W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 22, 2018 – 03:08 PM EST

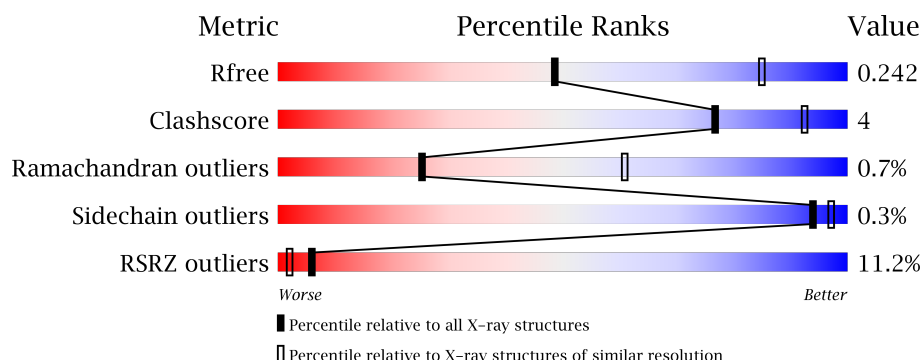|		
PDB ID	:	4LGD
Title	:	Structural Basis for Autoactivation of Human Mst2 Kinase and Its Regulation by RASSF5
Authors	:	Luo, X.; Ni, L.; Tomchick, D.R.
Deposited on	:	2013-06-27
Resolution	:	3.05 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
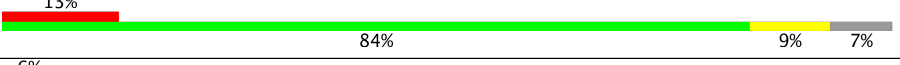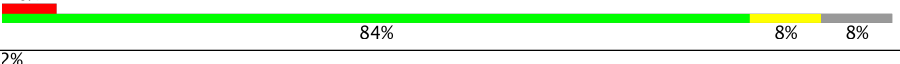*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		4
Ramachandran outliers		0.7%
Sidechain outliers		0.3%
RSRZ outliers		11.2%

Worse　　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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	378	15%　82%　11%　7%
1	B	378	13%　84%　9%　7%
1	C	378	6%　84%　8%　8%
1	D	378	2%　82%　7% · 11%
2	E	49	10%　84%　12% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	49	33% · 53% · 6% · 41%
2	G	49	6% · 86% · 12% ·
2	H	49	24% · 78% · · 18%

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
5	SO4	A	503	-	-	X	-
5	SO4	B	503	-	-	X	-
5	SO4	B	506	-	-	-	X
5	SO4	D	503	-	-	X	-
6	NA	C	504	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25637 atoms, of which 12852 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 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	H	N	O	S	0	0	0
			5690	1799	2865	479	530	17			
1	B	350	Total	C	H	N	O	S	0	0	0
			5698	1794	2879	480	528	17			
1	C	349	Total	C	H	N	O	S	0	0	0
			5706	1800	2879	482	528	17			
1	D	338	Total	C	H	N	O	S	0	0	0
			5486	1731	2765	463	511	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q13188
A	1	HIS	-	EXPRESSION TAG	UNP Q13188
A	2	HIS	-	EXPRESSION TAG	UNP Q13188
A	3	HIS	-	EXPRESSION TAG	UNP Q13188
A	4	HIS	-	EXPRESSION TAG	UNP Q13188
A	5	HIS	-	EXPRESSION TAG	UNP Q13188
A	6	HIS	-	EXPRESSION TAG	UNP Q13188
A	7	GLY	-	EXPRESSION TAG	UNP Q13188
A	8	SER	-	EXPRESSION TAG	UNP Q13188
A	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188
B	0	MET	-	EXPRESSION TAG	UNP Q13188
B	1	HIS	-	EXPRESSION TAG	UNP Q13188
B	2	HIS	-	EXPRESSION TAG	UNP Q13188
B	3	HIS	-	EXPRESSION TAG	UNP Q13188
B	4	HIS	-	EXPRESSION TAG	UNP Q13188
B	5	HIS	-	EXPRESSION TAG	UNP Q13188
B	6	HIS	-	EXPRESSION TAG	UNP Q13188
B	7	GLY	-	EXPRESSION TAG	UNP Q13188
B	8	SER	-	EXPRESSION TAG	UNP Q13188
B	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188
C	0	MET	-	EXPRESSION TAG	UNP Q13188

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	HIS	-	EXPRESSION TAG	UNP Q13188
C	2	HIS	-	EXPRESSION TAG	UNP Q13188
C	3	HIS	-	EXPRESSION TAG	UNP Q13188
C	4	HIS	-	EXPRESSION TAG	UNP Q13188
C	5	HIS	-	EXPRESSION TAG	UNP Q13188
C	6	HIS	-	EXPRESSION TAG	UNP Q13188
C	7	GLY	-	EXPRESSION TAG	UNP Q13188
C	8	SER	-	EXPRESSION TAG	UNP Q13188
C	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188
D	0	MET	-	EXPRESSION TAG	UNP Q13188
D	1	HIS	-	EXPRESSION TAG	UNP Q13188
D	2	HIS	-	EXPRESSION TAG	UNP Q13188
D	3	HIS	-	EXPRESSION TAG	UNP Q13188
D	4	HIS	-	EXPRESSION TAG	UNP Q13188
D	5	HIS	-	EXPRESSION TAG	UNP Q13188
D	6	HIS	-	EXPRESSION TAG	UNP Q13188
D	7	GLY	-	EXPRESSION TAG	UNP Q13188
D	8	SER	-	EXPRESSION TAG	UNP Q13188
D	146	ASN	ASP	ENGINEERED MUTATION	UNP Q13188

- Molecule 2 is a protein called Ras association domain family member 5, RASSF5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	47	Total 810	C 260	H 403	N 67	O 80	0	0	0
2	F	29	Total 489	C 155	H 246	N 39	O 49	0	0	0
2	G	48	Total 825	C 265	H 409	N 68	O 83	0	0	0
2	H	40	Total 697	C 226	H 346	N 57	O 68	0	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

ANP
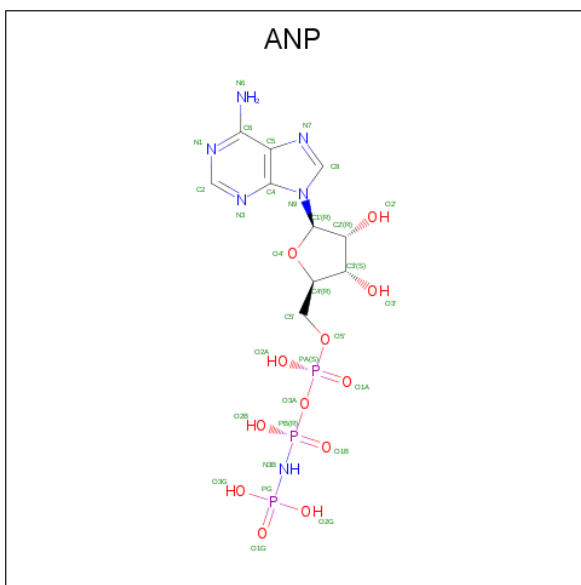
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	B	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	C	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		
3	D	1	Total	C	H	N	O	P	0	0
			46	10	15	6	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
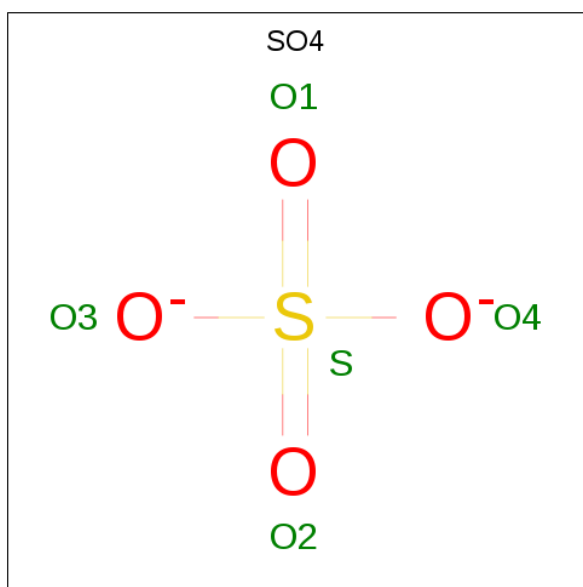
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

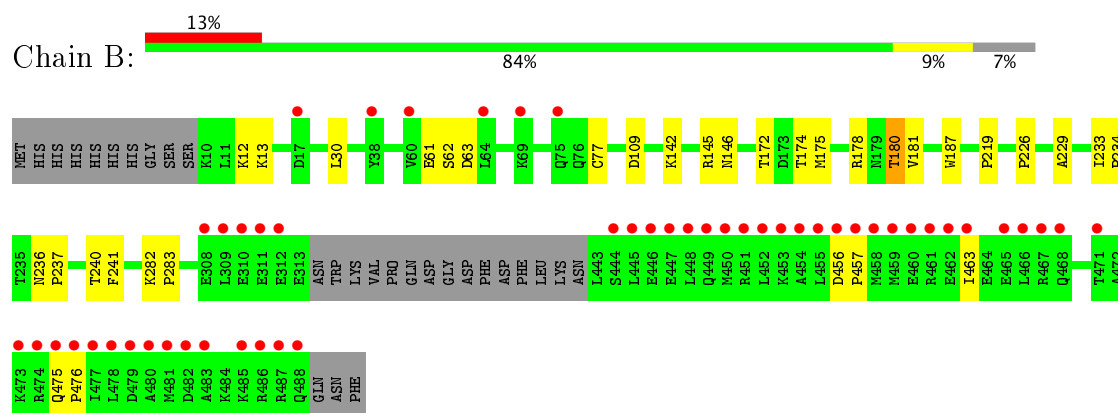| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Na	0	0
			1	1		
6	C	2	Total	Na	0	0
			2	2		

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 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 (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 3
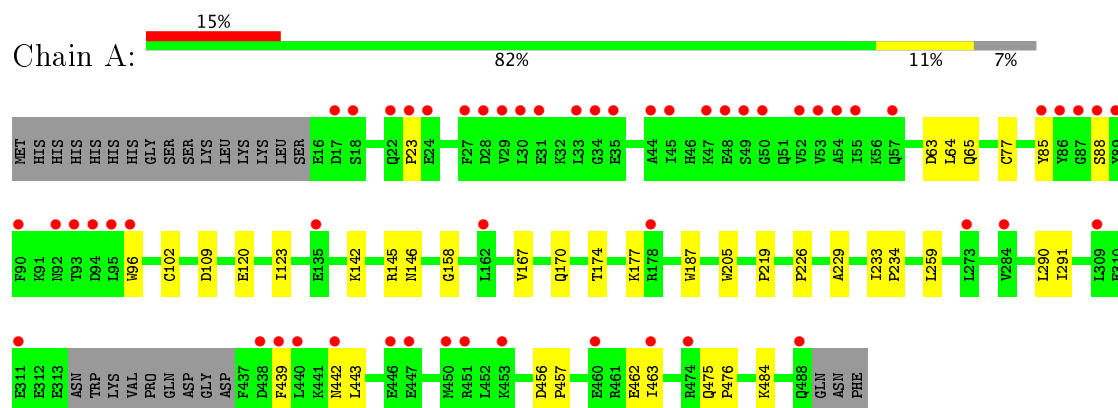
- Molecule 1: Serine/threonine-protein kinase 3

- Molecule 1: Serine/threonine-protein kinase 3

- Molecule 1: Serine/threonine-protein kinase 3

Chain D:

- Molecule 2: Ras association domain family member 5, RASSF5

Chain E:

- Molecule 2: Ras association domain family member 5, RASSF5

Chain F:

- Molecule 2: Ras association domain family member 5, RASSF5

Chain G:

- Molecule 2: Ras association domain family member 5, RASSF5

Chain H:
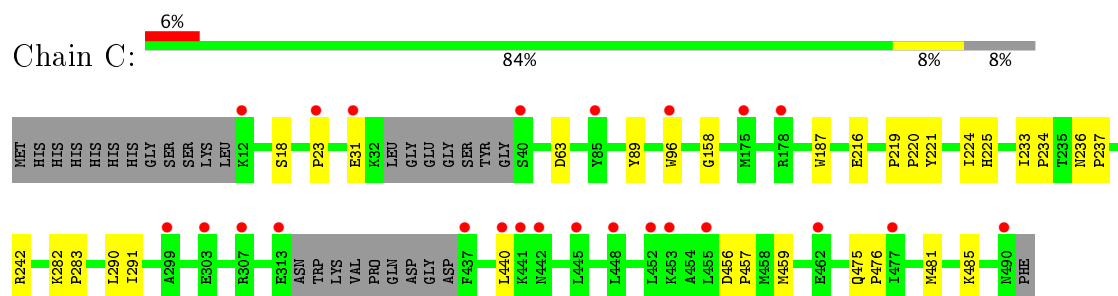
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.40Å 237.14Å 95.86Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.05 46.05 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-3.05) 98.6 (46.05-3.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.199 , 0.244 0.200 , 0.242	Depositor DCC
R_{free} test set	2522 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	1.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 94.3	EDS
L-test for twinning [2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25637	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NA, MG, ANP, 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	0.21	0/2879	0.38	0/3882
1	B	0.22	0/2871	0.41	0/3869
1	C	0.21	0/2879	0.38	0/3879
1	D	0.22	0/2773	0.40	0/3740
2	E	0.22	0/413	0.34	0/552
2	F	0.21	0/245	0.32	0/327
2	G	0.22	0/422	0.34	0/564
2	H	0.22	0/357	0.30	0/477
All	All	0.22	0/12839	0.39	0/17290

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	2825	2865	2858	25	0
1	B	2819	2879	2872	24	0
1	C	2827	2879	2872	17	0
1	D	2721	2765	2758	19	0
2	E	407	403	403	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	243	246	246	2	0
2	G	416	409	409	7	0
2	H	351	346	346	1	0
3	A	31	15	13	2	0
3	B	31	15	13	1	0
3	C	31	15	13	0	0
3	D	31	15	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	2	0
5	B	20	0	0	3	0
5	C	5	0	0	0	0
5	D	15	0	0	3	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
All	All	12785	12852	12816	90	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.

The worst 5 of 90 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:85:TYR:OH	1:A:88:SER:OG	2.08	0.71
1:D:145:ARG:NH1	5:D:503:SO4:S	2.72	0.63
1:B:145:ARG:NH1	5:B:503:SO4:S	2.73	0.61
1:B:145:ARG:NH1	5:B:503:SO4:O2	2.34	0.61
1:B:77:CYS:SG	1:B:142:LYS:NZ	2.73	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	346/378 (92%)	319 (92%)	24 (7%)	3 (1%)	20	55
1	B	346/378 (92%)	328 (95%)	16 (5%)	2 (1%)	28	64
1	C	343/378 (91%)	325 (95%)	16 (5%)	2 (1%)	28	64
1	D	334/378 (88%)	314 (94%)	16 (5%)	4 (1%)	15	47
2	E	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
2	F	27/49 (55%)	26 (96%)	1 (4%)	0	100	100
2	G	46/49 (94%)	46 (100%)	0	0	100	100
2	H	38/49 (78%)	38 (100%)	0	0	100	100
All	All	1525/1708 (89%)	1440 (94%)	74 (5%)	11 (1%)	25	61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	311	GLU
1	A	174	THR
1	C	31	GLU
1	D	174	THR
1	A	63	ASP

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	311/337 (92%)	309 (99%)	2 (1%)	89	95
1	B	311/337 (92%)	310 (100%)	1 (0%)	94	97
1	C	313/337 (93%)	313 (100%)	0	100	100
1	D	300/337 (89%)	299 (100%)	1 (0%)	94	97
2	E	45/46 (98%)	45 (100%)	0	100	100
2	F	28/46 (61%)	28 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	46/46 (100%)	46 (100%)	0	100	100
2	H	39/46 (85%)	39 (100%)	0	100	100
All	All	1393/1532 (91%)	1389 (100%)	4 (0%)	94	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	VAL
1	A	442	ASN
1	B	180	THR
1	D	290	LEU

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 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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
3	ANP	A	501	4	29,33,33	1.66	9 (31%)	28,52,52	2.27	4 (14%)
5	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.06	0
3	ANP	B	501	4	29,33,33	1.62	9 (31%)	28,52,52	2.25	5 (17%)
5	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.08	0
5	SO4	B	506	-	4,4,4	0.16	0	6,6,6	0.05	0
3	ANP	C	501	4	29,33,33	1.60	9 (31%)	28,52,52	2.27	5 (17%)
5	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.05	0
3	ANP	D	501	4	29,33,33	1.61	9 (31%)	28,52,52	2.30	5 (17%)
5	SO4	D	503	-	4,4,4	0.16	0	6,6,6	0.09	0
5	SO4	D	504	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.06	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
3	ANP	A	501	4	-	0/13/38/38	0/3/3/3
5	SO4	A	503	-	-	0/0/0/0	0/0/0/0
3	ANP	B	501	4	-	0/13/38/38	0/3/3/3
5	SO4	B	503	-	-	0/0/0/0	0/0/0/0
5	SO4	B	504	-	-	0/0/0/0	0/0/0/0
5	SO4	B	505	-	-	0/0/0/0	0/0/0/0
5	SO4	B	506	-	-	0/0/0/0	0/0/0/0
3	ANP	C	501	4	-	0/13/38/38	0/3/3/3
5	SO4	C	503	-	-	0/0/0/0	0/0/0/0
3	ANP	D	501	4	-	1/13/38/38	0/3/3/3
5	SO4	D	503	-	-	0/0/0/0	0/0/0/0
5	SO4	D	504	-	-	0/0/0/0	0/0/0/0
5	SO4	D	505	-	-	0/0/0/0	0/0/0/0

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	ANP	C2'-C1'	-3.51	1.48	1.53
3	B	501	ANP	C2'-C1'	-3.37	1.48	1.53
3	C	501	ANP	C2'-C1'	-3.33	1.48	1.53
3	A	501	ANP	C2'-C1'	-3.24	1.48	1.53
3	A	501	ANP	C2'-C3'	-2.35	1.47	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	ANP	N3-C2-N1	-10.15	120.02	128.86
3	C	501	ANP	N3-C2-N1	-9.95	120.19	128.86
3	B	501	ANP	N3-C2-N1	-9.73	120.38	128.86
3	D	501	ANP	N3-C2-N1	-9.68	120.43	128.86
3	B	501	ANP	PA-O3A-PB	-4.34	117.04	132.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	ANP	O1B-PB-N3B-PG

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ANP	2	0
5	A	503	SO4	2	0
3	B	501	ANP	1	0
5	B	503	SO4	3	0
5	D	503	SO4	2	0
5	D	504	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(Å²)	Q<0.9
1	A	350/378 (92%)	1.00	55 (15%)	2	1	98, 160, 251, 332	0
1	B	350/378 (92%)	0.84	51 (14%)	3	1	57, 98, 245, 293	0
1	C	349/378 (92%)	0.66	24 (6%)	18	7	72, 122, 204, 242	0
1	D	338/378 (89%)	0.45	8 (2%)	59	34	57, 92, 175, 232	0
2	E	47/49 (95%)	0.85	5 (10%)	7	2	97, 128, 163, 181	0
2	F	29/49 (59%)	2.58	16 (55%)	0	0	179, 258, 279, 304	0
2	G	48/49 (97%)	0.59	3 (6%)	21	8	62, 119, 154, 180	0
2	H	40/49 (81%)	1.31	12 (30%)	1	0	119, 153, 213, 255	0
All	All	1551/1708 (90%)	0.79	174 (11%)	6	2	57, 122, 238, 332	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	450	MET	8.9
1	C	440	LEU	7.5
1	A	88	SER	7.4
1	B	451	ARG	7.0
2	F	391	LYS	6.9

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(Å²)	Q<0.9
5	SO4	B	506	5/5	0.84	0.49	2.71	187,190,193,199	0
6	NA	C	504	1/1	0.34	0.37	2.48	103,103,103,103	0
5	SO4	D	505	5/5	0.87	0.34	1.03	128,150,162,168	0
3	ANP	C	501	31/31	0.75	0.34	0.90	140,192,243,292	0
3	ANP	D	501	31/31	0.95	0.28	0.27	57,93,183,229	0
5	SO4	B	503	5/5	0.92	0.24	0.04	108,110,116,132	0
5	SO4	D	504	5/5	0.76	0.28	-0.02	125,138,149,156	0
5	SO4	D	503	5/5	0.93	0.27	-0.09	77,78,105,145	0
3	ANP	B	501	31/31	0.95	0.27	-0.13	57,101,168,247	0
5	SO4	B	505	5/5	0.89	0.24	-0.32	113,128,140,166	0
3	ANP	A	501	31/31	0.74	0.26	-0.41	144,191,249,314	0
6	NA	D	506	1/1	0.89	0.22	-0.68	65,65,65,65	0
5	SO4	A	503	5/5	0.93	0.16	-1.24	133,149,152,155	0
6	NA	C	505	1/1	0.80	0.14	-1.27	189,189,189,189	0
5	SO4	B	504	5/5	0.83	0.18	-1.38	191,191,196,199	0
5	SO4	C	503	5/5	0.96	0.20	-1.57	94,96,107,133	0
4	MG	C	502	1/1	0.64	0.58	-	221,221,221,221	0
4	MG	A	502	1/1	0.88	0.59	-	219,219,219,219	0
4	MG	B	502	1/1	0.84	0.43	-	104,104,104,104	0
4	MG	D	502	1/1	0.92	0.55	-	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.