 P606 P607 P608 P609 P610 P611 P612 P613 P614 P615 P616 P617 P618 P619 P620 P621 P622 P623 P624 P625 P626 P627 P628 P629 P630 P631 P632 P633 P634 P635 P636 P637 P638 P639 P640 P641 P642 P643 P644 P645 P646 P647 P648 P649 P650 P651 P652 P653 P654 P655 P656 P657 P658 P659 P660 P661 P662 P663 P664 P665 P666 P667 P668 P669 P670 P671 P672 P673 P674 P675 P676 P677 P678 P679 P680 P681 P682 P683 P684 P685 P686 P687 P688 P689 P690 P691 P692 P693 P694 P695 P696 P697 P698 P699 P700 P701 P702 P703 P704 P705 P706 P707 P708 P709 P710 P711 P712 P713 P714 P715 P716 P717 P718 P719 P720 P721 P722 P723 P724 P725 P726 P727 P728 P729 P730 P731 P732 P733 P734 P735 P736 P737 P738 P739 P740 P741 P742 P743 P744 P745 P746 P747 P748 P749 P750 P751 P752 P753 P754 P755 P756 P757 P758 P759 P760 P761 P762 P763 P764 P765 P766 P767 P768 P769 P770 P771 P772 P773 P774 P775 P776 P777 P778 P779 P780 P781 P782 P783 P784 P785 P786 P787 P788 P789 P790 P791 P792 P793 P794 P795 P796 P797 P798 P799 P800 P801 P802 P803 P804 P805 P806 P807 P808 P809 P810 P811 P812 P813 P814 P815 P816 P817 P818 P819 P820 P821 P822 P823 P824 P825 P826 P827 P828 P829 P830 P831 P832 P833 P834 P835 P836 P837 P838 P839 P840 P841 P842 P843 P844 P845 P846 P847 P848 P849 P850 P851 P852 P853 P854 P855 P856 P857 P858 P859 P860 P861 P862 P863 P864 P865 P866 P867 P868 P869 P870 P871 P872 P873 P874 P875 P876 P877 P878 P879 P880 P881 P882 P883 P884 P885 P886 P887 P888 P889 P890 P891 P892 P893 P894 P895 P896 P897 P898 P899 P900 P901 P902 P903 P904 P905 P906 P907 P908 P909 P910 P911 P912 P913 P914 P915 P916 P917 P918 P919 P920 P921 P922 P923 P924 P925 P926 P927 P928 P929 P930 P931 P932 P933 P934 P935 P936 P937 P938 P939 P940 P941 P942 P943 P944 P945 P946 P947 P948 P949 P950 P951 P952 P953 P954 P955 P956 P957 P958 P959 P960 P961 P962 P963 P964 P965 P966 P967 P968 P969 P970 P971 P972 P973 P974 P975 P976 P977 P978 P979 P980 P981 P982 P983 P984 P985 P986 P987 P988 P989 P990 P991 P992 P993 P994 P995 P996 P997 P998 P999

Chain B:

3% 56% 29% 12%

Sequence of amino acids: MET, LYS, LYS, LYS, GLY, HIS, HIS, HIS, HIS, HIS, HIS, GLY, SER, ARG, ASP, ALA, ALA, ASP, D449, D454, I463, G464, S465, F468, G469, T470, V471, V482, K483, N484, L485, N486, A489, P490, T491, Q494, L495, F498, K499, N500, E501, V502, G503, V504, K507, T508, R509, H510, I513, F516.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.77Å 104.42Å 110.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.30 – 2.45 21.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (21.30-2.45) 89.8 (21.27-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.5 _2	Depositor
R, R_{free}	0.212 , 0.258 0.223 , 0.270	Depositor DCC
R_{free} test set	1107 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Reported twinning fraction	0.086 for -h,l,k	Depositor
Outliers	0 of 31341 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4100	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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, 0.333 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: 032

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	0.22	0/2014	0.39	0/2712
1	B	0.25	0/2069	0.42	0/2788
All	All	0.23	0/4083	0.40	0/5500

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
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	522	ALA	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	A	1974	0	1985	48	0
1	B	2028	0	2041	66	0
2	A	33	0	18	5	0
3	A	41	0	0	1	0
3	B	24	0	0	2	0
All	All	4100	0	4044	113	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 14.

The worst 5 of 113 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:491:THR:H	1:B:494:GLN:HE21	1.12	0.97
1:B:491:THR:H	1:B:494:GLN:NE2	1.77	0.83
1:B:623:GLU:OE1	1:B:701:ARG:HB3	1.79	0.81
1:B:454:ASP:CG	1:B:523:PRO:HG3	2.02	0.81
1:A:594:ASP:H	2:A:1:032:HN27	1.26	0.80

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	239/289 (83%)	225 (94%)	13 (5%)	1 (0%)	38	47
1	B	248/289 (86%)	234 (94%)	11 (4%)	3 (1%)	15	15
All	All	487/578 (84%)	459 (94%)	24 (5%)	4 (1%)	22	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	522	ALA
1	B	523	PRO
1	B	595	PHE
1	A	523	PRO

5.3.2 Protein sidechains ⓘ

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	215/251 (86%)	208 (97%)	7 (3%)	43	57
1	B	221/251 (88%)	212 (96%)	9 (4%)	35	48
All	All	436/502 (87%)	420 (96%)	16 (4%)	39	53

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	484	MET
1	B	502	VAL
1	B	637	SER
1	A	681	VAL
1	B	684	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	494	GLN
1	B	524	GLN
1	B	653	GLN
1	B	477	HIS
1	B	581	ASN

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
2	032	A	1	-	35,36,36	1.25	3 (8%)	41,53,53	0.96	1 (2%)

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	032	A	1	-	-	0/17/21/21	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	032	C16-C17	-3.54	1.46	1.50
2	A	1	032	C02-N03	2.31	1.35	1.31
2	A	1	032	S28-N27	3.85	1.72	1.62

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	032	C24-C18-C20	3.19	118.98	115.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	032	5	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	247/289 (85%)	0.01	16 (6%)	20 17	28, 58, 105, 156	0
1	B	254/289 (87%)	0.01	9 (3%)	44 41	25, 64, 107, 170	0
All	All	501/578 (86%)	0.01	25 (4%)	30 27	25, 61, 106, 170	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	642	PHE	4.8
1	B	468	PHE	4.4
1	B	465	SER	4.3
1	A	467	SER	4.1
1	A	640	TYR	4.0

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(\AA^2)	Q<0.9
2	032	A	1	33/33	0.95	0.12	-0.64	24,42,58,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.