



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X6K
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PI-103
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

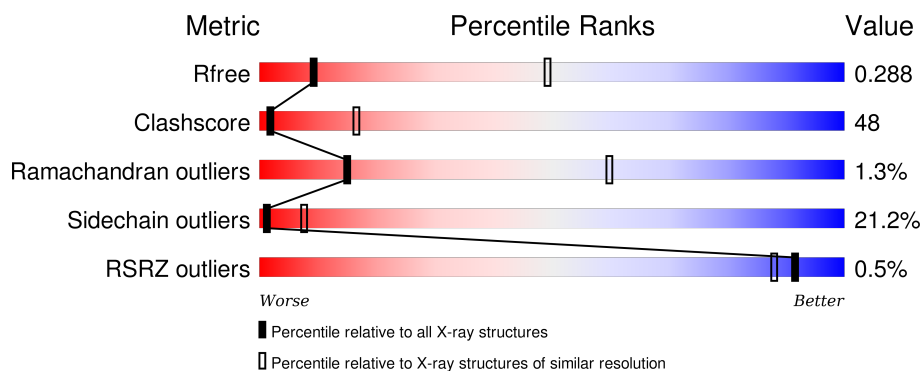
1 Overall quality at a glance

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	 31% 35% 12% • 21%
1	B	696	 33% 35% 10% • 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	X6K	A	1951	-	-	-	X
3	X6K	B	1950	-	-	X	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9062 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	550	Total	C	N	O	S	0	0	0
			4497	2906	765	799	27			
1	B	550	Total	C	N	O	S	0	0	0
			4498	2907	766	798	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	ALA	GLY	ENGINEERED MUTATION	UNP Q9W1M7
B	455	ALA	GLY	ENGINEERED MUTATION	UNP Q9W1M7

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



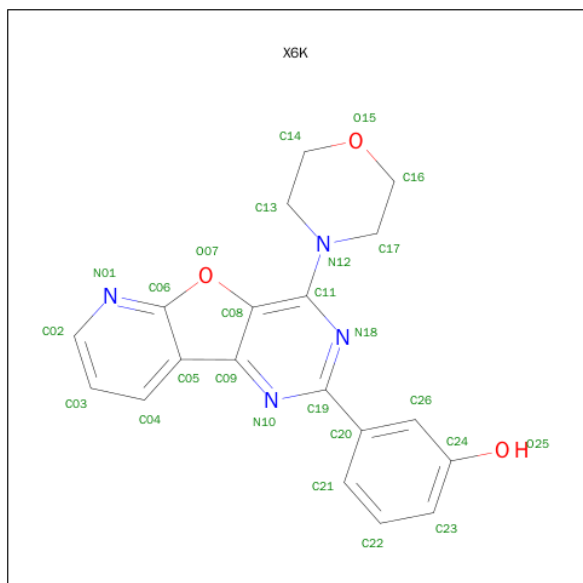
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3-(4-MORPHOLIN-4-YLPYRIDO[3',2':4,5]FURO[3,2-D]PYRIMIDIN-2-YL)PHENOL (three-letter code: X6K) (formula: C₁₉H₁₆N₄O₃).

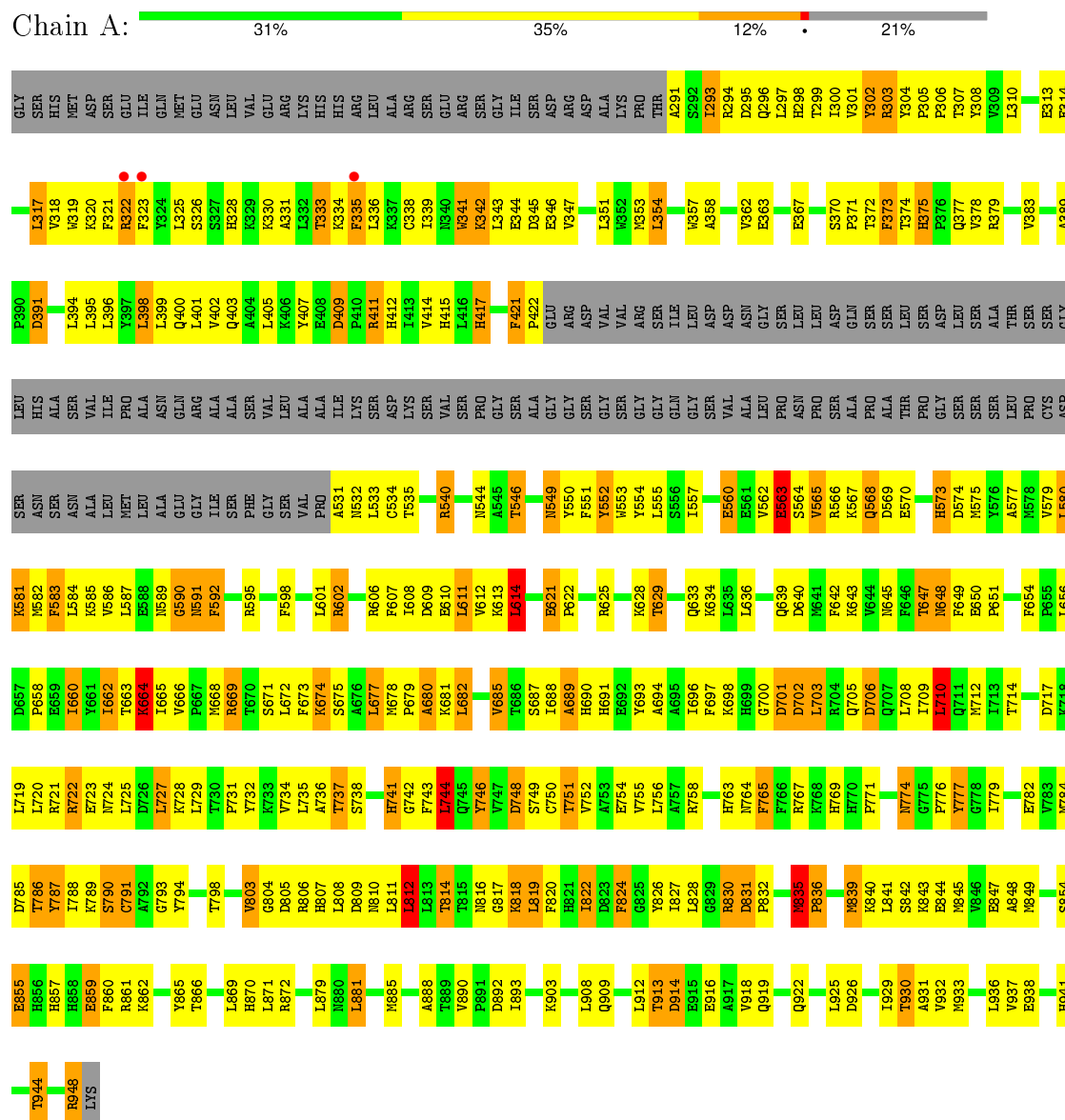


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	4	3		
3	B	1	Total	C	N	O	0	0
			26	19	4	3		

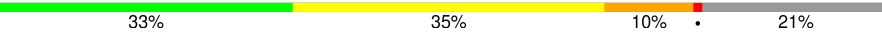
3 Residue-property plots

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

Chain B: 

GLY	SER	HIS	MET	ASP	SER	GLU	ILE	GLN	MET	GLU	ASN	VAL	VAL	GLU	ARG	LYS	HIS	HIS	ARG	LEU	ALA	ARG	SER	GLU	ARG	ASP	ASP	ASP	ALA	LYS	PRO	THR	A291	R294	H298	T299	I300	V301	Y302	R303	Y304	P305	P306	T307	Y308	V309	L310	S311	S312	E313	E314	Q315	D316			
L317	V318	W319	K320	F321	R322	F323	S326	S327	R328	K329	L332	T333	K334	F335	L336	K337	C338	I339	W341	K342	L343	E344	D345	E346	A350	L351	L354	W357	A358	P359	K360	E363	L366	L369	S370	P371	T372	F373	T374	K375	P376	Q377	V378	K379	L380	Y381	A382	V383	S384	R385						
L386	D391	D392	L393	L394	L395	L396	Y397	L398	L399	Q400	L401	V402	Q403	A404	L405	K406	Y407	E408	P410	R411	H412	I413	L416	H417	G418	C419	E423	ARG	ASP	VAL	VAL	ARG	SER	ILE	LEU	ASP	ASN	GLY	SER	LEU	ASP	GLN	SER	LEU	ASP	LEU	ALA	THR	SER	SER						
GLY	LEU	ALA	SER	ASN	VAL	ILE	PRO	ALA	ASN	GLN	ARG	ALA	SER	VAL	LEU	ALA	ILE	LYS	SER	ASP	LYS	SER	VAL	SER	PRO	GLY	ALA	GLY	ASP	GLY	VAL	VAL	ALA	LEU	PRO	ASN	PRO	SER	ALA	ALA	PRO	THR	GLY	SER	SER	LEU	PRO	CYS								
ASP	SER	ASN	SER	ASN	ALA	LEU	MET	LEU	LEU	GLU	GLY	ILE	SER	PHE	SER	VAL	PRO	A531	D532	L533	C534	W535	F536	L537	I538	Q539	R540	A541	N544	A545	T546	L547	A548	N549	Y550	F551	T552	N553	V554	L555	S556	L557	E560	V561	V562	E563	SER	VAL	R566	K567	N645	Q568	D569	E570	H573	D574
M575	Y576	A577	M578	K581	M582	L587	G590	N591	F592	R595	F598	Y599	N600	A603	Q604	R605	R606	F607	I608	D609	E610	L611	V612	K613	L614	V618	E621	N624	R625	N626	K627	K631	F632	Q633	L635	E638	Q639	D640	K643	V644	N645	Q646	T647	N648	F649	E650										
P651	I652	P653	P655	P658	T663	K664	P667	M668	R669	T670	S671	L672	F673	Q674	S675	A676	M677	M678	P679	A680	K681	L682	T683	F684	V685	H690	Y693	I696	F697	K698	H699	G700	D701	D702	L703	R704	Q705	D706	Q707	L708	I709	L710	Q711	M712	T713	T714	L715	L719	R722	E723						
L729	F730	F731	Y732	K733	V734	L735	A736	T737	S738	W739	K740	H741	F742	F743	L744	Q745	Y746	V747	D748	S749	C750	T751	E754	V755	L756	A757	F758	E759	I762	H763	N764	F765	F766	R767	H770	F771	C772	G775	F776	Y777	G778	I779	E782	V783	T786	Y787	I788	T789	L799	L801						
G802	V803	G804	D805	R806	D809	N810	L811	L812	L813	T814	T815	N816	F820	H821	I822	D823	F824	G825	Y826	I827	L828	G829	R830	K833	P834	M839	K840	L841	S842	K843	E844	M845	Y846	E847	A848	I852	H857	H858	E859	F860	R861	K862	Q863	C864	Y865	A867	Y868	L869	H870	L871	R872	R873				
H874	A875	H876	N880	L881	F882	S883	H884	H885	H886	D887	A888	T889	W890	F891	D892	L895	K902	E906	I907	L908	Q909	L912	T913	D914	E915	E916	W918	Q919	I920	L921	Q922	S923	D926	T930	A931	V932	L936	V937	H941	T944	Q945	Y946	Y949													

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.44Å 155.68Å 244.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.74 – 3.50 61.74 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.74-3.50) 99.5 (61.74-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.235 , 0.296 0.230 , 0.288	Depositor DCC
R_{free} test set	1340 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	110.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 27069 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9062	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: X6K, SO4

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	0.58	1/4607 (0.0%)	0.86	6/6240 (0.1%)
1	B	0.51	1/4607 (0.0%)	0.68	2/6237 (0.0%)
All	All	0.55	2/9214 (0.0%)	0.77	8/12477 (0.1%)

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	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	SER	CB-OG	10.06	1.55	1.42
1	A	590	GLY	C-O	7.84	1.36	1.23

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	710	LEU	CA-CB-CG	-7.23	98.68	115.30
1	A	818	LYS	N-CA-C	-6.73	92.82	111.00
1	B	310	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	611	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	744	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	ASN	Peptide
1	A	590	GLY	Mainchain
1	A	591	ASN	Mainchain
1	A	664	LYS	Peptide
1	A	680	ALA	Peptide

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	4497	0	4533	413	1
1	B	4498	0	4533	453	1
2	A	10	0	0	2	0
2	B	5	0	0	1	0
3	A	26	0	16	3	0
3	B	26	0	16	9	0
All	All	9062	0	9098	863	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 48.

The worst 5 of 863 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:664:LYS:CG	1:B:685:VAL:HG21	1.52	1.39
1:A:677:LEU:HD22	1:A:700:GLY:HA3	1.22	1.21
1:A:827:ILE:HG22	1:A:828:LEU:HG	1.25	1.11
1:A:591:ASN:O	1:A:595:ARG:HD3	1.48	1.11
1:B:672:LEU:HD21	1:B:678:MET:HB2	1.27	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:391:ASP:OD2	1:A:724:ASN:OD1[6_555]	1.87	0.33
1:B:600:ASN:ND2	1:B:782:GLU:OE2[8_565]	2.11	0.09

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	546/696 (78%)	507 (93%)	34 (6%)	5 (1%)	21	68
1	B	544/696 (78%)	519 (95%)	16 (3%)	9 (2%)	11	54
All	All	1090/1392 (78%)	1026 (94%)	50 (5%)	14 (1%)	15	60

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	664	LYS
1	A	731	PRO
1	B	408	GLU
1	B	778	GLY
1	A	563	GLU

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	495/612 (81%)	382 (77%)	113 (23%)	1	6
1	B	494/612 (81%)	397 (80%)	97 (20%)	1	9
All	All	989/1224 (81%)	779 (79%)	210 (21%)	1	7

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	830	ARG

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Mol	Chain	Res	Type
1	B	310	LEU
1	B	822	ILE
1	A	839	MET
1	A	913	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	919	GLN
1	B	328	HIS
1	B	870	HIS
1	B	298	HIS
1	B	356	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](#)

5 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	SO4	A	1949	-	4,4,4	0.11	0	6,6,6	0.14	0
2	SO4	A	1950	-	4,4,4	0.28	0	6,6,6	0.26	0
3	X6K	A	1951	-	26,30,30	2.36	8 (30%)	33,43,43	2.43	8 (24%)
3	X6K	B	1950	-	26,30,30	2.30	8 (30%)	33,43,43	2.55	9 (27%)
2	SO4	B	1951	-	4,4,4	0.29	0	6,6,6	0.07	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
2	SO4	A	1949	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1950	-	-	0/0/0/0	0/0/0/0
3	X6K	A	1951	-	-	0/8/16/16	0/4/5/5
3	X6K	B	1950	-	-	0/8/16/16	0/4/5/5
2	SO4	B	1951	-	-	0/0/0/0	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1951	X6K	C05-C06	-2.66	1.35	1.42
3	B	1950	X6K	C05-C06	-2.45	1.36	1.42
3	A	1951	X6K	C09-N10	-2.19	1.31	1.36
3	B	1950	X6K	C09-N10	-2.10	1.31	1.36
3	B	1950	X6K	C11-N12	2.49	1.45	1.36

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1951	X6K	N10-C19-N18	-9.18	120.28	126.20
3	B	1950	X6K	N10-C19-N18	-9.04	120.37	126.20
3	B	1950	X6K	C13-N12-C11	-3.62	108.52	117.56
3	B	1950	X6K	C03-C02-N01	-2.48	120.05	123.94
3	A	1951	X6K	C13-N12-C11	-2.38	111.61	117.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	SO4	1	0
2	A	1950	SO4	1	0
3	A	1951	X6K	3	0
3	B	1950	X6K	9	0
2	B	1951	SO4	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	550/696 (79%)	-0.23	3 (0%) 91 88	18, 62, 117, 129	0
1	B	550/696 (79%)	-0.19	3 (0%) 91 88	48, 75, 126, 135	0
All	All	1100/1392 (79%)	-0.21	6 (0%) 91 88	18, 69, 121, 135	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	690	HIS	2.7
1	A	322	ARG	2.5
1	A	323	PHE	2.4
1	B	341	TRP	2.3
1	A	335	PHE	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
3	X6K	B	1950	26/26	0.85	0.52	2.13	113,121,125,125	0
3	X6K	A	1951	26/26	0.89	0.35	2.02	114,119,123,123	0
2	SO4	A	1949	5/5	0.87	0.23	1.26	145,145,145,146	0
2	SO4	B	1951	5/5	0.65	0.17	-	194,194,194,194	0
2	SO4	A	1950	5/5	0.93	0.35	-	146,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.