



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:54 AM GMT

PDB ID : 3QAQ
Title : Crystal structure of PI3K-gamma in complex with triazine-benzimidazole 1
Authors : Whittington, D.A.; Tang, J.; Yakowec, P.
Deposited on : 2011-01-11
Resolution : 2.90 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
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

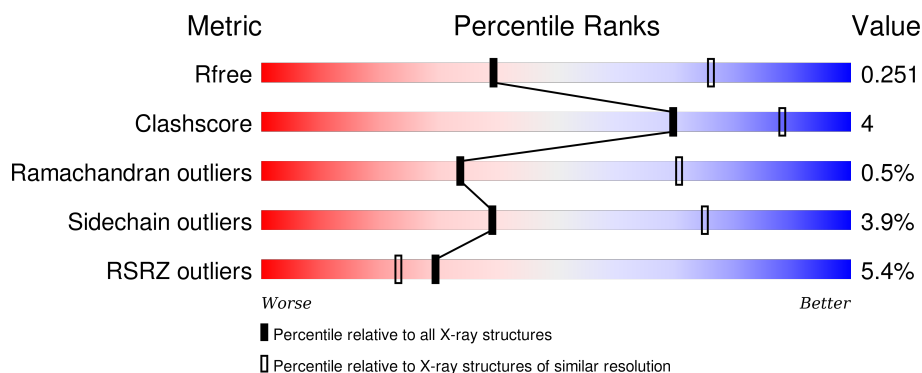
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	960	<div> <div>5%</div> <div>74%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6828 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	837	Total	C	N	O	S	0	0	0
			6773	4350	1155	1234	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: SO4) (formula: O₄S).



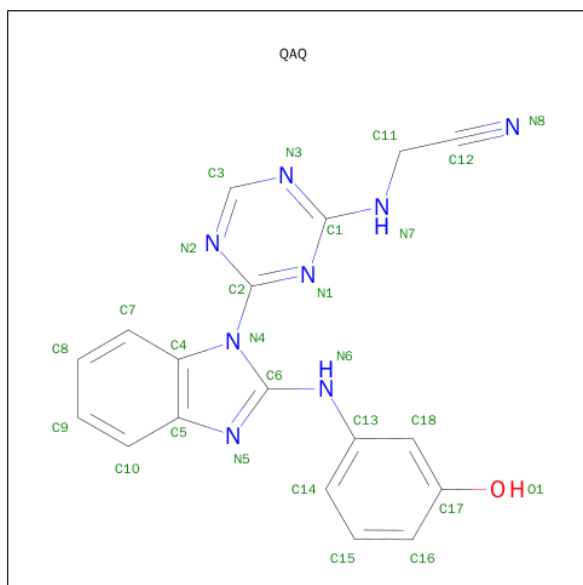
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is [(4-{2-[(3-HYDROXYPHENYL)AMINO]-1H-BENZIMIDAZOL-1-YL}-1,3,5-TRIAZIN-2-YL)AMINO]ACETONITRILE (three-letter code: QAQ) (formula: C₁₈H₁₄N₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	18	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.40 Å 68.58 Å 106.50 Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.90) 99.6 (29.48-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.265 0.205 , 0.251	Depositor DCC
R_{free} test set	1688 reflections (7.79%)	DCC
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23343 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6828	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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: QAQ, 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	0.57	6/6915 (0.1%)	0.53	1/9352 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	918	GLU	CD-OE1	31.13	1.59	1.25
1	A	918	GLU	CD-OE2	10.39	1.37	1.25
1	A	905	GLU	CD-OE1	8.68	1.35	1.25
1	A	904	ASP	CG-OD2	7.74	1.43	1.25
1	A	905	GLU	CD-OE2	7.36	1.33	1.25
1	A	904	ASP	CG-OD1	6.18	1.39	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	918	GLU	OE1-CD-OE2	6.25	130.80	123.30

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	6773	0	6812	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	0	0
3	A	27	0	13	1	0
4	A	13	0	0	0	0
All	All	6828	0	6825	61	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 (61) 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:564:LEU:HD11	1:A:1048:ILE:HG22	1.79	0.65
1:A:947:ARG:NH2	1:A:963:ILE:O	2.30	0.64
1:A:799:GLU:CD	1:A:799:GLU:H	2.00	0.64
1:A:707:ARG:HA	1:A:710:GLN:OE1	1.99	0.63
1:A:497:PHE:HE2	1:A:1045:LYS:HG3	1.65	0.61
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.81	0.60
1:A:947:ARG:HH11	1:A:948:HIS:HE1	1.49	0.60
1:A:1000:LYS:HA	1:A:1076:ARG:HH22	1.67	0.59
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.83	0.59
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.87	0.56
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.35	0.56
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.88	0.55
1:A:576:TRP:O	1:A:579:ARG:HB2	2.06	0.55
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.89	0.55
1:A:947:ARG:NH2	1:A:964:ASP:O	2.40	0.54
1:A:707:ARG:H	1:A:707:ARG:HH11	1.57	0.53
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.91	0.53
1:A:782:SER:HA	1:A:793:ALA:O	2.10	0.52
1:A:240:THR:HG23	1:A:243:ALA:H	1.75	0.52
1:A:181:VAL:O	1:A:185:MET:HG2	2.08	0.52
1:A:639:ASN:O	1:A:643:ILE:HG23	2.10	0.51
1:A:354:LEU:HD12	1:A:527:ILE:HG22	1.91	0.51
1:A:629:GLN:HG3	1:A:1029:ILE:HG13	1.94	0.50
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.95	0.49
1:A:758:ASP:N	1:A:809:LYS:HZ1	2.10	0.48
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.96	0.48
1:A:931:SER:HB3	1:A:960:LEU:HB3	1.96	0.48
1:A:908:ASN:HA	1:A:911:LEU:HD12	1.97	0.47
1:A:995:MET:O	1:A:1005:HIS:HB2	2.15	0.47
3:A:1103:QAA:N6	3:A:1103:QAA:N2	2.61	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:SD	1:A:282:VAL:HG21	2.56	0.46
1:A:467:LEU:O	1:A:476:ARG:HD2	2.16	0.45
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.49	0.45
1:A:701:SER:O	1:A:705:GLN:HG2	2.17	0.45
1:A:483:HIS:CD2	1:A:510:LYS:HD3	2.52	0.45
1:A:355:TRP:HA	1:A:421:LYS:HB2	1.99	0.45
1:A:640:VAL:O	1:A:643:ILE:HG12	2.17	0.44
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.98	0.44
1:A:624:VAL:O	1:A:628:MET:HG2	2.18	0.44
1:A:487:ILE:HG22	1:A:488:SER:N	2.32	0.44
1:A:370:ILE:HD12	1:A:371:PRO:HD2	1.99	0.43
1:A:921:PHE:O	1:A:925:VAL:HG23	2.18	0.43
1:A:497:PHE:HZ	1:A:1045:LYS:HE3	1.83	0.43
1:A:776:ASN:HD22	1:A:777:SER:H	1.67	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.19	0.43
1:A:915:SER:HA	1:A:916:PRO:HD3	1.90	0.42
1:A:777:SER:HA	1:A:778:GLN:HA	1.67	0.42
1:A:589:TYR:O	1:A:593:PHE:HD1	2.02	0.42
1:A:629:GLN:HG2	1:A:1029:ILE:CD1	2.49	0.42
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.19	0.42
1:A:432:GLN:HB3	1:A:460:LEU:HD11	2.01	0.42
1:A:843:LEU:HD13	1:A:1034:MET:HG3	2.02	0.42
1:A:158:ILE:HG23	1:A:717:LEU:HD23	2.02	0.41
1:A:947:ARG:NH1	1:A:948:HIS:HE1	2.16	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.20	0.41
1:A:278:ASP:HB2	1:A:784:ARG:HH12	1.85	0.41
1:A:901:ALA:HA	1:A:902:PHE:CD1	2.56	0.41
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.04	0.40
1:A:707:ARG:H	1:A:707:ARG:NH1	2.18	0.40
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.96	0.40
1:A:779:LEU:HD23	1:A:780:PRO:O	2.21	0.40

There are no symmetry-related clashes.

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	815/960 (85%)	764 (94%)	47 (6%)	4 (0%)	34 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	ARG
1	A	145	GLU
1	A	896	VAL
1	A	759	VAL

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	751/857 (88%)	722 (96%)	29 (4%)	39 75

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
1	A	235	VAL
1	A	269	ASP
1	A	305	VAL
1	A	354	LEU
1	A	381	VAL
1	A	395	CYS
1	A	459	GLN
1	A	470	ASP
1	A	544	ARG
1	A	555	LEU
1	A	662	GLN
1	A	683	LYS
1	A	707	ARG
1	A	769	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	776	ASN
1	A	823	LEU
1	A	824	SER
1	A	841	ASP
1	A	865	LEU
1	A	875	LYS
1	A	902	PHE
1	A	909	HIS
1	A	931	SER
1	A	948	HIS
1	A	959	ASN
1	A	981	GLU
1	A	982	ARG
1	A	1039	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	389	HIS
1	A	391	GLN
1	A	577	HIS
1	A	734	GLN
1	A	743	GLN
1	A	773	ASN
1	A	776	ASN
1	A	951	ASN
1	A	959	ASN

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	0.18	0	6,6,6	0.16	0
3	QAQ	A	1103	-	28,30,30	1.43	3 (10%)	31,41,41	2.94	8 (25%)
2	SO4	A	2	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	A	3	-	4,4,4	0.20	0	6,6,6	0.12	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	QAQ	A	1103	-	-	0/5/12/12	0/4/4/4
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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	QAQ	C4-N4	-3.90	1.34	1.39
3	A	1103	QAQ	C13-N6	-2.93	1.34	1.40
3	A	1103	QAQ	C2-N2	3.18	1.34	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	QAQ	N3-C1-N1	-6.81	119.42	126.67
3	A	1103	QAQ	N2-C2-N1	-6.32	118.51	126.44
3	A	1103	QAQ	N2-C3-N3	-4.92	120.37	128.67
3	A	1103	QAQ	C11-C12-N8	-3.55	172.93	177.99
3	A	1103	QAQ	N2-C2-N4	2.54	119.29	115.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	QAQ	N7-C1-N1	2.80	122.47	117.21
3	A	1103	QAQ	C2-N1-C1	6.72	120.10	114.04
3	A	1103	QAQ	C3-N2-C2	8.51	121.13	114.06

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
3	A	1103	QAQ	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

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, 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	837/960 (87%)	0.15	45 (5%)	29 23	52, 93, 140, 175	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	998	SER	6.8
1	A	916	PRO	4.9
1	A	532	HIS	4.8
1	A	895	THR	4.4
1	A	497	PHE	4.2
1	A	320	LYS	4.0
1	A	488	SER	4.0
1	A	351	THR	3.8
1	A	525	HIS	3.8
1	A	533	GLN	3.7
1	A	228	THR	3.7
1	A	1043	THR	3.6
1	A	270	PHE	3.5
1	A	1042	LEU	3.4
1	A	936	CYS	3.2
1	A	248	PHE	3.2
1	A	999	GLY	3.1
1	A	894	SER	3.1
1	A	759	VAL	3.1
1	A	319	ARG	3.0
1	A	457	LYS	3.0
1	A	986	VAL	3.0
1	A	145	GLU	2.8
1	A	356	ASP	2.8
1	A	924	ALA	2.8
1	A	511	GLU	2.7
1	A	496	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	231	GLN	2.7
1	A	1000	LYS	2.6
1	A	526	PRO	2.6
1	A	900	GLY	2.6
1	A	378	ASP	2.4
1	A	1041	GLN	2.4
1	A	754	ALA	2.2
1	A	1001	LYS	2.2
1	A	957	THR	2.2
1	A	148	GLN	2.2
1	A	321	GLU	2.2
1	A	309	THR	2.2
1	A	1040	PRO	2.2
1	A	985	PHE	2.1
1	A	967	HIS	2.1
1	A	530	PRO	2.0
1	A	945	GLY	2.0
1	A	144	SER	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
3	QAQ	A	1103	27/27	0.92	0.24	1.50	87,89,92,93	0
2	SO4	A	3	5/5	0.94	0.22	1.47	135,135,135,136	0
2	SO4	A	1	5/5	0.92	0.14	-1.24	124,125,125,125	0
2	SO4	A	2	5/5	0.94	0.11	-1.62	116,117,117,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.