Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:48 PM GMT

PDB ID	:	5EDS
Title	:	Crystal structure of human PI3K-gamma in complex with benzimidazole inhibitor 5
Authors	:	Whittington, D.A.; Tang, J.; Yakowec, P.
Deposited on	:	2015-10-21
Resolution	:	2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

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 2.80 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		0.277
Clashscore		8
Ramachandran outliers		0.6%
Sidechain outliers		2.0%
RSRZ outliers		5.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
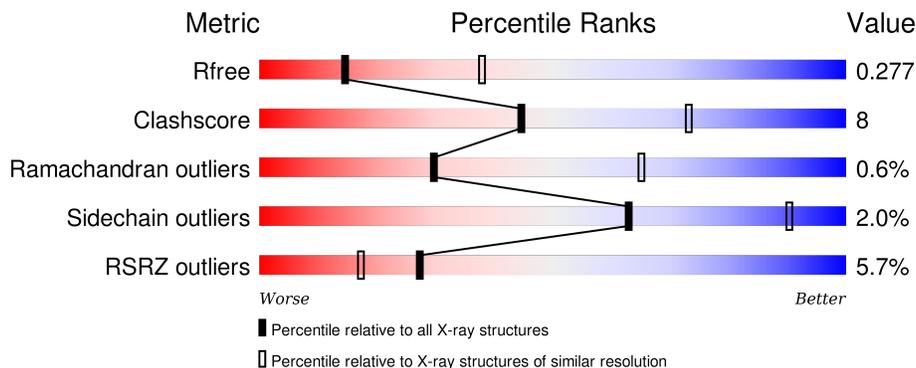
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	959	5% / 69% 16% · 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6736 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total 6674	C 4293	N 1137	O 1210	S 34	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
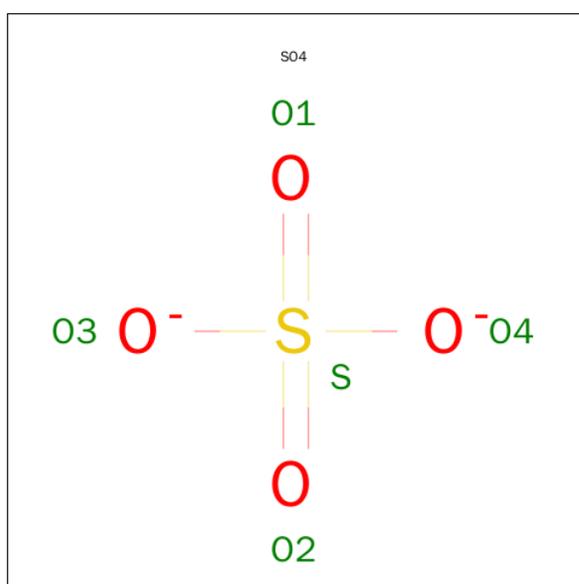
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 4-azanyl-6-[[(1 {S})-1-[6-fluoranyl-1-(3-methylsulfonylphenyl)benzimidazol-2-yl]ethyl]amino]pyrimidine-5-carbonitrile (three-letter code: 5MT) (formula: $C_{21}H_{18}FN_7O_2S$).
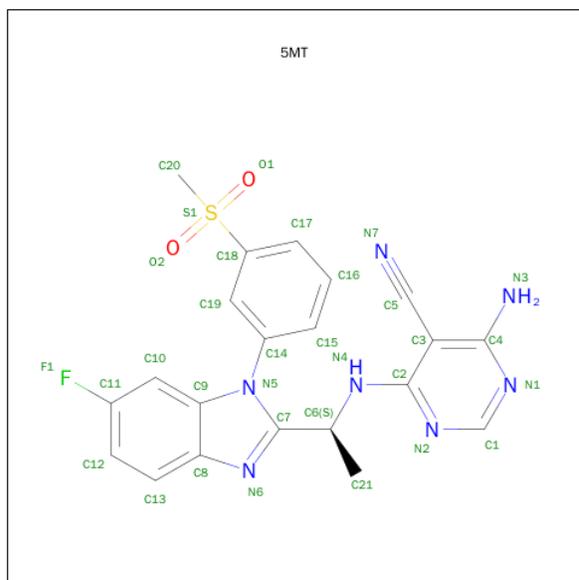
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	32	21	1	7	2	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	15	15	15	0	0

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform
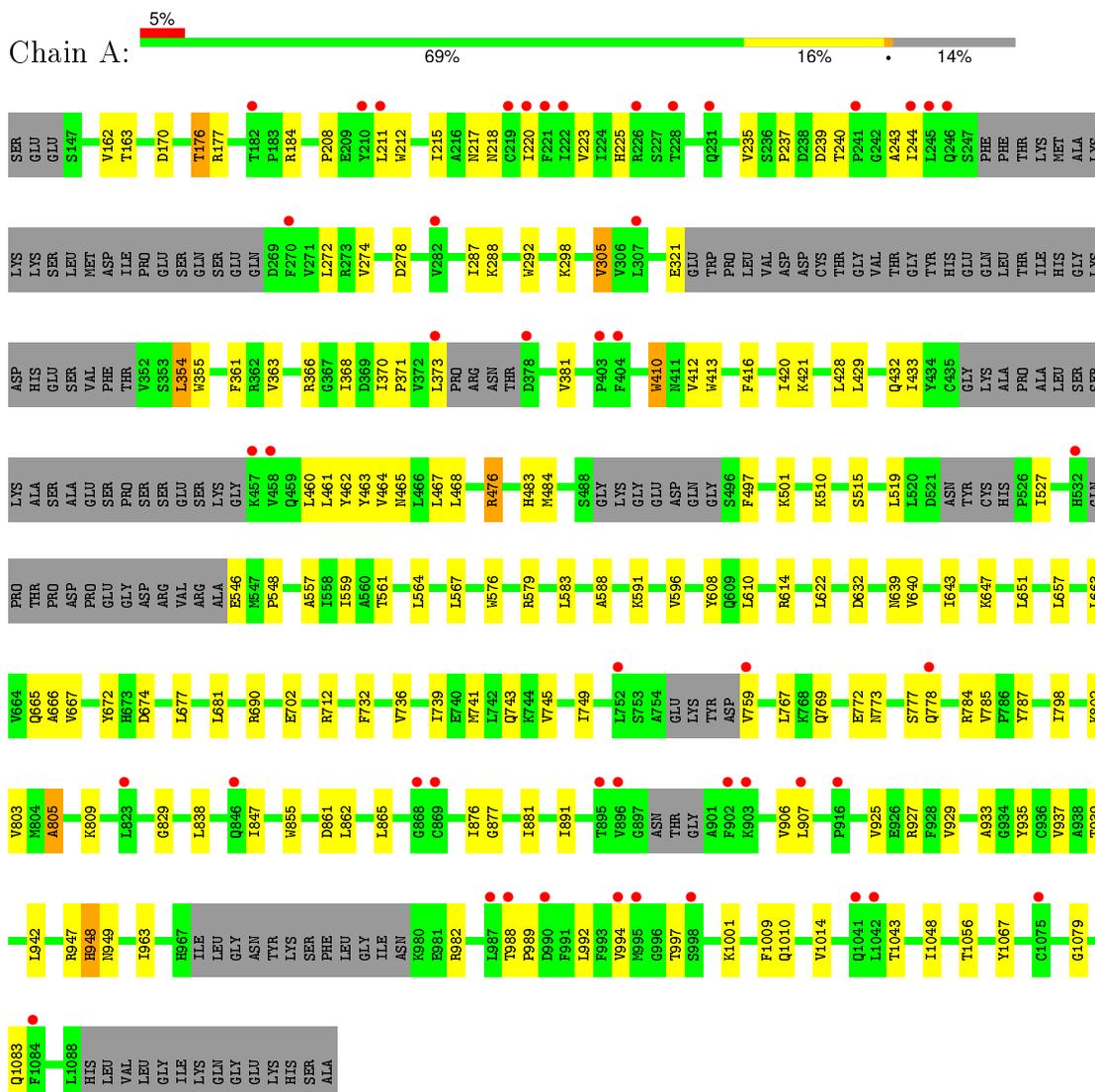
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.30Å 68.23Å 106.62Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 41.01 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-2.80) 98.2 (41.01-2.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.273 0.209 , 0.277	Depositor DCC
R_{free} test set	1832 reflections (7.74%)	DCC
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.7	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 25882 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6736	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MT, 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	0.51	1/6815 (0.0%)	0.57	0/9215

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	TRP	CD2-CE2	5.12	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6674	0	6738	106	0
2	A	15	0	0	0	0
3	A	32	0	18	0	0
4	A	15	0	0	0	0
All	All	6736	0	6756	106	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 8.

All (106) 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:749:ILE:HD13	1:A:767:LEU:HD13	1.55	0.89
1:A:354:LEU:HD12	1:A:527:ILE:HG22	1.55	0.87
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.62	0.81
1:A:497:PHE:O	1:A:1043:THR:HB	1.83	0.78
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.70	0.73
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.71	0.73
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.73	0.70
1:A:907:LEU:HD23	1:A:994:VAL:HG21	1.73	0.69
1:A:240:THR:HG23	1:A:243:ALA:H	1.58	0.68
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.78	0.65
1:A:935:TYR:O	1:A:939:THR:HG23	1.98	0.64
1:A:567:LEU:HD21	1:A:591:LYS:HD3	1.84	0.60
1:A:354:LEU:HD12	1:A:527:ILE:CG2	2.32	0.60
1:A:743:GLN:HG3	1:A:876:ILE:HD13	1.85	0.57
1:A:759:VAL:HG22	1:A:809:LYS:HZ3	1.69	0.57
1:A:798:ILE:H	1:A:798:ILE:HD12	1.70	0.57
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.87	0.56
1:A:749:ILE:CD1	1:A:767:LEU:HD13	2.33	0.56
1:A:759:VAL:HG11	1:A:805:ALA:HA	1.87	0.55
1:A:759:VAL:HG13	1:A:809:LYS:HZ3	1.72	0.55
1:A:666:ALA:HB3	1:A:677:LEU:HD21	1.89	0.54
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.37	0.54
1:A:933:ALA:O	1:A:937:VAL:HG23	2.08	0.54
1:A:212:TRP:O	1:A:215:ILE:HG22	2.07	0.54
1:A:579:ARG:HG2	1:A:610:LEU:HD22	1.90	0.54
1:A:640:VAL:O	1:A:643:ILE:HG12	2.08	0.53
1:A:769:GLN:NE2	1:A:773:ASN:OD1	2.37	0.53
1:A:579:ARG:CG	1:A:610:LEU:HD22	2.39	0.52
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.90	0.52
1:A:759:VAL:HG22	1:A:809:LYS:NZ	2.25	0.51
1:A:220:ILE:CD1	1:A:287:ILE:HD13	2.41	0.50
1:A:244:ILE:HD11	1:A:287:ILE:HG21	1.92	0.50
1:A:861:ASP:C	1:A:862:LEU:HD12	2.32	0.50
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.92	0.50
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.45	0.50
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.93	0.50
1:A:657:LEU:HD11	1:A:690:ARG:HD3	1.93	0.50
1:A:583:LEU:HD22	1:A:610:LEU:CD1	2.42	0.49
1:A:287:ILE:HD12	1:A:288:LYS:N	2.27	0.49
1:A:208:PRO:HG2	1:A:211:LEU:HD12	1.93	0.49
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HB3	1:A:305:VAL:CG2	2.41	0.48
1:A:278:ASP:HB2	1:A:784:ARG:HH12	1.78	0.48
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	1.95	0.48
1:A:855:TRP:CE3	1:A:862:LEU:HD13	2.49	0.48
1:A:947:ARG:NH2	1:A:963:ILE:O	2.47	0.48
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.13	0.48
1:A:287:ILE:C	1:A:287:ILE:HD12	2.34	0.47
1:A:741:MET:HE2	1:A:778:GLN:HB3	1.96	0.47
1:A:925:VAL:HG13	1:A:994:VAL:HG12	1.95	0.47
1:A:162:VAL:CG1	1:A:177:ARG:HD2	2.44	0.47
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.97	0.47
1:A:732:PHE:O	1:A:736:VAL:HG23	2.14	0.47
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.96	0.46
1:A:665:GLN:NE2	1:A:702:GLU:OE2	2.29	0.46
1:A:632:ASP:C	1:A:632:ASP:OD1	2.52	0.46
1:A:366:ARG:NH1	1:A:519:LEU:HD22	2.30	0.46
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.84	0.46
1:A:373:LEU:O	1:A:373:LEU:HD23	2.15	0.46
1:A:170:ASP:OD2	1:A:476:ARG:NH2	2.47	0.46
1:A:745:VAL:O	1:A:749:ILE:HD12	2.16	0.46
1:A:907:LEU:HD23	1:A:994:VAL:CG2	2.46	0.46
1:A:759:VAL:HG13	1:A:809:LYS:NZ	2.31	0.46
1:A:559:ILE:CD1	1:A:588:ALA:HB2	2.45	0.46
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.97	0.45
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.97	0.45
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.42	0.45
1:A:663:LEU:HB3	1:A:681:LEU:HD21	1.99	0.45
1:A:777:SER:HA	1:A:778:GLN:HA	1.72	0.45
1:A:184:ARG:NH1	1:A:321:GLU:OE2	2.50	0.45
1:A:527:ILE:HD12	1:A:527:ILE:N	2.31	0.44
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.47	0.44
1:A:235:VAL:HG13	1:A:239:ASP:OD2	2.17	0.44
1:A:244:ILE:CD1	1:A:287:ILE:HG21	2.48	0.44
1:A:355:TRP:HA	1:A:421:LYS:HB2	2.00	0.44
1:A:223:VAL:HG12	1:A:225:HIS:CD2	2.52	0.44
1:A:862:LEU:N	1:A:862:LEU:HD12	2.33	0.44
1:A:745:VAL:HG12	1:A:749:ILE:CD1	2.48	0.43
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.48	0.43
1:A:745:VAL:HG12	1:A:749:ILE:HD12	2.01	0.43
1:A:614:ARG:CZ	1:A:643:ILE:HG22	2.47	0.43
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:TRP:CZ3	1:A:596:VAL:HG22	2.53	0.43
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.01	0.42
1:A:847:ILE:HG21	1:A:942:LEU:HD21	2.01	0.42
1:A:220:ILE:HD11	1:A:287:ILE:CD1	2.49	0.42
1:A:464:VAL:HG11	1:A:484:MET:HG2	2.00	0.42
1:A:211:LEU:HD21	1:A:298:LYS:HA	2.02	0.42
1:A:891:ILE:O	1:A:906:VAL:HG11	2.19	0.42
1:A:1056:THR:HG21	1:A:1067:TYR:CD2	2.54	0.42
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.83	0.42
1:A:988:THR:HG21	1:A:1083:GLN:HE21	1.84	0.42
1:A:772:GLU:HG3	1:A:798:ILE:HG21	2.02	0.42
1:A:370:ILE:HD12	1:A:371:PRO:HD2	2.02	0.42
1:A:220:ILE:HD11	1:A:287:ILE:HD13	2.02	0.41
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.47	0.41
1:A:667:VAL:HG12	1:A:712:ARG:HD3	2.01	0.41
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.85	0.41
1:A:464:VAL:CG1	1:A:484:MET:HG2	2.50	0.41
1:A:483:HIS:CD2	1:A:510:LYS:HD3	2.55	0.41
1:A:745:VAL:CG1	1:A:749:ILE:HD11	2.51	0.41
1:A:785:VAL:HG11	1:A:787:TYR:CE1	2.56	0.41
1:A:467:LEU:HD13	1:A:672:TYR:CE1	2.56	0.40
1:A:948:HIS:N	1:A:948:HIS:ND1	2.69	0.40
1:A:461:LEU:HB3	1:A:462:TYR:CD1	2.56	0.40
1:A:557:ALA:O	1:A:561:THR:HG23	2.21	0.40

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	801/959 (84%)	753 (94%)	43 (5%)	5 (1%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	1079	GLY
1	A	949	ASN
1	A	805	ALA
1	A	548	PRO

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	742/857 (87%)	727 (98%)	15 (2%)	63	90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	THR
1	A	218	ASN
1	A	305	VAL
1	A	354	LEU
1	A	381	VAL
1	A	410	TRP
1	A	476	ARG
1	A	515	SER
1	A	546	GLU
1	A	739	ILE
1	A	802	LYS
1	A	865	LEU
1	A	927	ARG
1	A	948	HIS
1	A	982	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	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)

4 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	1201	-	4,4,4	0.40	0	6,6,6	0.15	0
2	SO4	A	1202	-	4,4,4	0.42	0	6,6,6	0.22	0
2	SO4	A	1203	-	4,4,4	0.43	0	6,6,6	0.16	0
3	5MT	A	1204	-	34,35,35	2.05	7 (20%)	41,52,52	1.47	7 (17%)

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	1201	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1202	-	-	0/0/0/0	0/0/0/0

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Full wwPDB X-ray Structure Validation Report

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1203	-	-	0/0/0/0	0/0/0/0
3	5MT	A	1204	-	-	0/16/20/20	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1204	5MT	C14-N5	-8.73	1.33	1.46
3	A	1204	5MT	C9-N5	-4.89	1.32	1.39
3	A	1204	5MT	C3-C4	-2.08	1.39	1.42
3	A	1204	5MT	O2-S1	2.01	1.50	1.44
3	A	1204	5MT	O1-S1	2.09	1.51	1.44
3	A	1204	5MT	C10-C11	2.19	1.39	1.35
3	A	1204	5MT	C7-C6	2.31	1.54	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1204	5MT	C3-C2-N2	-4.10	117.39	121.23
3	A	1204	5MT	O2-S1-O1	-3.68	109.68	117.73
3	A	1204	5MT	N1-C1-N2	-3.44	122.74	128.65
3	A	1204	5MT	C12-C11-C10	-2.43	119.91	123.26
3	A	1204	5MT	O1-S1-C18	2.27	110.27	108.29
3	A	1204	5MT	C20-S1-C18	2.27	107.36	104.67
3	A	1204	5MT	C2-C3-C5	2.46	122.69	119.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	823/959 (85%)	0.27	47 (5%)	27	17	41, 82, 132, 165	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	GLN	5.9
1	A	895	THR	4.8
1	A	220	ILE	4.5
1	A	221	PHE	4.5
1	A	988	THR	4.0
1	A	896	VAL	3.8
1	A	998	SER	3.7
1	A	1042	LEU	3.7
1	A	270	PHE	3.6
1	A	1041	GLN	3.6
1	A	823	LEU	3.6
1	A	532	HIS	3.6
1	A	457	LYS	3.4
1	A	222	ILE	3.3
1	A	987	LEU	3.3
1	A	1075	CYS	3.3
1	A	219	CYS	3.3
1	A	307	LEU	3.2
1	A	228	THR	2.7
1	A	907	LEU	2.7
1	A	373	LEU	2.6
1	A	246	GLN	2.6
1	A	210	TYR	2.5
1	A	995	MET	2.5
1	A	846	GLN	2.5
1	A	245	LEU	2.4
1	A	990	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	211	LEU	2.4
1	A	916	PRO	2.4
1	A	244	ILE	2.4
1	A	869	CYS	2.3
1	A	458	VAL	2.3
1	A	759	VAL	2.3
1	A	903	LYS	2.3
1	A	378	ASP	2.3
1	A	994	VAL	2.3
1	A	226	ARG	2.3
1	A	1084	PHE	2.3
1	A	868	GLY	2.2
1	A	778	GLN	2.2
1	A	282	VAL	2.2
1	A	182	THR	2.2
1	A	404	PHE	2.2
1	A	902	PHE	2.1
1	A	403	PRO	2.1
1	A	241	PRO	2.0
1	A	752	LEU	2.0

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($Å^2$)	Q<0.9
2	SO4	A	1202	5/5	0.92	0.17	-0.35	87,87,103,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	SO4	A	1203	5/5	0.87	0.30	-0.39	87,96,103,104	0
3	5MT	A	1204	32/32	0.95	0.19	-0.60	64,87,104,116	0
2	SO4	A	1201	5/5	0.94	0.15	-0.72	104,113,115,115	0

6.5 Other polymers (i)

There are no such residues in this entry.