Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:58 am BST

PDB ID	:	1W2F
Title	:	Human Inositol (1,4,5)-trisphosphate 3-kinase substituted with selenomethionine
Authors	:	Gonzalez, B.; Schell, M.J.; Irvine, R.F.; Williams, R.L.
Deposited on	:	2004-07-01
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

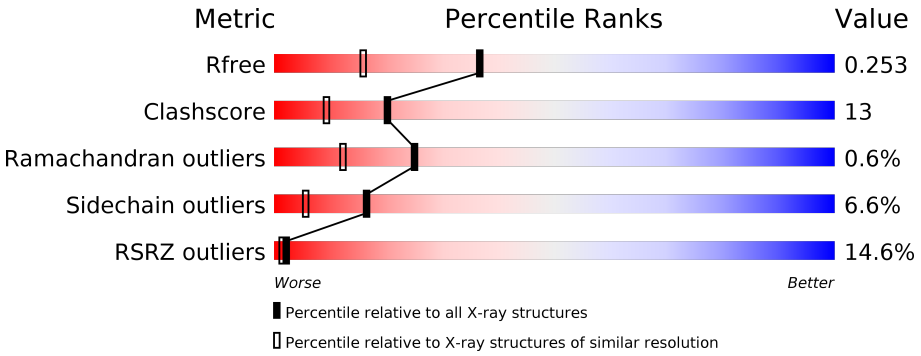
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. 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	276	8% 73% 24% .
1	B	276	20% 66% 30% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4690 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.

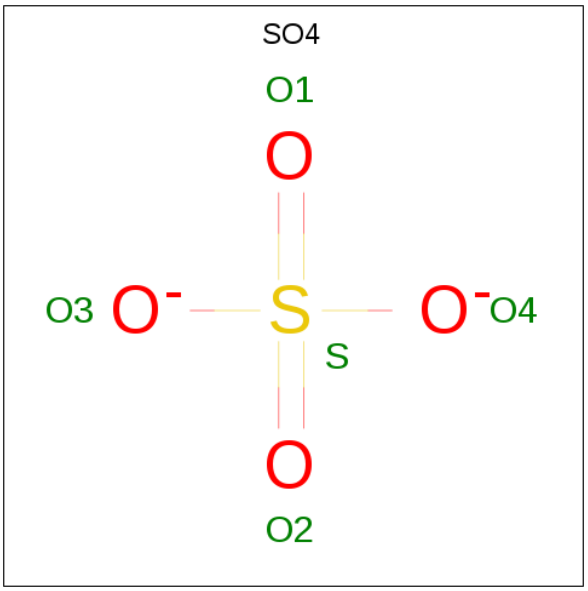
- Molecule 1 is a protein called INOSITOL-TRISPHOSPHATE 3-KINASE A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	Se	0	0	0
			2215	1386	403	413	7	6			
1	B	272	Total	C	N	O	S	Se	0	0	0
			2190	1372	397	408	7	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	SER	ALA	conflict	UNP P23677
B	187	SER	ALA	conflict	UNP P23677

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

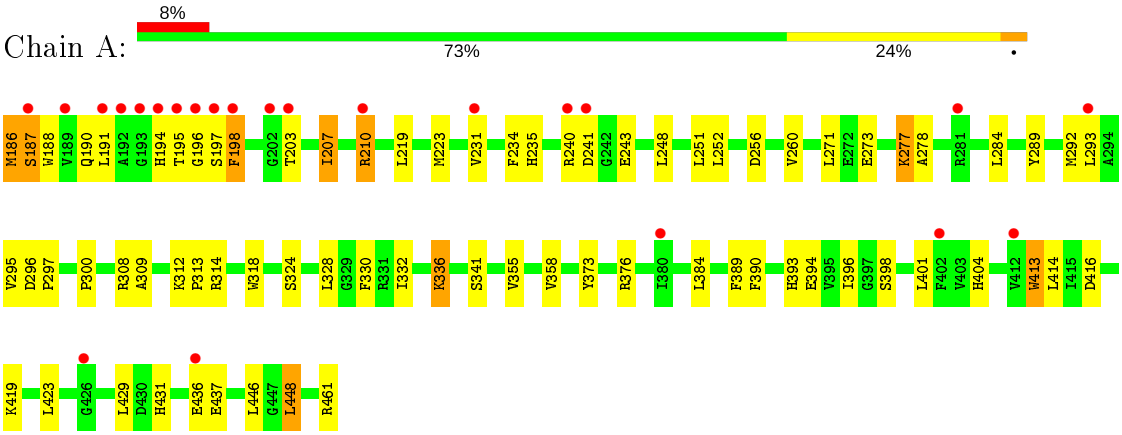
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	145	Total O 145 145	0	0
3	B	120	Total O 120 120	0	0

3 Residue-property plots (i)

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.

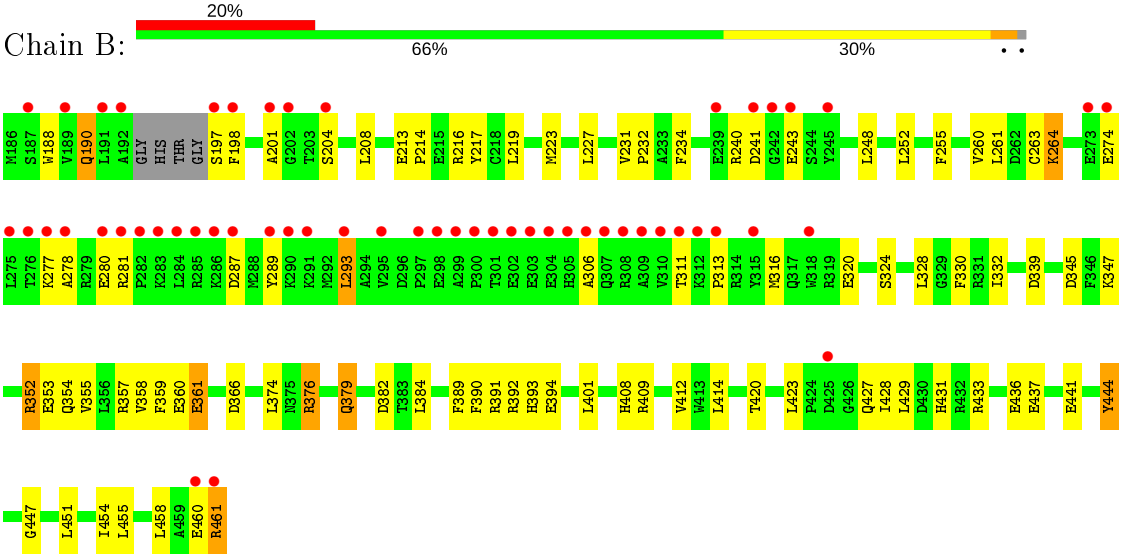
• Molecule 1: INOSITOL-TRISPHOSPHATE 3-KINASE A

Chain A:



• Molecule 1: INOSITOL-TRISPHOSPHATE 3-KINASE A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.30Å 95.80Å 180.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 1.80 45.09 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.5 (45.17-1.80) 91.5 (45.09-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.241 0.372 , 0.253	Depositor DCC
R_{free} test set	4887 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 35.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4690	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: 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	1.05	1/2253 (0.0%)	0.94	3/3025 (0.1%)
1	B	0.99	3/2226 (0.1%)	0.95	6/2987 (0.2%)
All	All	1.02	4/4479 (0.1%)	0.94	9/6012 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	CYS	CB-SG	-5.96	1.72	1.81
1	B	444	TYR	CD2-CE2	-5.94	1.30	1.39
1	B	444	TYR	CD1-CE1	-5.56	1.31	1.39
1	A	413	TRP	CB-CG	-5.53	1.40	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	352	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	376	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	296	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	241	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	287	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	376	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	382	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	256	ASP	CB-CG-OD2	5.08	122.87	118.30

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	2215	0	2190	51	0
1	B	2190	0	2169	61	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	A	145	0	0	3	0
3	B	120	0	0	1	1
All	All	4690	0	4359	110	1

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 13.

All (110) 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:B:376:ARG:HH11	1:B:379:GLN:HE22	1.23	0.87
1:A:390:PHE:CE2	1:A:431:HIS:CD2	2.67	0.82
1:B:358:VAL:O	1:B:361:GLU:HG3	1.85	0.76
1:B:423:LEU:HD11	1:B:429:LEU:HG	1.71	0.72
1:B:289:TYR:CE2	1:B:293:LEU:HD21	2.26	0.71
1:B:289:TYR:CE1	1:B:293:LEU:HD11	2.27	0.70
1:A:373:TYR:OH	1:A:404:HIS:HD2	1.76	0.68
1:B:217:TYR:CE2	1:B:393:HIS:HE1	2.13	0.66
1:B:217:TYR:OH	1:B:393:HIS:HE1	1.77	0.65
1:A:188:TRP:HB3	1:A:252:LEU:HG	1.81	0.62
1:B:289:TYR:CZ	1:B:293:LEU:HD21	2.36	0.61
1:A:390:PHE:CE2	1:A:431:HIS:HD2	2.18	0.61
1:A:404:HIS:HE1	3:A:2101:HOH:O	1.83	0.61
1:B:217:TYR:OH	1:B:393:HIS:CE1	2.54	0.60
1:B:190:GLN:HG3	1:B:198:PHE:CG	2.37	0.59
1:B:366:ASP:OD2	1:B:408:HIS:HD2	1.85	0.59
1:B:392:ARG:HD2	1:B:427:GLN:O	2.03	0.58
1:A:436:GLU:O	1:A:437:GLU:C	2.42	0.57
1:A:190:GLN:HG2	1:A:198:PHE:CE1	2.40	0.57
1:B:217:TYR:CZ	1:B:393:HIS:HE1	2.22	0.57
1:A:389:PHE:CD1	1:A:393:HIS:CE1	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ILE:HD13	1:A:358:VAL:HG11	1.88	0.56
1:A:373:TYR:OH	1:A:404:HIS:CD2	2.57	0.56
1:B:460:GLU:O	1:B:461:ARG:C	2.44	0.55
1:A:195:THR:HG21	1:A:210:ARG:HD2	1.89	0.54
1:B:231:VAL:HG12	1:B:414:LEU:HB2	1.89	0.54
1:A:190:GLN:HG2	1:A:198:PHE:CD1	2.43	0.54
1:A:195:THR:HG21	1:A:210:ARG:CD	2.38	0.53
1:A:191:LEU:HD11	1:A:336:LYS:HD3	1.90	0.52
1:A:292:MSE:HE2	1:A:300:PRO:HG3	1.91	0.52
1:B:217:TYR:CE2	1:B:393:HIS:CE1	2.96	0.52
1:A:235:HIS:HE1	3:A:2018:HOH:O	1.92	0.52
1:B:332:ILE:HD13	1:B:358:VAL:HG11	1.92	0.51
1:B:444:TYR:C	1:B:444:TYR:CD2	2.84	0.51
1:A:332:ILE:HD13	1:A:358:VAL:CG1	2.42	0.49
1:A:390:PHE:CZ	1:A:431:HIS:CD2	3.00	0.49
1:B:217:TYR:HE2	1:B:393:HIS:CE1	2.31	0.49
1:A:330:PHE:CZ	1:A:355:VAL:HG11	2.48	0.49
1:B:394:GLU:O	1:B:420:THR:HA	2.13	0.48
1:B:278:ALA:HB2	1:B:313:PRO:HG2	1.96	0.48
1:A:187:SER:OG	1:A:190:GLN:NE2	2.46	0.48
1:B:376:ARG:NH1	1:B:379:GLN:HE22	2.00	0.48
1:B:324:SER:HB2	1:B:328:LEU:HD12	1.96	0.48
1:B:227:LEU:HD11	1:B:384:LEU:HD23	1.96	0.48
1:A:231:VAL:HG12	1:A:414:LEU:HB2	1.96	0.47
1:B:391:ARG:HE	1:B:428:ILE:HG21	1.79	0.47
1:A:271:LEU:HD21	1:A:419:LYS:O	2.14	0.47
1:A:429:LEU:HD12	1:A:431:HIS:HE1	1.80	0.47
1:B:401:LEU:O	1:B:412:VAL:HA	2.15	0.47
1:B:359:PHE:CZ	1:B:451:LEU:HD11	2.49	0.47
1:A:190:GLN:HG2	1:A:198:PHE:CZ	2.49	0.47
1:A:390:PHE:CD2	1:A:431:HIS:CD2	3.03	0.47
1:A:295:VAL:CG2	1:B:339:ASP:HB3	2.45	0.47
1:A:324:SER:HB2	1:A:328:LEU:HD12	1.96	0.46
1:B:188:TRP:HB3	1:B:252:LEU:HG	1.98	0.46
1:A:186:MSE:HA	1:A:190:GLN:OE1	2.15	0.46
1:B:353:GLU:HG3	1:B:357:ARG:NH1	2.30	0.46
1:B:390:PHE:CE2	1:B:431:HIS:CD2	3.03	0.46
1:B:328:LEU:O	1:B:447:GLY:HA2	2.15	0.46
1:B:201:ALA:HB2	1:B:208:LEU:HG	1.96	0.46
1:B:264:LYS:CE	3:B:2024:HOH:O	2.63	0.45
1:B:376:ARG:HH11	1:B:379:GLN:NE2	2.03	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:MSE:SE	1:B:234:PHE:H	2.49	0.45
1:A:394:GLU:HG2	1:A:396:ILE:HG12	1.99	0.45
1:A:398:SER:HA	1:A:416:ASP:O	2.18	0.44
1:A:260:VAL:CG1	1:A:401:LEU:HD11	2.47	0.44
1:B:436:GLU:O	1:B:437:GLU:C	2.55	0.44
1:A:429:LEU:HB2	1:A:431:HIS:CE1	2.52	0.44
1:B:213:GLU:N	1:B:214:PRO:CD	2.80	0.44
1:B:219:LEU:HD13	1:B:248:LEU:HD21	1.98	0.44
1:B:219:LEU:O	1:B:223:MSE:HG2	2.18	0.44
1:B:389:PHE:O	1:B:393:HIS:HD2	2.00	0.44
1:B:374:LEU:HG	1:B:455:LEU:HB3	2.00	0.44
1:B:227:LEU:HD21	1:B:384:LEU:HD23	1.99	0.44
1:B:293:LEU:HD13	1:B:293:LEU:N	2.32	0.44
1:A:292:MSE:HG2	1:A:318:TRP:CE3	2.54	0.43
1:A:429:LEU:HD12	1:A:431:HIS:CE1	2.53	0.43
1:B:231:VAL:HB	1:B:232:PRO:HD2	2.00	0.43
1:A:293:LEU:HD12	1:A:297:PRO:HA	2.01	0.43
1:B:274:GLU:O	1:B:313:PRO:HG2	2.18	0.43
1:B:379:GLN:HE21	1:B:379:GLN:HB3	1.50	0.43
1:B:260:VAL:CG1	1:B:401:LEU:HD11	2.47	0.43
1:B:255:PHE:CE1	1:B:409:ARG:HG2	2.53	0.43
1:A:187:SER:O	1:A:190:GLN:HB2	2.19	0.43
1:A:312:LYS:HB3	1:A:313:PRO:HD3	2.01	0.43
1:B:433:ARG:CG	1:B:441:GLU:HG3	2.49	0.43
1:B:352:ARG:HG3	1:B:454:ILE:HD11	2.00	0.43
1:A:186:MSE:HG2	1:A:191:LEU:CD2	2.49	0.43
1:A:219:LEU:HD13	1:A:248:LEU:HD21	2.00	0.43
1:A:278:ALA:HB2	1:A:313:PRO:HG2	2.01	0.43
1:B:354:GLN:O	1:B:358:VAL:HG23	2.19	0.43
1:B:332:ILE:HD13	1:B:358:VAL:CG1	2.49	0.42
1:A:289:TYR:CE2	1:A:293:LEU:HD22	2.55	0.42
1:B:360:GLU:HA	1:B:458:LEU:HD21	2.02	0.42
1:A:194:HIS:HE2	1:A:416:ASP:CG	2.23	0.42
1:B:261:LEU:C	1:B:261:LEU:HD23	2.39	0.42
1:A:223:MSE:SE	1:A:234:PHE:H	2.52	0.42
1:A:196:GLY:HA2	1:A:198:PHE:CZ	2.55	0.42
1:A:284:LEU:HB3	1:A:309:ALA:HB1	2.02	0.42
1:B:461:ARG:HA	1:B:461:ARG:HD2	1.80	0.41
1:A:384:LEU:HD22	1:A:390:PHE:CD1	2.56	0.41
1:B:255:PHE:CD1	1:B:409:ARG:HD3	2.55	0.41
1:B:316:MSE:O	1:B:320:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:HG22	1:A:248:LEU:HB2	2.03	0.41
1:A:273:GLU:O	1:A:277:LYS:HD3	2.20	0.41
1:A:341:SER:HB2	1:B:345:ASP:HA	2.03	0.41
1:A:251:LEU:HD22	1:A:413:TRP:CE2	2.57	0.40
1:B:330:PHE:CZ	1:B:355:VAL:HG11	2.56	0.40
1:A:384:LEU:HD12	1:A:448:LEU:HD12	2.02	0.40
3:A:2084:HOH:O	1:B:347:LYS:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2097:HOH:O	3:B:2098:HOH:O[3_555]	2.14	0.06

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	274/276 (99%)	267 (97%)	6 (2%)	1 (0%)	34 21
1	B	268/276 (97%)	258 (96%)	8 (3%)	2 (1%)	22 10
All	All	542/552 (98%)	525 (97%)	14 (3%)	3 (1%)	25 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	306	ALA
1	A	198	PHE
1	B	280	GLU

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	237/231 (103%)	220 (93%)	17 (7%)	14 4
1	B	235/231 (102%)	221 (94%)	14 (6%)	19 7
All	All	472/462 (102%)	441 (93%)	31 (7%)	16 5

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	MSE
1	A	187	SER
1	A	197	SER
1	A	203	THR
1	A	207	ILE
1	A	210	ARG
1	A	240	ARG
1	A	241	ASP
1	A	243	GLU
1	A	277	LYS
1	A	308	ARG
1	A	314	ARG
1	A	336	LYS
1	A	423	LEU
1	A	446	LEU
1	A	448	LEU
1	A	461	ARG
1	B	190	GLN
1	B	197	SER
1	B	204	SER
1	B	216	ARG
1	B	240	ARG
1	B	243	GLU
1	B	264	LYS
1	B	277	LYS
1	B	281	ARG
1	B	293	LEU

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Mol	Chain	Res	Type
1	B	311	THR
1	B	361	GLU
1	B	379	GLN
1	B	461	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	235	HIS
1	A	404	HIS
1	A	450	ASN
1	B	190	GLN
1	B	317	GLN
1	B	379	GLN
1	B	393	HIS
1	B	408	HIS

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	1462	-	4,4,4	0.24	0	6,6,6	0.22	0
2	SO4	B	1462	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	A	1464	-	4,4,4	0.16	0	6,6,6	0.37	0
2	SO4	A	1463	-	4,4,4	0.17	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	270/276 (97%)	0.60	23 (8%)	10	8	8, 18, 59, 73	0
1	B	266/276 (96%)	1.10	55 (20%)	1	0	7, 20, 61, 76	0
All	All	536/552 (97%)	0.85	78 (14%)	2	1	7, 19, 61, 76	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	GLY	12.6
1	A	195	THR	11.2
1	B	306	ALA	9.8
1	A	198	PHE	7.7
1	B	187	SER	7.7
1	B	284	LEU	7.6
1	B	202	GLY	6.8
1	B	300	PRO	6.6
1	B	297	PRO	6.3
1	B	286	LYS	6.0
1	B	307	GLN	5.8
1	B	191	LEU	5.8
1	A	197	SER	5.8
1	B	310	VAL	5.5
1	B	311	THR	5.1
1	A	196	GLY	5.0
1	B	308	ARG	4.8
1	B	287	ASP	4.6
1	B	301	THR	4.5
1	A	241	ASP	4.4
1	B	312	LYS	4.4
1	B	189	VAL	4.4
1	B	299	ALA	4.3
1	B	282	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	283	LYS	4.1
1	B	204	SER	4.1
1	B	281	ARG	4.1
1	A	187	SER	4.1
1	B	198	PHE	4.1
1	A	194	HIS	4.0
1	B	241	ASP	3.8
1	B	242	GLY	3.7
1	A	192	ALA	3.7
1	B	290	LYS	3.6
1	A	193	GLY	3.6
1	B	303	GLU	3.5
1	B	289	TYR	3.4
1	A	210	ARG	3.3
1	B	192	ALA	3.1
1	A	189	VAL	3.1
1	B	295	VAL	3.0
1	B	275	LEU	3.0
1	B	293	LEU	2.9
1	B	278	ALA	2.9
1	B	315	TYR	2.9
1	B	461	ARG	2.7
1	B	302	GLU	2.7
1	B	305	HIS	2.6
1	B	239	GLU	2.6
1	A	240	ARG	2.6
1	B	197	SER	2.6
1	B	280	GLU	2.6
1	A	412	VAL	2.6
1	B	273	GLU	2.5
1	B	304	GLU	2.5
1	A	436	GLU	2.5
1	B	298	GLU	2.5
1	B	243	GLU	2.5
1	A	203	THR	2.5
1	B	425	ASP	2.4
1	B	277	LYS	2.4
1	B	274	GLU	2.4
1	B	245	TYR	2.3
1	B	291	LYS	2.3
1	B	309	ALA	2.3
1	B	313	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	293	LEU	2.3
1	B	460	GLU	2.2
1	A	191	LEU	2.2
1	A	281	ARG	2.2
1	A	231	VAL	2.2
1	A	426	GLY	2.1
1	B	318	TRP	2.1
1	A	402	PHE	2.1
1	A	380	ILE	2.1
1	B	201	ALA	2.1
1	B	285	ARG	2.0
1	B	276	THR	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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	SO4	A	1462	5/5	0.83	0.16	65,65,68,68	0
2	SO4	A	1463	5/5	0.83	0.25	70,71,72,72	0
2	SO4	B	1462	5/5	0.86	0.23	82,83,83,84	0
2	SO4	A	1464	5/5	0.87	0.18	73,75,75,76	0

6.5 Other polymers (i)

There are no such residues in this entry.