



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:24 am GMT

PDB ID : 3S2A  
Title : Crystal structure of PI3K-gamma in complex with a quinoline inhibitor  
Authors : Whittington, D.A.; Tang, J.; Yakowec, P.  
Deposited on : 2011-05-16  
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

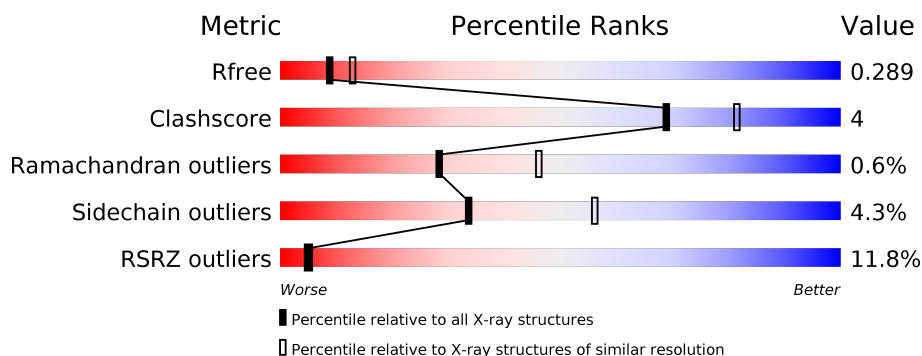
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

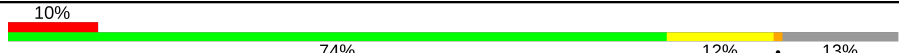
The reported resolution of this entry is 2.55 Å.

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))
$R_{free}$	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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  $\geq 3$ , 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	960	

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
2	SO4	A	3	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6822 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	834	Total	C	N	O	S	0	0	0
			6744	4329	1148	1233	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



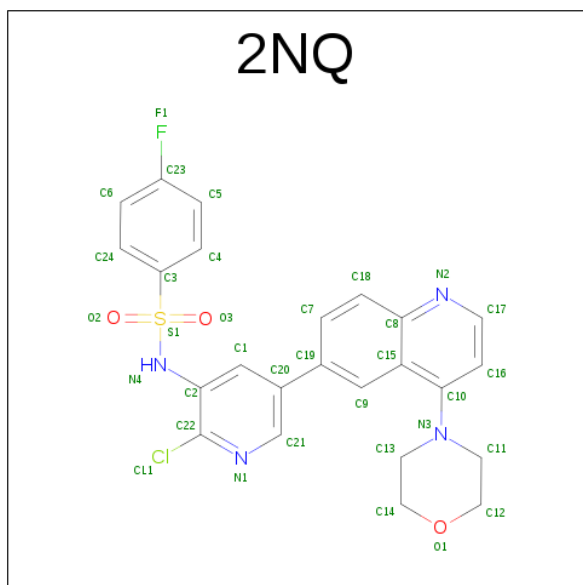
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is N-{2-CHLORO-5-[4-(MORPHOLIN-4-YL)QUINOLIN-6-YL]PYRIDIN-3-YL}-4-FLUOROBENZENESULFONAMIDE (three-letter code: 2NQ) (formula: C<sub>24</sub>H<sub>20</sub>ClFN<sub>4</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	
			34	24	1	1	4	3	1	0

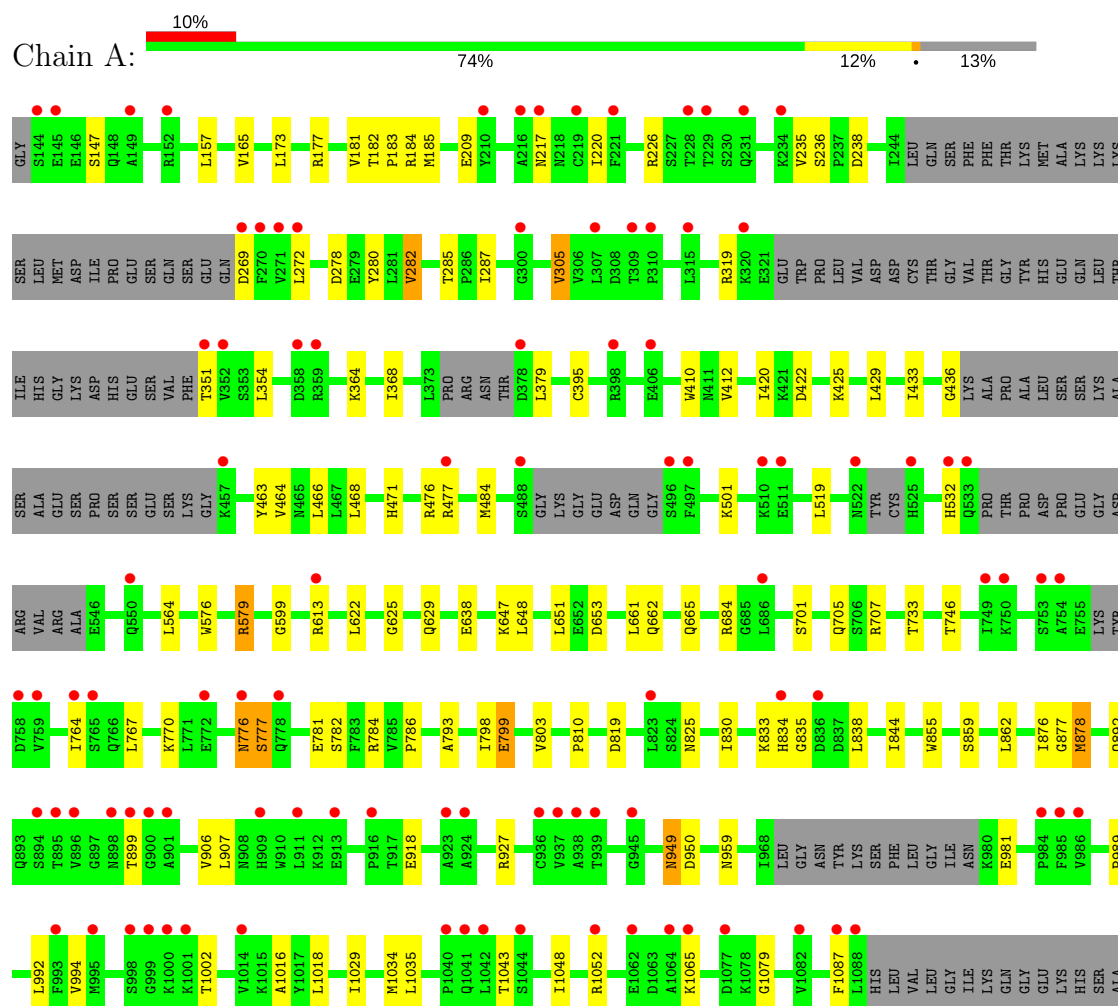
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		

### 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 ( $\text{RSRZ} > 2$ ). 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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.47Å 68.17Å 107.35Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 29.32 – 2.55	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.00-2.55) 93.5 (29.32-2.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.234 , 0.301 0.224 , 0.289	Depositor DCC
$R_{free}$ test set	1623 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6822	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 2NQ, 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	0.40	1/6886 (0.0%)	0.53	0/9317

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	918	GLU	CD-OE2	7.33	1.33	1.25

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	6744	0	6772	56	0
2	A	15	0	0	0	0
3	A	34	0	20	3	0
4	A	29	0	0	0	0
All	All	6822	0	6792	59	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.

All (59) 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:629:GLN:HG2	1:A:1029:ILE:HG13	1.49	0.93
3:A:1103:2NQ:H6	3:A:1103:2NQ:C11	2.16	0.76
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.76	0.68
3:A:1103:2NQ:H8	3:A:1103:2NQ:H6	1.77	0.67
1:A:181:VAL:O	1:A:185:MET:HG2	1.99	0.63
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.82	0.60
1:A:147:SER:OG	1:A:319:ARG:NH2	2.35	0.60
1:A:830:ILE:HD13	1:A:878:MET:HE3	1.84	0.58
1:A:653:ASP:OD1	1:A:684:ARG:NH2	2.25	0.56
1:A:220:ILE:HD11	1:A:287:ILE:HD13	1.88	0.55
1:A:799:GLU:CD	1:A:799:GLU:H	2.10	0.55
3:A:1103:2NQ:C9	3:A:1103:2NQ:C11	2.85	0.54
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.89	0.54
1:A:182:THR:HB	1:A:183:PRO:HD3	1.90	0.53
1:A:782:SER:HA	1:A:793:ALA:O	2.09	0.53
1:A:776:ASN:HD22	1:A:777:SER:N	2.07	0.52
1:A:425:LYS:HD3	1:A:638:GLU:OE1	2.09	0.52
1:A:834:HIS:CG	1:A:835:GLY:N	2.77	0.52
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.91	0.51
1:A:471:HIS:H	1:A:471:HIS:CD2	2.29	0.50
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.92	0.50
1:A:464:VAL:HB	1:A:484:MET:HG2	1.94	0.50
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.91	0.50
1:A:862:LEU:HD21	1:A:1016:ALA:HB2	1.93	0.50
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.94	0.49
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.94	0.49
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.94	0.49
1:A:855:TRP:CD2	1:A:862:LEU:HD13	2.48	0.49
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.95	0.49
1:A:157:LEU:HD21	1:A:733:THR:HA	1.96	0.48
1:A:278:ASP:HB2	1:A:784:ARG:HH12	1.78	0.48
1:A:625:GLY:O	1:A:629:GLN:HG3	2.15	0.47
1:A:810:PRO:HB3	1:A:833:LYS:HG3	1.96	0.47
1:A:949:ASN:H	1:A:949:ASN:HD22	1.60	0.47
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.96	0.46
1:A:280:TYR:HB3	1:A:282:VAL:CG2	2.46	0.46
1:A:379:LEU:HB3	1:A:436:GLY:O	2.15	0.46
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.50	0.46
1:A:648:LEU:O	1:A:651:LEU:HB2	2.16	0.46
1:A:613:ARG:O	1:A:613:ARG:HG2	2.15	0.46
1:A:235:VAL:HG12	1:A:236:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:ASP:N	1:A:950:ASP:OD1	2.51	0.44
1:A:786:PRO:HD2	1:A:878:MET:HE1	1.99	0.44
1:A:701:SER:O	1:A:705:GLN:HG2	2.18	0.44
1:A:798:ILE:H	1:A:798:ILE:HD12	1.82	0.43
1:A:576:TRP:O	1:A:579:ARG:HB2	2.17	0.43
1:A:830:ILE:HD13	1:A:878:MET:CE	2.49	0.43
1:A:422:ASP:HB3	1:A:599:GLY:O	2.17	0.43
1:A:272:LEU:HB3	1:A:305:VAL:HG21	2.00	0.43
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	2.01	0.42
1:A:907:LEU:HD23	1:A:994:VAL:HG21	2.01	0.42
1:A:287:ILE:HG13	1:A:287:ILE:H	1.70	0.42
1:A:989:PRO:HA	1:A:992:LEU:HD12	2.01	0.42
1:A:661:LEU:O	1:A:665:GLN:HG2	2.20	0.41
1:A:892:GLN:HE22	1:A:906:VAL:HB	1.85	0.41
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.60	0.41
1:A:173:LEU:O	1:A:177:ARG:HG3	2.20	0.41
1:A:767:LEU:HD22	1:A:803:VAL:HG23	2.03	0.41
1:A:1018:LEU:HD11	1:A:1065:LYS:HE2	2.03	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	814/960 (85%)	772 (95%)	37 (4%)	5 (1%)	28 46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	777	SER
1	A	825	ASN
1	A	1079	GLY

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	579	ARG

### 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	748/857 (87%)	716 (96%)	32 (4%)	33 56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	VAL
1	A	184	ARG
1	A	226	ARG
1	A	238	ASP
1	A	269	ASP
1	A	282	VAL
1	A	285	THR
1	A	305	VAL
1	A	351	THR
1	A	354	LEU
1	A	395	CYS
1	A	420	ILE
1	A	477	ARG
1	A	532	HIS
1	A	662	GLN
1	A	707	ARG
1	A	746	THR
1	A	764	ILE
1	A	770	LYS
1	A	776	ASN
1	A	781	GLU
1	A	799	GLU
1	A	819	ASP
1	A	876	ILE

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Mol	Chain	Res	Type
1	A	878	MET
1	A	899	THR
1	A	927	ARG
1	A	949	ASN
1	A	959	ASN
1	A	981	GLU
1	A	1002	THR
1	A	1087	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	HIS
1	A	391	GLN
1	A	471	HIS
1	A	662	GLN
1	A	705	GLN
1	A	734	GLN
1	A	776	ASN
1	A	949	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1010	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	1	-	4,4,4	0.16	0	6,6,6	0.05	0
3	2NQ	A	1103	-	37,38,38	2.11	7 (18%)	50,55,55	2.11	12 (24%)
2	SO4	A	2	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	A	3	-	4,4,4	0.17	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	1	-	-	0/0/0/0	0/0/0/0
3	2NQ	A	1103	-	-	0/19/27/27	0/5/5/5
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	2NQ	C2-N4	-4.81	1.34	1.42
3	A	1103	2NQ	C19-C20	-3.66	1.39	1.49
3	A	1103	2NQ	C3-S1	-3.38	1.71	1.76
3	A	1103	2NQ	C22-N1	2.27	1.35	1.32
3	A	1103	2NQ	C11-N3	2.39	1.50	1.46
3	A	1103	2NQ	O2-S1	6.42	1.50	1.43
3	A	1103	2NQ	O3-S1	6.50	1.50	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	2NQ	O3-S1-O2	-7.62	109.81	119.55
3	A	1103	2NQ	C20-C21-N1	-2.57	119.98	124.24
3	A	1103	2NQ	C16-C17-N2	-2.49	120.72	124.58
3	A	1103	2NQ	C16-C10-N3	-2.20	118.84	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	2NQ	O2-S1-C3	2.64	111.22	107.95
3	A	1103	2NQ	C17-N2-C8	2.64	121.08	116.89
3	A	1103	2NQ	C1-C20-C21	2.75	119.67	116.96
3	A	1103	2NQ	C3-S1-N4	2.84	110.48	106.83
3	A	1103	2NQ	CL1-C22-N1	2.89	120.31	115.88
3	A	1103	2NQ	C15-C10-N3	3.02	123.74	118.71
3	A	1103	2NQ	C13-N3-C11	3.73	119.47	111.57
3	A	1103	2NQ	C21-N1-C22	6.73	121.90	117.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	2NQ	3	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	834/960 (86%)	0.67	98 (11%) 5 5	42, 80, 140, 187	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	895	THR	7.5
1	A	228	THR	6.7
1	A	270	PHE	6.4
1	A	999	GLY	6.1
1	A	916	PRO	5.8
1	A	1000	LYS	5.7
1	A	1041	GLN	5.4
1	A	749	ILE	5.3
1	A	1042	LEU	5.2
1	A	764	ILE	5.2
1	A	231	GLN	5.2
1	A	998	SER	4.8
1	A	1040	PRO	4.6
1	A	216	ALA	4.6
1	A	525	HIS	4.6
1	A	533	GLN	4.6
1	A	898	ASN	4.6
1	A	315	LEU	4.5
1	A	993	PHE	4.4
1	A	986	VAL	4.3
1	A	351	THR	4.2
1	A	1065	LYS	3.8
1	A	497	PHE	3.6
1	A	924	ALA	3.6
1	A	496	SER	3.5
1	A	144	SER	3.5
1	A	758	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1062	GLU	3.3
1	A	759	VAL	3.3
1	A	1001	LYS	3.2
1	A	894	SER	3.1
1	A	271	VAL	3.1
1	A	909	HIS	3.1
1	A	145	GLU	3.1
1	A	532	HIS	3.0
1	A	937	VAL	3.0
1	A	995	MET	3.0
1	A	1088	LEU	3.0
1	A	320	LYS	3.0
1	A	511	GLU	3.0
1	A	985	PHE	2.9
1	A	269	ASP	2.9
1	A	923	ALA	2.9
1	A	229	THR	2.9
1	A	217	ASN	2.9
1	A	307	LEU	2.9
1	A	152	ARG	2.8
1	A	359	ARG	2.8
1	A	899	THR	2.8
1	A	221	PHE	2.7
1	A	1064	ALA	2.7
1	A	753	SER	2.7
1	A	823	LEU	2.7
1	A	939	THR	2.7
1	A	310	PRO	2.7
1	A	352	VAL	2.6
1	A	936	CYS	2.6
1	A	754	ALA	2.5
1	A	913	GLU	2.6
1	A	896	VAL	2.5
1	A	1087	PHE	2.5
1	A	488	SER	2.5
1	A	938	ALA	2.5
1	A	358	ASP	2.5
1	A	772	GLU	2.5
1	A	477	ARG	2.5
1	A	1077	ASP	2.5
1	A	522	ASN	2.4
1	A	778	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1014	VAL	2.3
1	A	219	CYS	2.3
1	A	210	TYR	2.3
1	A	510	LYS	2.3
1	A	901	ALA	2.3
1	A	309	THR	2.3
1	A	272	LEU	2.3
1	A	234	LYS	2.3
1	A	750	LYS	2.3
1	A	776	ASN	2.3
1	A	1052	ARG	2.2
1	A	398	ARG	2.2
1	A	836	ASP	2.2
1	A	900	GLY	2.2
1	A	378	ASP	2.2
1	A	765	SER	2.2
1	A	457	LYS	2.2
1	A	1082	VAL	2.1
1	A	300	GLY	2.1
1	A	834	HIS	2.1
1	A	911	LEU	2.1
1	A	550	GLN	2.1
1	A	613	ARG	2.1
1	A	1044	SER	2.0
1	A	686	LEU	2.0
1	A	149	ALA	2.0
1	A	945	GLY	2.0
1	A	406	GLU	2.0
1	A	984	PRO	2.0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	A	3	5/5	0.86	0.27	4.73	115,115,115,115	0
2	SO4	A	2	5/5	0.93	0.18	0.65	74,75,76,76	0
3	2NQ	A	1103	34/34	0.94	0.14	-0.55	73,74,75,75	0
2	SO4	A	1	5/5	0.90	0.15	-0.97	117,117,117,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.