



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X6J
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PIK-93
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.
Deposited on : 2010-02-17
Resolution : 3.50 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 (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

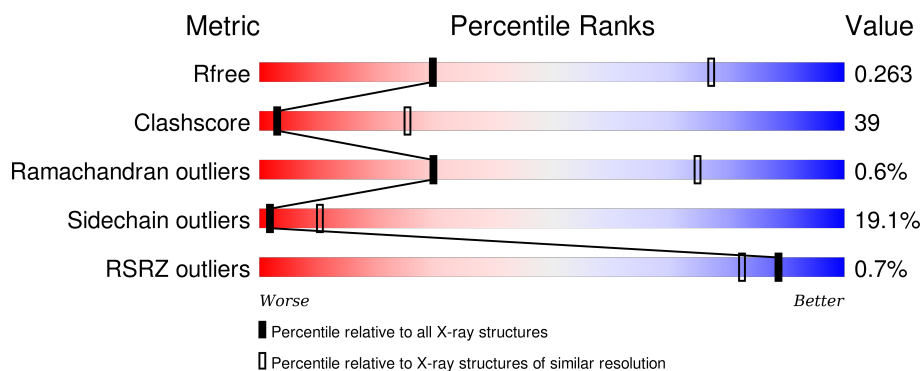
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	696	 34% 34% 10% 22%
1	B	696	 34% 34% 10% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8967 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.

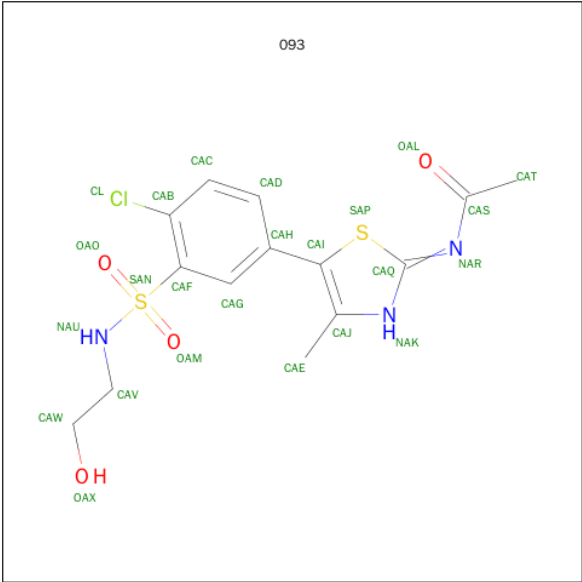
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4457	2882	757	791	27			
1	B	546	Total	C	N	O	S	0	0	0
			4462	2886	759	790	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	EXPRESSION TAG	UNP Q9W1M7
A	255	SER	-	EXPRESSION TAG	UNP Q9W1M7
A	256	HIS	-	EXPRESSION TAG	UNP Q9W1M7
A	257	MET	-	EXPRESSION TAG	UNP Q9W1M7
A	455	ALA	GLY	ENGINEERED MUTATION	UNP Q9W1M7
B	254	GLY	-	EXPRESSION TAG	UNP Q9W1M7
B	255	SER	-	EXPRESSION TAG	UNP Q9W1M7
B	256	HIS	-	EXPRESSION TAG	UNP Q9W1M7
B	257	MET	-	EXPRESSION TAG	UNP Q9W1M7
B	455	ALA	GLY	ENGINEERED MUTATION	UNP Q9W1M7

- Molecule 2 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIAZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).

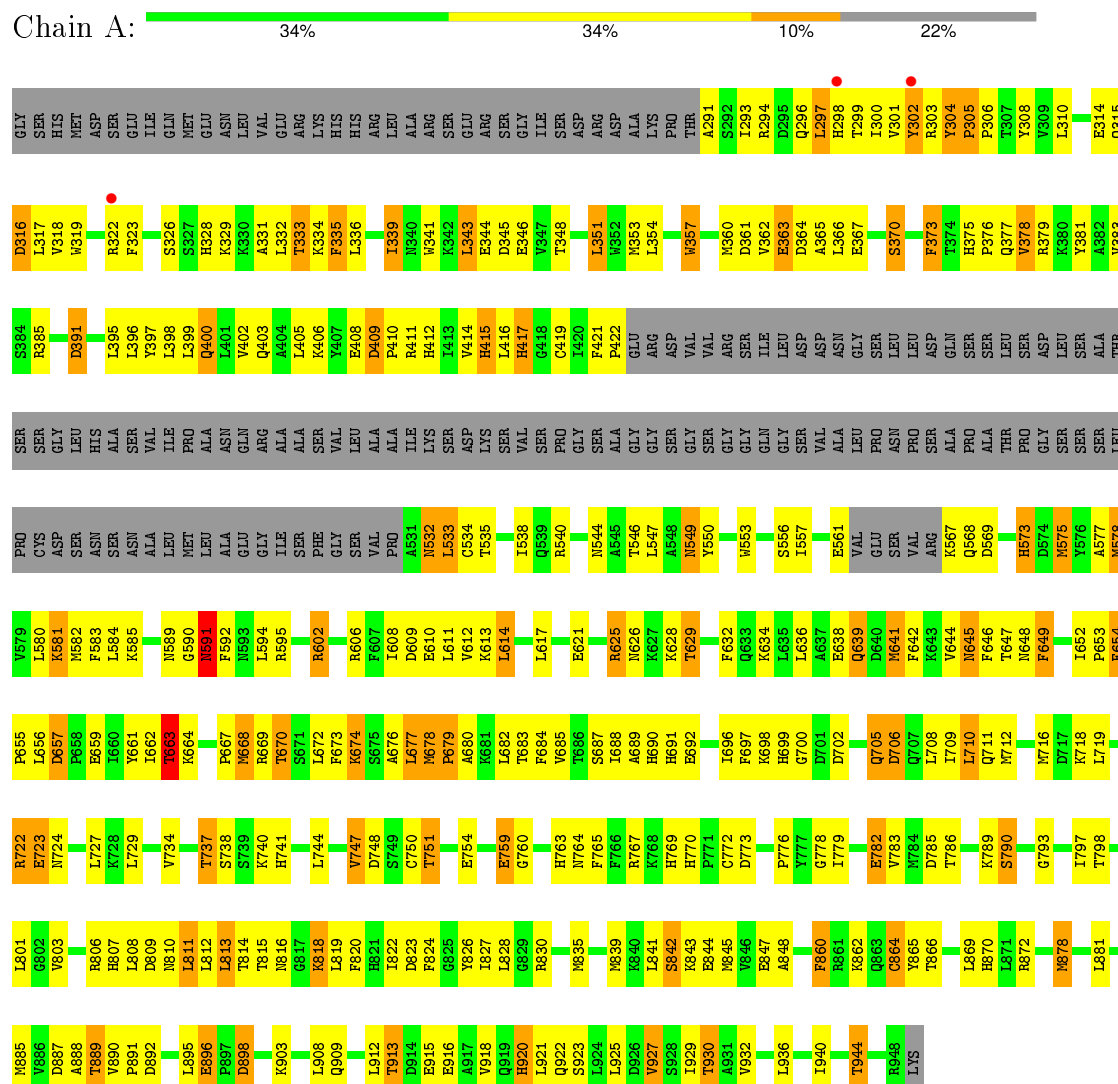


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		
2	B	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		

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: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



• Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



F882	D805	Y732	P653	K581	LEU	THR	A382	E314	GLY
A888	R806	Y733	F654	M582	PRO	SER	A382	Q315	SER
T889	H807	A733	P655	V586	CYS	HIS	R385	D316	HIS
H890	L808	L656	V586	L587	ASP	GLY	R385	L317	MET
P891	D809	L735	D657	L587	SER	LEU	Q388	V318	ASP
D892	N810	A736	P658	Q590	ASN	HIS	Q388	W319	SER
L893	L811	T737	Y661	G590	SER	ALA	Q388	K320	GLU
A894	L812	S738	I662	M591	ASN	SER	D391	F321	ILE
L895	L813	S739	I662	L594	ALA	VAL	E392	R322	GLN
E896	T814	K740	T663	L594	LEU	ILE	D393	K322	MET
P897	T815	H741	K664	R595	MET	PRO	L325	L325	GLU
G817	N816	G742	P667	F598	LEU	ALA	L398	S326	ASN
D898	G817	F743	P667	Y599	ALA	ASN	L399	S327	LEU
K899	K818	L744	T670	M600	GLU	GLN	Q400	K328	VAL
K903	L819	V747	S671	L601	GLY	ARG	L401	K329	GLU
E906	F820	D748	L672	R602	ILE	ALA	V402	K330	ARG
I907	H821	S749	F673	K603	SER	ALA	L405	A331	LYS
D923	D823	G750	P679	Q604	PHE	SER	L406	L332	HIS
L908	F824	T751	L677	R605	GLY	VAL	Y407	T333	HIS
Q909	G825	A753	M678	Q605	SER	LEU	E408	K334	ARG
L912	Y826	E754	P679	I608	VAL	ALA	F335	F335	LEU
T913	I827	E754	V685	D609	PRO	ALA	K337	K337	ALA
E916	L828	V755	T686	E610	ASP	ILE	C338	C338	ARG
A917	G829	L756	T686	L611	LYS	LYS	H412	SER	SER
Q919	R830	A757	H691	L614	ASP	ASP	I413	GLU	GLU
Q922	M835	R758	I696	V618	LYS	LYS	V414	ARG	ARG
S923	P836	E759	F697	V618	GLY	GLY	H415	SER	SER
V927	P837	H763	K698	E621	VAL	VAL	L416	ILE	ILE
A931	P838	I764	H699	E621	SER	SER	C419	SER	SER
V932	M839	F765	H699	G623	PRO	PRO	I420	ASP	ASP
I933	K840	R766	G700	G623	GLY	GLY	F421	ARG	ARG
F934	L841	R767	D702	R625	ALA	ALA	T348	ASP	ASP
E938	S842	F771	L703	M626	LYS	LYS	E423	LYS	LYS
Q939	K843	G772	R704	K627	GLY	GLY	ASP	PRO	PRO
F943	A848	D773	Q705	K628	SER	SER	VAL	THR	THR
T944	P849	P776	D706	T629	GLY	GLY	VAL	K291	K291
Q945	G850	Y777	Q707	E630	ARG	ARG	VAL	S292	S292
V946	G851	G778	L708	F632	GLY	GLY	ARG	I293	I293
G948	I852	I779	I709	K631	ILE	ILE	ASP	K294	K294
K949	S853	I779	L710	Q633	GLU	GLU	ILE	D295	D295
F943	S854	Y782	Q711	K634	VAL	VAL	LEU	Q296	Q296
Q945	E855	V783	M712	L635	SER	SER	ASP	D861	D861
V946	E859	T786	T714	L636	ASP	ASP	ASP	H296	H296
I947	F860	Y787	L715	Q639	LEU	LEU	D864	T299	T299
R948	R861	I788	M716	D640	ALA	ALA	A365	I300	I300
K949	K862	I788	D717	M641	PRO	PRO	L366	V301	V301
	Y865	C791	R721	K643	ASN	ASN	E367	Y302	Y302
	T866	Y794	E723	M644	PRO	PRO	L368	R303	R303
	N876	Y794	T723	M645	SER	SER	L369	Y304	Y304
	V877	T798	M724	T647	ALA	ALA	S370	P305	P305
	M878	Y799	L725	M648	THR	THR	P371	P306	P306
	L879	Y803	K728	P649	PRO	PRO	T372	T307	T307
	N880	G804	L729	L652	GLY	GLY	F373	Y308	Y308
	L881				SER	SER	T374	V309	V309
					ASP	ASP	H375	L310	L310
					LEU	LEU	P376	S311	S311
					SER	SER	Q377	S312	S312
					SER	SER	V378	E313	E313

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.95Å 156.33Å 242.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.62 – 3.50 61.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.62-3.50) 99.5 (61.62-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.272 0.225 , 0.263	Depositor DCC
R_{free} test set	1313 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 26700 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 093

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	0.61	1/4566 (0.0%)	0.84	1/6183 (0.0%)
1	B	0.48	0/4571	0.69	2/6189 (0.0%)
All	All	0.55	1/9137 (0.0%)	0.77	3/12372 (0.0%)

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	A	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	864	CYS	CB-SG	-6.21	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	A	818	LYS	N-CA-C	-5.24	96.86	111.00
1	B	710	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	591	ASN	Mainchain
1	A	663	THR	Mainchain
1	A	680	ALA	Peptide
1	A	737	THR	Mainchain

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	4457	0	4490	348	1
1	B	4462	0	4499	348	1
2	A	24	0	16	8	0
2	B	24	0	16	6	0
All	All	8967	0	9021	697	2

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 39.

The worst 5 of 697 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:375:HIS:CD2	1:A:377:GLN:H	1.54	1.24
1:B:311:SER:HB3	1:B:314:GLU:CB	1.76	1.15
1:B:299:THR:HB	1:B:303:ARG:HH11	1.10	1.14
1:A:705:GLN:HG2	1:A:890:VAL:HG13	1.22	1.13
1:A:629:THR:HB	1:A:672:LEU:HD12	1.18	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:TYR:OH	1:A:782:GLU:OE1[6_555]	2.07	0.13
1:B:391:ASP:OD2	1:B:724:ASN:ND2[8_565]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	539/696 (77%)	505 (94%)	30 (6%)	4 (1%)	26	72
1	B	540/696 (78%)	517 (96%)	20 (4%)	3 (1%)	30	75
All	All	1079/1392 (78%)	1022 (95%)	50 (5%)	7 (1%)	30	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	SER
1	A	305	PRO
1	B	408	GLU
1	A	304	TYR
1	A	591	ASN

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	490/612 (80%)	398 (81%)	92 (19%)	2	11
1	B	490/612 (80%)	395 (81%)	95 (19%)	2	10
All	All	980/1224 (80%)	793 (81%)	187 (19%)	2	10

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	896	GLU

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Mol	Chain	Res	Type
1	B	321	PHE
1	B	839	MET
1	A	920	HIS
1	B	297	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	807	HIS
1	A	922	GLN
1	B	876	ASN
1	A	810	ASN
1	B	403	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](#)

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	093	A	1949	-	21,25,25	3.73	13 (61%)	24,36,36	2.78	11 (45%)
2	093	B	1950	-	21,25,25	3.97	14 (66%)	24,36,36	3.05	11 (45%)

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	093	A	1949	-	-	0/17/19/19	0/2/2/2
2	093	B	1950	-	-	2/17/19/19	0/2/2/2

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1950	093	CAB-CAF	-2.38	1.36	1.40
2	A	1949	093	CAB-CAF	-2.33	1.36	1.40
2	A	1949	093	CAC-CAB	2.33	1.44	1.39
2	B	1950	093	CAB-CL	2.37	1.79	1.73
2	A	1949	093	CAF-SAN	2.69	1.81	1.77

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1949	093	OAQ-SAN-OAM	-8.14	108.74	119.54
2	B	1950	093	OAQ-SAN-OAM	-6.51	110.90	119.54
2	B	1950	093	CAB-CAF-SAN	-6.29	119.44	123.30
2	B	1950	093	CAF-CAB-CL	-5.28	117.70	121.54
2	A	1949	093	CAB-CAF-SAN	-3.74	121.01	123.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1950	093	OAL-CAS-NAR-CAQ
2	B	1950	093	CAT-CAS-NAR-CAQ

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	093	8	0
2	B	1950	093	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 [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	545/696 (78%)	-0.26	3 (0%) 90 85	32, 55, 105, 116	0
1	B	546/696 (78%)	-0.15	5 (0%) 85 78	43, 65, 116, 123	0
All	All	1091/1392 (78%)	-0.20	8 (0%) 89 82	32, 61, 107, 123	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	TRP	3.1
1	A	302	TYR	2.7
1	B	636	LEU	2.5
1	B	423	GLU	2.2
1	A	322	ARG	2.2

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	093	A	1949	24/24	0.89	0.31	1.79	87,97,104,107	0
2	093	B	1950	24/24	0.91	0.35	1.08	101,108,117,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.