wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:32 AM GMT

PDB ID	:	3MDB
Title	:	Crystal structure of the ternary complex of full length centaurin alpha-1, KIF13B FHA domain, and IP4
Authors	:	Shen, L.; Tong, Y.; Tempel, W.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on	:	2010-03-30
Resolution	:	2.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

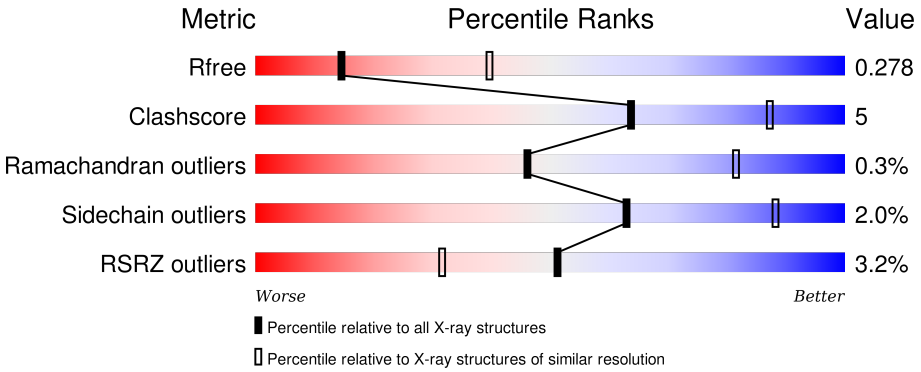
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	124	2% 65% 13% • 21%
1	B	124	5% 61% 15% • 23%
2	C	392	3% 81% 12% 7%
2	D	392	2% 80% 10% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7107 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 Kinesin-like protein KIF13B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			737	468	129	135	5			
1	B	95	Total	C	N	O	S	0	0	0
			716	458	124	129	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	MET	-	EXPRESSION TAG	UNP Q9NQT8
A	423	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	424	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	425	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	426	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	427	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	428	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	429	SER	-	EXPRESSION TAG	UNP Q9NQT8
A	430	SER	-	EXPRESSION TAG	UNP Q9NQT8
A	431	GLY	-	EXPRESSION TAG	UNP Q9NQT8
A	432	ARG	-	EXPRESSION TAG	UNP Q9NQT8
A	433	GLU	-	EXPRESSION TAG	UNP Q9NQT8
A	434	ASN	-	EXPRESSION TAG	UNP Q9NQT8
A	435	LEU	-	EXPRESSION TAG	UNP Q9NQT8
A	436	TYR	-	EXPRESSION TAG	UNP Q9NQT8
A	437	PHE	-	EXPRESSION TAG	UNP Q9NQT8
A	438	GLN	-	EXPRESSION TAG	UNP Q9NQT8
A	439	GLY	-	EXPRESSION TAG	UNP Q9NQT8
B	422	MET	-	EXPRESSION TAG	UNP Q9NQT8
B	423	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	424	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	425	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	426	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	427	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	428	HIS	-	EXPRESSION TAG	UNP Q9NQT8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	SER	-	EXPRESSION TAG	UNP Q9NQT8
B	430	SER	-	EXPRESSION TAG	UNP Q9NQT8
B	431	GLY	-	EXPRESSION TAG	UNP Q9NQT8
B	432	ARG	-	EXPRESSION TAG	UNP Q9NQT8
B	433	GLU	-	EXPRESSION TAG	UNP Q9NQT8
B	434	ASN	-	EXPRESSION TAG	UNP Q9NQT8
B	435	LEU	-	EXPRESSION TAG	UNP Q9NQT8
B	436	TYR	-	EXPRESSION TAG	UNP Q9NQT8
B	437	PHE	-	EXPRESSION TAG	UNP Q9NQT8
B	438	GLN	-	EXPRESSION TAG	UNP Q9NQT8
B	439	GLY	-	EXPRESSION TAG	UNP Q9NQT8

- Molecule 2 is a protein called Arf-GAP with dual PH domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	365	Total	C	N	O	S	0	0	0
			2883	1843	510	517	13			
2	D	353	Total	C	N	O	S	0	0	0
			2730	1753	471	494	12			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	EXPRESSION TAG	UNP O75689
C	-16	HIS	-	EXPRESSION TAG	UNP O75689
C	-15	HIS	-	EXPRESSION TAG	UNP O75689
C	-14	HIS	-	EXPRESSION TAG	UNP O75689
C	-13	HIS	-	EXPRESSION TAG	UNP O75689
C	-12	HIS	-	EXPRESSION TAG	UNP O75689
C	-11	HIS	-	EXPRESSION TAG	UNP O75689
C	-10	SER	-	EXPRESSION TAG	UNP O75689
C	-9	SER	-	EXPRESSION TAG	UNP O75689
C	-8	GLY	-	EXPRESSION TAG	UNP O75689
C	-7	ARG	-	EXPRESSION TAG	UNP O75689
C	-6	GLU	-	EXPRESSION TAG	UNP O75689
C	-5	ASN	-	EXPRESSION TAG	UNP O75689
C	-4	LEU	-	EXPRESSION TAG	UNP O75689
C	-3	TYR	-	EXPRESSION TAG	UNP O75689
C	-2	PHE	-	EXPRESSION TAG	UNP O75689
C	-1	GLN	-	EXPRESSION TAG	UNP O75689
C	0	GLY	-	EXPRESSION TAG	UNP O75689
C	241	SER	GLY	SEE REMARK 999	UNP O75689

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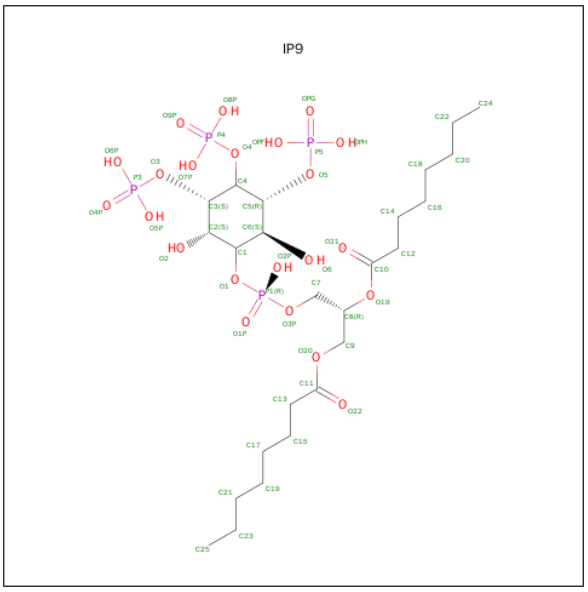
Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	MET	-	EXPRESSION TAG	UNP O75689
D	-16	HIS	-	EXPRESSION TAG	UNP O75689
D	-15	HIS	-	EXPRESSION TAG	UNP O75689
D	-14	HIS	-	EXPRESSION TAG	UNP O75689
D	-13	HIS	-	EXPRESSION TAG	UNP O75689
D	-12	HIS	-	EXPRESSION TAG	UNP O75689
D	-11	HIS	-	EXPRESSION TAG	UNP O75689
D	-10	SER	-	EXPRESSION TAG	UNP O75689
D	-9	SER	-	EXPRESSION TAG	UNP O75689
D	-8	GLY	-	EXPRESSION TAG	UNP O75689
D	-7	ARG	-	EXPRESSION TAG	UNP O75689
D	-6	GLU	-	EXPRESSION TAG	UNP O75689
D	-5	ASN	-	EXPRESSION TAG	UNP O75689
D	-4	LEU	-	EXPRESSION TAG	UNP O75689
D	-3	TYR	-	EXPRESSION TAG	UNP O75689
D	-2	PHE	-	EXPRESSION TAG	UNP O75689
D	-1	GLN	-	EXPRESSION TAG	UNP O75689
D	0	GLY	-	EXPRESSION TAG	UNP O75689
D	241	SER	GLY	SEE REMARK 999	UNP O75689

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is (2R)-3-{[(R)-{[(1S,2S,3R,4S,5S,6S)-2,6-DIHYDROXY-3,4,5-TRIS(PHOSPHONOOXY)CYCLOHEXYL]OXY}(HYDROXY)PHOSPHORYL]OXY}PROPANE-1,2-DIYL DIOCTANOATE (three-letter code: IP9) (formula: $C_{25}H_{50}O_{22}P_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O P 28 6 18 4	0	0

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

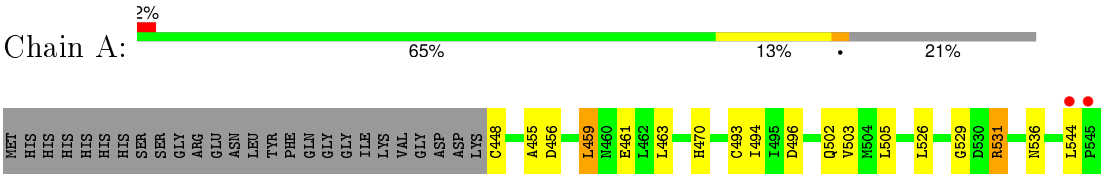
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total X 1 1	1	0
5	A	2	Total X 2 2	2	0
5	D	5	Total X 5 5	5	0
5	C	3	Total X 3 3	3	0

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.

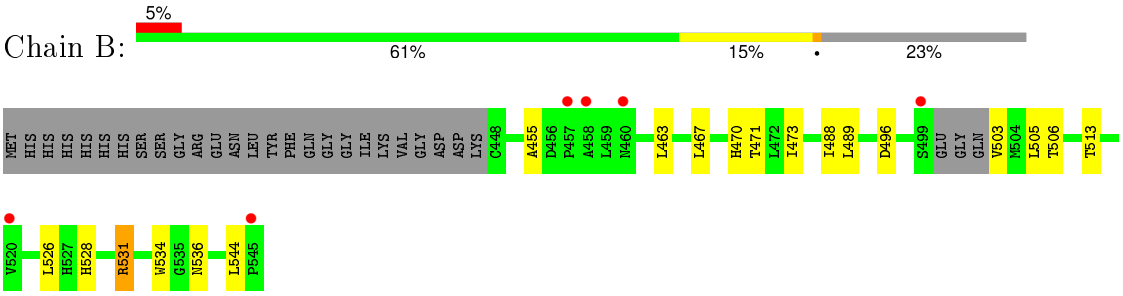
- Molecule 1: Kinesin-like protein KIF13B

Chain A:



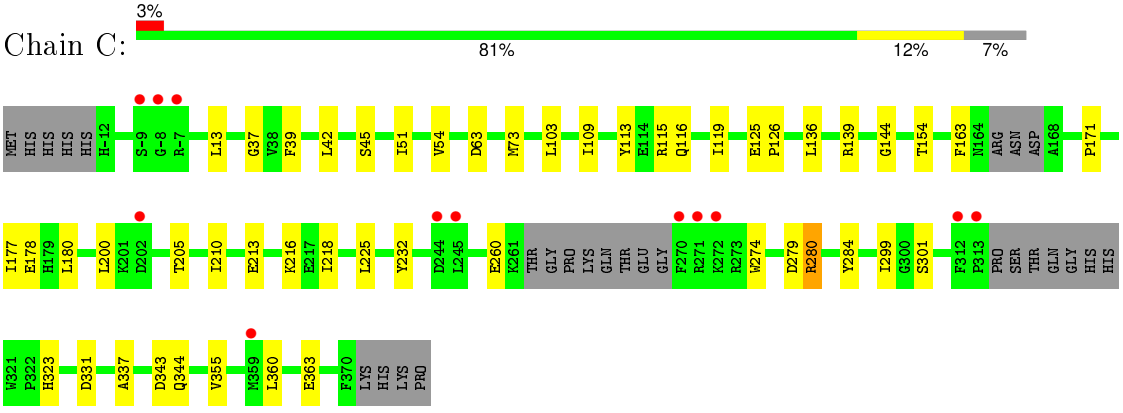
- Molecule 1: Kinesin-like protein KIF13B

Chain B:



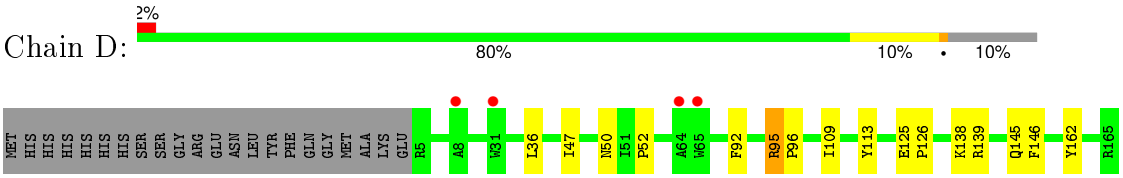
- Molecule 2: Arf-GAP with dual PH domain-containing protein 1

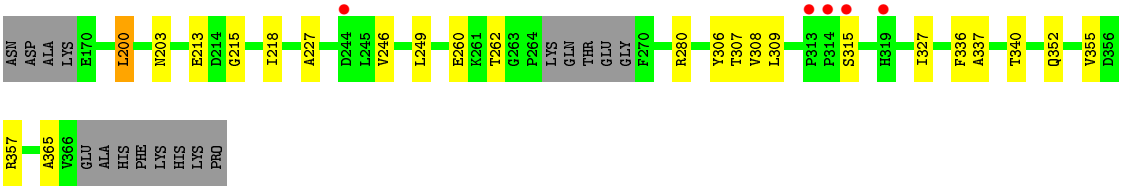
Chain C:



- Molecule 2: Arf-GAP with dual PH domain-containing protein 1

Chain D:




ASN ASP ALA LYS E170 L200 N203 E213 D214 G215 I218 A227 D244 L245 V246 L249 E260 K261 T262 G263 P264 LYS GLN THR GLU GLY F270 R280 Y306 T307 V308 L309 P313 P314 S315 H319 I327 F336 A337 T340 Q352 V355 D356

R357 A365 V366 GLU ALA HIS PHE LYS HIS LYS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.80Å 115.80Å 189.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.95 29.44 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.44-2.95) 100.0 (29.44-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.225 , 0.277 0.226 , 0.278	Depositor DCC
R_{free} test set	977 reflections (3.65%)	DCC
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 27736 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7107	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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.*

[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: UNX, ZN, IP9

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	0.50	0/754	0.63	0/1029
1	B	0.51	0/731	0.58	0/999
2	C	0.58	0/2966	0.61	0/4018
2	D	0.56	0/2812	0.57	0/3819
All	All	0.56	0/7263	0.59	0/9865

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

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	737	0	693	12	0
1	B	716	0	688	15	0
2	C	2883	0	2660	27	0
2	D	2730	0	2480	19	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	28	0	8	1	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	3	0	0	0	0
5	D	5	0	0	0	0
All	All	7107	0	6529	71	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 5.

The worst 5 of 71 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)
2:C:136:LEU:HD13	2:C:210:ILE:HD12	1.67	0.77
2:C:200:LEU:HD13	2:C:205:THR:OG1	1.91	0.71
1:A:536:ASN:ND2	2:C:213:GLU:OE1	2.32	0.63
1:B:470:HIS:ND1	1:B:496:ASP:OD1	2.32	0.62
2:D:138:LYS:HE3	2:D:162:TYR:CZ	2.35	0.61

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	96/124 (77%)	92 (96%)	4 (4%)	0	100	100
1	B	91/124 (73%)	86 (94%)	5 (6%)	0	100	100
2	C	357/392 (91%)	339 (95%)	17 (5%)	1 (0%)	46	81
2	D	347/392 (88%)	328 (94%)	17 (5%)	2 (1%)	30	70
All	All	891/1032 (86%)	845 (95%)	43 (5%)	3 (0%)	46	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	365	ALA
2	C	279	ASP
2	D	315	SER

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	78/110 (71%)	74 (95%)	4 (5%)	29 67
1	B	77/110 (70%)	76 (99%)	1 (1%)	76 92
2	C	278/334 (83%)	273 (98%)	5 (2%)	66 89
2	D	256/334 (77%)	252 (98%)	4 (2%)	70 90
All	All	689/888 (78%)	675 (98%)	14 (2%)	63 88

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	154	THR
2	C	280	ARG
2	D	200	LEU
2	C	63	ASP
2	D	95	ARG

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)

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)

Of 14 ligands modelled in this entry, 11 are unknown and 2 are 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	IP9	C	375	-	28,28,51	1.64	8 (28%)	38,46,72	1.01	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
4	IP9	C	375	-	-	0/20/44/73	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	375	IP9	P1-O3P	2.11	1.62	1.54
4	C	375	IP9	P3-O6P	2.35	1.63	1.54
4	C	375	IP9	P5-O5	2.36	1.67	1.60
4	C	375	IP9	P5-OPH	2.37	1.63	1.54
4	C	375	IP9	P3-O5P	2.39	1.63	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	375	IP9	P4-O4-C4	2.09	126.58	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	375	IP9	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	98/124 (79%)	-0.06	2 (2%)	68	48	47, 65, 85, 92	0
1	B	95/124 (76%)	0.07	6 (6%)	23	12	51, 73, 91, 100	0
2	C	365/392 (93%)	-0.09	12 (3%)	50	31	30, 55, 92, 101	0
2	D	353/392 (90%)	-0.11	9 (2%)	61	39	35, 58, 91, 107	0
All	All	911/1032 (88%)	-0.08	29 (3%)	51	32	30, 60, 91, 107	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	312	PHE	5.8
2	C	-8	GLY	4.0
2	D	315	SER	3.3
2	D	314	PRO	3.2
2	C	270	PHE	3.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	ZN	D	401	1/1	0.99	0.08	-1.23	68,68,68,68	0
4	IP9	C	375	28/51	0.94	0.12	-1.51	60,66,69,70	0
3	ZN	C	401	1/1	1.00	0.09	-1.52	38,38,38,38	0
5	UNX	D	377	1/1	-	-	-	0,0,0,0	1
5	UNX	C	377	1/1	-	-	-	0,0,0,0	1
5	UNX	B	11	1/1	-	-	-	0,0,0,0	1
5	UNX	D	375	1/1	-	-	-	0,0,0,0	1
5	UNX	C	376	1/1	-	-	-	0,0,0,0	1
5	UNX	A	5	1/1	-	-	-	0,0,0,0	1
5	UNX	D	376	1/1	-	-	-	0,0,0,0	1
5	UNX	C	378	1/1	-	-	-	0,0,0,0	1
5	UNX	A	1	1/1	-	-	-	0,0,0,0	1
5	UNX	D	378	1/1	-	-	-	0,0,0,0	1
5	UNX	D	379	1/1	-	-	-	0,0,0,0	1

6.5 Other polymers

There are no such residues in this entry.