Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:08 PM GMT

PDB ID	:	4WWO
Title	:	Crystal structure of human PI3K-gamma in complex with phenylquinoline inhibitor N-{(1S)-1-[8-chloro-2-(3-fluorophenyl)quinolin-3-yl]ethyl}-9H-purin-6-amine
Authors	:	Whittington, D.A.; Tang, J.; Yakowec, P.
Deposited on	:	2014-11-11
Resolution	:	2.30 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 (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 2.30 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		0.267
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		2.6%
RSRZ outliers		15.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
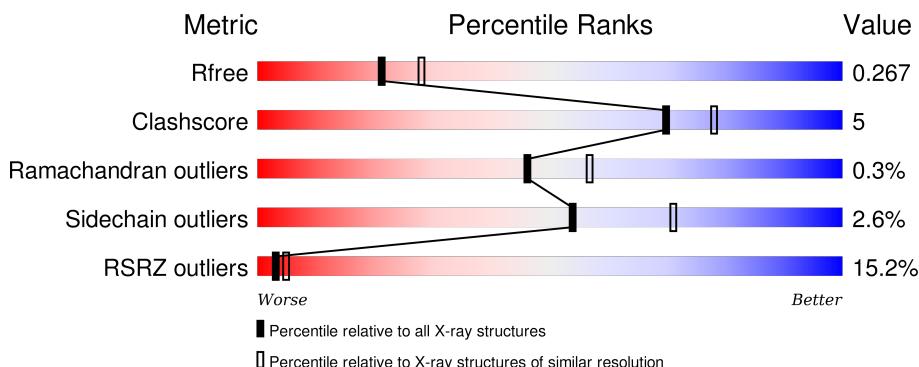
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	13% — 75% — 9% · 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6732 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	814	Total 6594	C 4239	N 1125	O 1196	S 34	0	0	0

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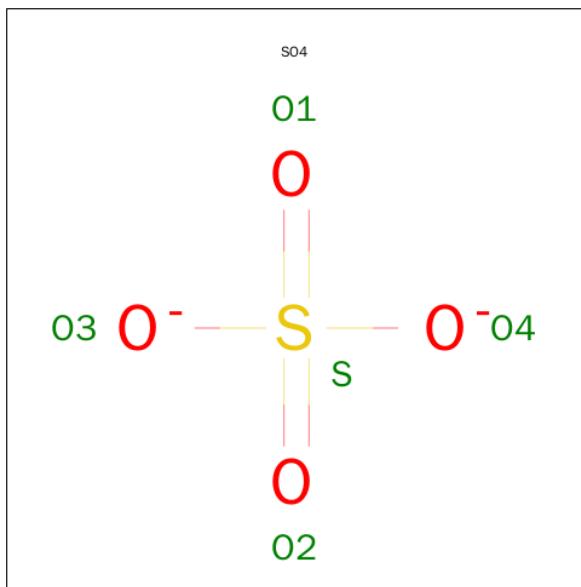
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

- Molecule 3 is N-{(1S)-1-[8-chloro-2-(3-fluorophenyl)quinolin-3-yl]ethyl}-9H-purin-6-amine

(three-letter code: 3VD) (formula: $C_{22}H_{16}ClFN_6$).
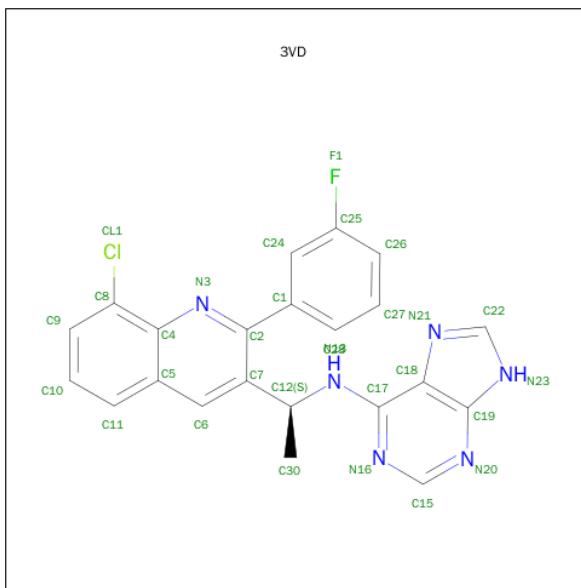
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	0	0
			30	22	1	1	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total	O	0	0
			88	88		

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
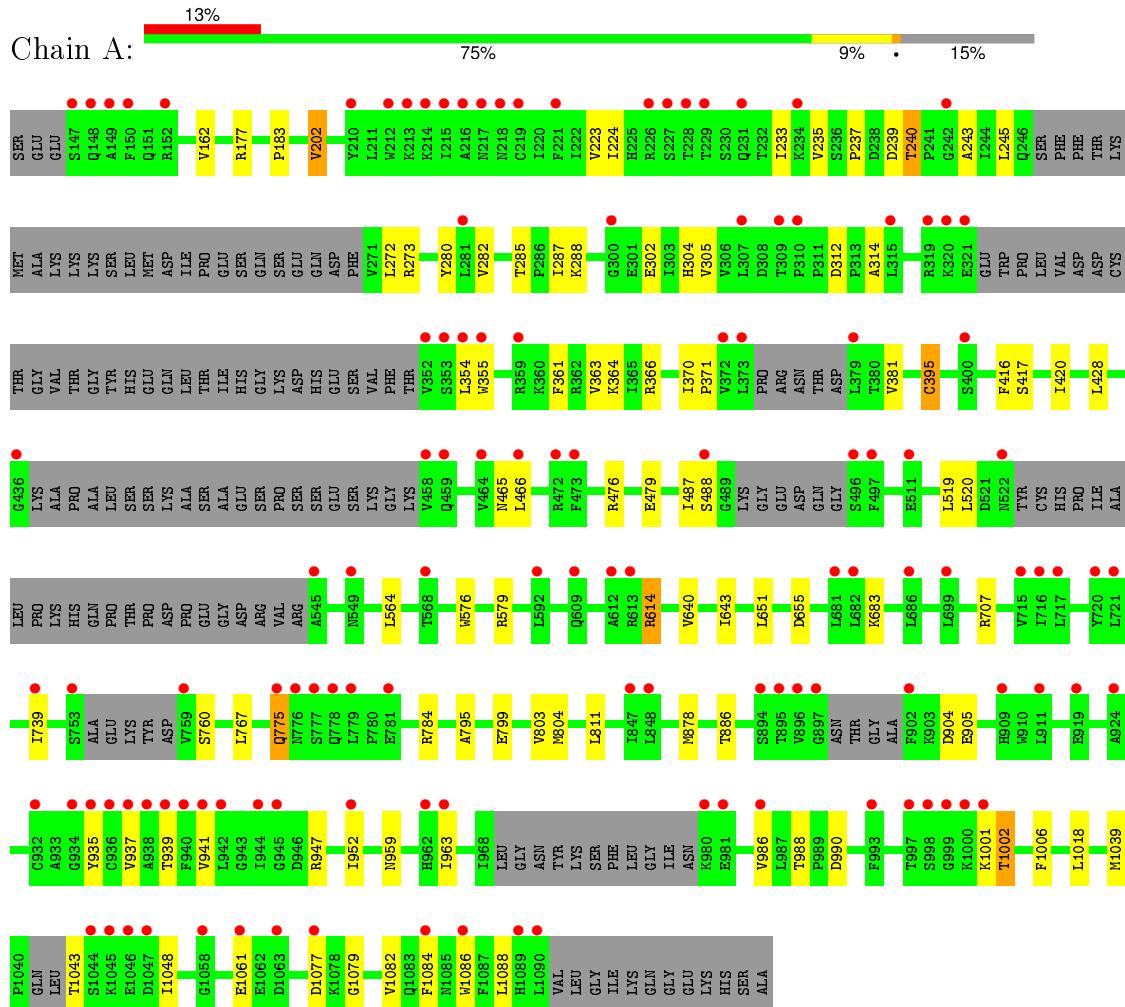
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	145.90Å 68.17Å 107.38Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 28.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.30) 99.6 (28.81-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.21 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.274 0.215 , 0.267	Depositor DCC
R_{free} test set	2350 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.6	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 46680 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6732	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: 3VD, 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	0.53	1/6732 (0.0%)	0.60	0/9104

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	TRP	CD2-CE2	5.45	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	6594	0	6647	60	0
2	A	20	0	0	0	0
3	A	30	0	16	1	0
4	A	88	0	0	1	0
All	All	6732	0	6663	60	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.

All (60) 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:767:LEU:HD22	1:A:803:VAL:HG23	1.50	0.91
1:A:272:LEU:HB3	1:A:305:VAL:HG21	1.55	0.86
1:A:1018:LEU:HD22	1:A:1061:GLU:OE1	1.87	0.74
1:A:947:ARG:NH2	1:A:963:ILE:O	2.24	0.71
1:A:240:THR:HG23	1:A:243:ALA:H	1.56	0.71
1:A:202:VAL:CG2	1:A:285:THR:HG21	2.23	0.69
1:A:223:VAL:O	1:A:305:VAL:HG12	1.97	0.65
1:A:162:VAL:HG12	1:A:177:ARG:HD2	1.79	0.65
1:A:202:VAL:HG21	1:A:285:THR:HG21	1.79	0.64
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.24	0.64
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.79	0.64
1:A:363:VAL:HG23	1:A:520:LEU:HD23	1.81	0.62
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.81	0.62
1:A:366:ARG:NH1	1:A:479:GLU:OE1	2.38	0.56
1:A:803:VAL:HG22	1:A:811:LEU:HD23	1.89	0.55
1:A:1002:THR:HG22	1:A:1006:PHE:CD2	2.42	0.54
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.90	0.53
1:A:272:LEU:HD22	1:A:305:VAL:CG1	2.38	0.53
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.90	0.53
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.44	0.52
1:A:370:ILE:HD12	1:A:371:PRO:HD2	1.91	0.51
1:A:937:VAL:O	1:A:941:VAL:HG23	2.12	0.50
1:A:245:LEU:HD11	1:A:272:LEU:HG	1.93	0.49
1:A:1082:VAL:HG12	1:A:1086:TRP:CD1	2.48	0.48
1:A:1001:LYS:O	1:A:1002:THR:HG23	2.13	0.48
1:A:739:ILE:HD12	1:A:739:ILE:C	2.34	0.48
1:A:202:VAL:HG22	1:A:285:THR:HG21	1.94	0.47
1:A:366:ARG:NH1	1:A:519:LEU:HB2	2.29	0.47
1:A:804:MET:HB2	3:A:1205:3VD:C9	2.45	0.46
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.96	0.46
1:A:273:ARG:O	1:A:305:VAL:HG23	2.15	0.46
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.97	0.46
1:A:361:PHE:HA	1:A:420:ILE:CD1	2.46	0.46
1:A:904:ASP:O	1:A:990:ASP:HA	2.16	0.46
1:A:224:ILE:HD12	1:A:233:ILE:HD13	1.97	0.46
1:A:1002:THR:HG22	1:A:1006:PHE:CE2	2.50	0.45
1:A:235:VAL:HG13	1:A:239:ASP:HB2	1.99	0.45
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.35	0.45
1:A:935:TYR:O	1:A:939:THR:HG23	2.16	0.45
1:A:287:ILE:HD12	1:A:288:LYS:N	2.32	0.45
1:A:302:GLU:HG3	1:A:304:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG22	1:A:235:VAL:HG23	1.99	0.44
1:A:952:ILE:HD11	1:A:986:VAL:HG21	1.98	0.44
1:A:162:VAL:CG1	1:A:177:ARG:HD2	2.47	0.44
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.17	0.44
1:A:395:CYS:SG	1:A:417:SER:OG	2.75	0.43
1:A:614:ARG:HG2	1:A:614:ARG:O	2.17	0.43
1:A:1084:PHE:CZ	1:A:1088:LEU:HD11	2.53	0.43
1:A:272:LEU:CB	1:A:305:VAL:HG21	2.39	0.42
1:A:640:VAL:O	1:A:643:ILE:HG12	2.18	0.42
1:A:428:LEU:HD22	1:A:465:ASN:HB3	2.01	0.42
1:A:487:ILE:CG2	1:A:488:SER:N	2.82	0.41
1:A:683:LYS:NZ	4:A:1374:HOH:O	2.36	0.41
1:A:487:ILE:HG22	1:A:488:SER:N	2.35	0.41
1:A:361:PHE:HD2	1:A:416:PHE:CD1	2.39	0.41
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	2.02	0.41
1:A:775:GLN:OE1	1:A:795:ALA:HB1	2.20	0.41
1:A:878:MET:HB2	1:A:878:MET:HE2	2.00	0.41
1:A:476:ARG:HG2	1:A:520:LEU:HD12	2.03	0.41
1:A:364:LYS:HB3	1:A:519:LEU:HB3	2.01	0.41

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	792/959 (83%)	761 (96%)	29 (4%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1079	GLY
1	A	760	SER

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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	732/857 (85%)	713 (97%)	19 (3%)	54 71

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	A	202	VAL
1	A	240	THR
1	A	354	LEU
1	A	381	VAL
1	A	395	CYS
1	A	614	ARG
1	A	707	ARG
1	A	775	GLN
1	A	784	ARG
1	A	799	GLU
1	A	886	THR
1	A	905	GLU
1	A	959	ASN
1	A	988	THR
1	A	1002	THR
1	A	1039	MET
1	A	1043	THR
1	A	1077	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	846	GLN
1	A	959	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)

5 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	0.46	0	6,6,6	0.13	0
2	SO4	A	1202	-	4,4,4	0.47	0	6,6,6	0.27	0
2	SO4	A	1203	-	4,4,4	0.52	0	6,6,6	0.27	0
2	SO4	A	1204	-	4,4,4	0.53	0	6,6,6	0.31	0
3	3VD	A	1205	-	29,34,34	2.13	5 (17%)	33,49,49	2.75	10 (30%)

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
2	SO4	A	1203	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1204	-	-	0/0/0/0	0/0/0/0
3	3VD	A	1205	-	-	0/11/12/12	0/5/5/5

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All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1205	3VD	C1-C2	-9.45	1.38	1.49
3	A	1205	3VD	C8-C4	-2.25	1.40	1.42
3	A	1205	3VD	C19-N20	-2.07	1.33	1.37
3	A	1205	3VD	C7-C12	2.11	1.54	1.52
3	A	1205	3VD	C6-C7	2.25	1.39	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1205	3VD	N20-C15-N16	-8.62	122.29	128.89
3	A	1205	3VD	C30-C12-C7	-4.57	106.88	111.40
3	A	1205	3VD	C19-C18-N21	-2.88	106.83	109.48
3	A	1205	3VD	C24-C1-C2	-2.66	115.61	120.05
3	A	1205	3VD	C26-C25-C24	-2.43	120.21	123.35
3	A	1205	3VD	C5-C4-N3	-2.35	119.35	122.64
3	A	1205	3VD	C28-C1-C2	2.06	123.81	120.60
3	A	1205	3VD	C2-N3-C4	4.60	121.59	118.15
3	A	1205	3VD	C4-C8-CL1	6.03	122.26	118.80
3	A	1205	3VD	C15-N16-C17	6.57	121.21	116.48

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	1205	3VD	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	814/959 (84%)	0.92	124 (15%) [3] [5]		37, 76, 133, 178	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	9.0
1	A	895	THR	8.3
1	A	226	ARG	8.1
1	A	228	THR	8.0
1	A	458	VAL	7.2
1	A	545	ALA	7.1
1	A	980	LYS	6.9
1	A	1089	HIS	6.6
1	A	511	GLU	6.3
1	A	777	SER	5.9
1	A	231	GLN	5.8
1	A	999	GLY	5.8
1	A	759	VAL	5.6
1	A	778	GLN	5.5
1	A	147	SER	5.3
1	A	152	ARG	5.2
1	A	1058	GLY	5.2
1	A	993	PHE	5.1
1	A	379	LEU	5.1
1	A	227	SER	5.1
1	A	221	PHE	5.0
1	A	937	VAL	4.8
1	A	1000	LYS	4.6
1	A	779	LEU	4.6
1	A	896	VAL	4.5
1	A	436	GLY	4.4
1	A	986	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	234	LYS	4.3
1	A	352	VAL	4.2
1	A	217	ASN	4.2
1	A	894	SER	4.2
1	A	938	ALA	4.2
1	A	717	LEU	4.1
1	A	1077	ASP	4.1
1	A	315	LEU	4.1
1	A	613	ARG	4.0
1	A	353	SER	4.0
1	A	355	TRP	4.0
1	A	310	PRO	3.9
1	A	215	ILE	3.9
1	A	149	ALA	3.8
1	A	497	PHE	3.8
1	A	998	SER	3.7
1	A	945	GLY	3.7
1	A	776	ASN	3.7
1	A	320	LYS	3.7
1	A	150	PHE	3.7
1	A	229	THR	3.6
1	A	1090	LEU	3.5
1	A	148	GLN	3.5
1	A	941	VAL	3.4
1	A	522	ASN	3.4
1	A	936	CYS	3.3
1	A	307	LEU	3.3
1	A	1044	SER	3.2
1	A	359	ARG	3.2
1	A	939	THR	3.2
1	A	720	TYR	3.1
1	A	716	ILE	3.1
1	A	944	ILE	3.1
1	A	373	LEU	3.0
1	A	300	GLY	3.0
1	A	592	LEU	3.0
1	A	459	GLN	2.9
1	A	781	GLU	2.9
1	A	473	PHE	2.9
1	A	942	LEU	2.9
1	A	699	LEU	2.9
1	A	682	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	911	LEU	2.8
1	A	319	ARG	2.8
1	A	686	LEU	2.7
1	A	715	VAL	2.7
1	A	739	ILE	2.7
1	A	372	VAL	2.7
1	A	354	LEU	2.7
1	A	212	TRP	2.7
1	A	924	ALA	2.7
1	A	464	VAL	2.7
1	A	934	GLY	2.6
1	A	466	LEU	2.6
1	A	902	PHE	2.6
1	A	935	TYR	2.6
1	A	309	THR	2.5
1	A	1046	GLU	2.5
1	A	1045	LYS	2.5
1	A	775	GLN	2.5
1	A	919	GLU	2.5
1	A	997	THR	2.5
1	A	472	ARG	2.4
1	A	940	PHE	2.4
1	A	1001	LYS	2.4
1	A	321	GLU	2.4
1	A	549	ASN	2.4
1	A	612	ALA	2.4
1	A	897	GLY	2.4
1	A	219	CYS	2.4
1	A	218	ASN	2.3
1	A	1063	ASP	2.3
1	A	952	ILE	2.3
1	A	1047	ASP	2.3
1	A	932	CYS	2.3
1	A	909	HIS	2.3
1	A	214	LYS	2.2
1	A	1086	TRP	2.2
1	A	210	TYR	2.2
1	A	681	LEU	2.2
1	A	1084	PHE	2.2
1	A	847	ILE	2.2
1	A	962	HIS	2.2
1	A	609	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	721	LEU	2.1
1	A	963	ILE	2.1
1	A	568	THR	2.1
1	A	848	LEU	2.1
1	A	213	LYS	2.1
1	A	1061	GLU	2.1
1	A	981	GLU	2.0
1	A	281	LEU	2.0
1	A	400	SER	2.0
1	A	488	SER	2.0
1	A	753	SER	2.0
1	A	242	GLY	2.0
1	A	496	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
2	SO4	A	1202	5/5	0.95	0.18	-0.34	61,65,85,87	0
2	SO4	A	1203	5/5	0.94	0.15	-0.59	78,79,91,102	0
2	SO4	A	1201	5/5	0.95	0.15	-0.60	68,86,90,90	0
3	3VD	A	1205	30/30	0.93	0.14	-0.63	54,64,77,95	0
2	SO4	A	1204	5/5	0.89	0.15	-2.70	77,85,109,112	0

6.5 Other polymers (i)

There are no such residues in this entry.