



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:41 PM GMT

PDB ID : 1W2F
Title : HUMAN INOSITOL (1,4,5)-TRISPHOSPHATE3-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 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/ValidationPDFNotes.html>

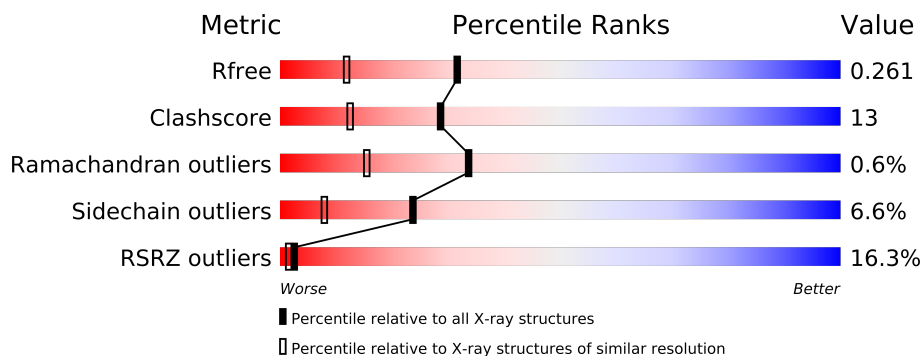
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	276	
1	B	276	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1463	-	X
2	SO4	A	1464	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4690 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

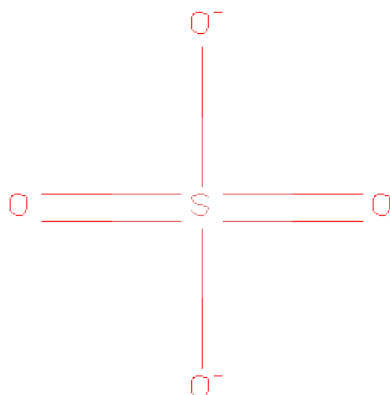
- Molecule 1 is a protein called INOSITOL-TRISPHOSPHATE3-KINASE A.

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: O₄S).



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

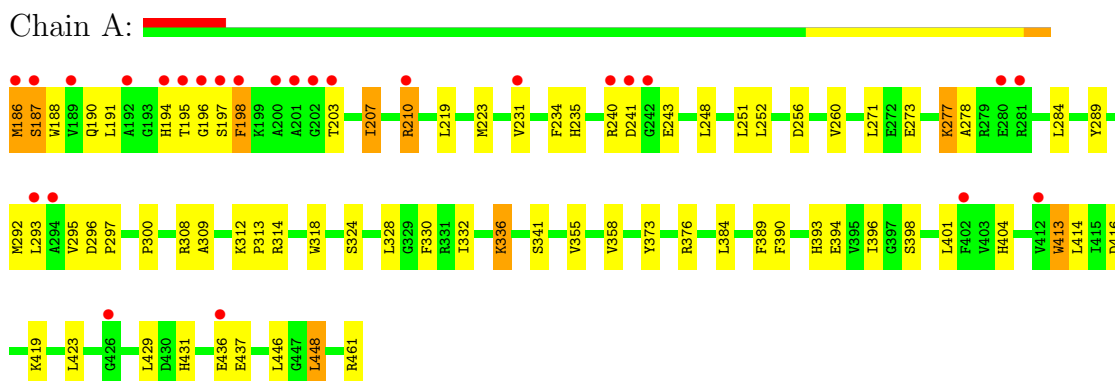
- Molecule 3 is water.

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

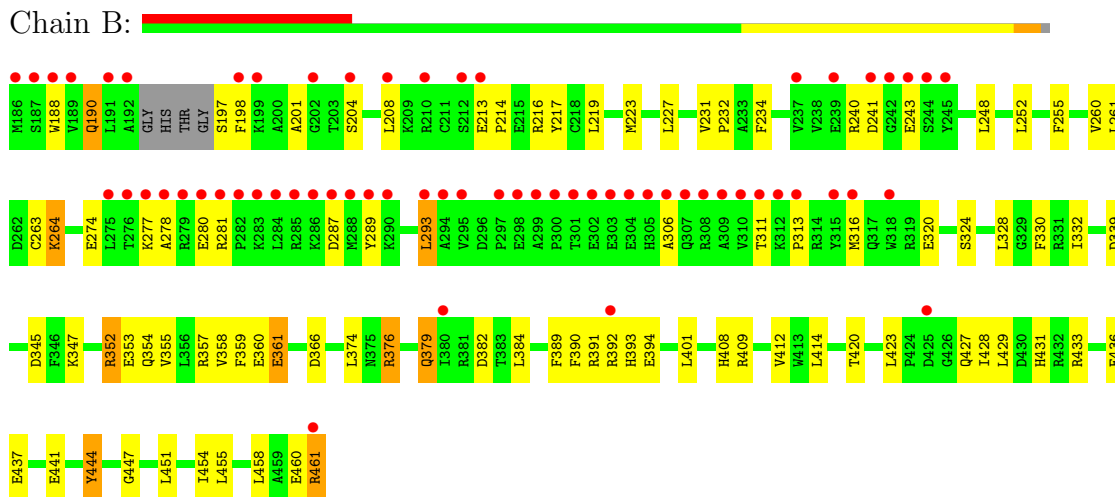
3 Residue-property plots

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: INOSITOL-TRISPHOSPHATE3-KINASE A



• Molecule 1: INOSITOL-TRISPHOSPHATE3-KINASE A



4 Data and refinement statistics

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) 91.6 (45.09-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.241 0.243 , 0.261	Depositor DCC
R_{free} test set	2576 reflections (4.60%)	DCC
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 , 22.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 96919 reflections	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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:227:LEU:HD11	1:B:384:LEU:HD23	1.96	0.48
1:B:324:SER:HB2	1:B:328:LEU:HD12	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:429:LEU:HD12	1:A:431:HIS:HE1	1.80	0.47
1:A:271:LEU:HD21	1:A:419:LYS:O	2.14	0.47
1:B:401:LEU:O	1:B:412:VAL:HA	2.15	0.47
1:A:190:GLN:HG2	1:A:198:PHE:CZ	2.49	0.47
1:B:359:PHE:CZ	1:B:451:LEU:HD11	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:328:LEU:O	1:B:447:GLY:HA2	2.15	0.46
1:B:390:PHE:CE2	1:B:431:HIS:CD2	3.03	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
1:B:223:MSE:SE	1:B:234:PHE:H	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:394:GLU:HG2	1:A:396:ILE:HG12	1.99	0.45
1:B:436:GLU:O	1:B:437:GLU:C	2.55	0.44
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: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:N	1:B:293:LEU:HD13	2.32	0.44
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:292:MSE:HG2	1:A:318:TRP:CE3	2.54	0.43
1:B:379:GLN:HE21	1:B:379:GLN:HB3	1.50	0.43
1:B:274:GLU:O	1:B:313:PRO:HG2	2.18	0.43
1:B:260:VAL:CG1	1:B:401:LEU:HD11	2.47	0.43
1:A:293:LEU:HD12	1:A:297:PRO:HA	2.01	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:278:ALA:HB2	1:A:313:PRO:HG2	2.01	0.43
1:A:219:LEU:HD13	1:A:248:LEU:HD21	2.00	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(Å)
3:B:2097:HOH:O	3:B:2098:HOH:O[3.555]	2.14	0.06

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	274/276 (99%)	267 (97%)	6 (2%)	1 (0%)	43	25
1	B	268/276 (97%)	258 (96%)	8 (3%)	2 (1%)	30	13
All	All	542/552 (98%)	525 (97%)	14 (3%)	3 (1%)	33	15

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 ⓘ

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%)	21	6
1	B	235/231 (102%)	221 (94%)	14 (6%)	27	10
All	All	472/462 (102%)	441 (93%)	31 (7%)	24	8

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
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 chains 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	0.17	0	6,6,6	0.15	0
2	SO4	A	1463	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	A	1464	-	4,4,4	0.09	0	6,6,6	0.31	0
2	SO4	B	1462	-	4,4,4	0.20	0	6,6,6	0.21	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	1462	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1463	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1464	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1462	-	-	0/0/0/0	0/0/0/0

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.

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, 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	276/276 (100%)	0.82	26 (9%) 9 6	8, 18, 60, 73	0
1	B	272/276 (98%)	1.40	64 (23%) 1 1	7, 20, 61, 82	0
All	All	548/552 (99%)	1.11	90 (16%) 2 1	7, 19, 61, 82	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	GLY	16.6
1	A	195	THR	12.9
1	B	187	SER	11.1
1	B	284	LEU	9.6
1	A	198	PHE	8.7
1	B	202	GLY	8.6
1	A	197	SER	8.5
1	B	306	ALA	7.6
1	A	186	MSE	7.6
1	B	286	LYS	7.2
1	B	186	MSE	6.5
1	B	300	PRO	6.4
1	B	297	PRO	6.3
1	A	241	ASP	6.2
1	B	191	LEU	6.2
1	B	283	LYS	5.9
1	B	198	PHE	5.8
1	B	301	THR	5.3
1	B	312	LYS	4.9
1	B	308	ARG	4.8
1	B	289	TYR	4.8
1	A	196	GLY	4.7
1	B	307	GLN	4.7
1	B	282	PRO	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	241	ASP	4.6
1	B	278	ALA	4.5
1	B	204	SER	4.5
1	A	194	HIS	4.3
1	B	290	LYS	4.3
1	B	245	TYR	4.3
1	B	310	VAL	4.2
1	B	287	ASP	4.1
1	A	210	ARG	4.0
1	B	311	THR	3.9
1	B	281	ARG	3.8
1	A	189	VAL	3.7
1	B	242	GLY	3.7
1	B	299	ALA	3.7
1	A	192	ALA	3.7
1	B	316	MSE	3.5
1	B	192	ALA	3.5
1	B	425	ASP	3.5
1	B	237	VAL	3.5
1	B	303	GLU	3.4
1	B	243	GLU	3.4
1	B	461	ARG	3.4
1	B	285	ARG	3.3
1	B	293	LEU	3.3
1	B	189	VAL	3.3
1	B	275	LEU	3.1
1	B	309	ALA	3.0
1	A	201	ALA	3.0
1	B	305	HIS	3.0
1	A	240	ARG	2.9
1	A	187	SER	2.9
1	B	239	GLU	2.9
1	B	277	LYS	2.9
1	B	294	ALA	2.8
1	B	212	SER	2.8
1	B	244	SER	2.8
1	B	295	VAL	2.7
1	B	288	MSE	2.7
1	B	280	GLU	2.7
1	B	298	GLU	2.6
1	A	412	VAL	2.6
1	B	208	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	203	THR	2.5
1	B	302	GLU	2.5
1	B	276	THR	2.5
1	A	281	ARG	2.4
1	B	188	TRP	2.4
1	A	426	GLY	2.4
1	B	313	PRO	2.4
1	B	213	GLU	2.4
1	A	293	LEU	2.4
1	A	436	GLU	2.3
1	B	392	ARG	2.3
1	B	304	GLU	2.3
1	B	210	ARG	2.3
1	B	279	ARG	2.2
1	B	318	TRP	2.2
1	A	294	ALA	2.2
1	A	402	PHE	2.2
1	B	315	TYR	2.1
1	A	280	GLU	2.1
1	A	242	GLY	2.1
1	B	380	ILE	2.1
1	B	199	LYS	2.1
1	A	231	VAL	2.0
1	A	200	ALA	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 ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	1463	5/5	0.18	39.67	70,71,72,72	0
2	SO4	A	1464	5/5	0.19	4.33	73,75,75,76	0
2	SO4	A	1462	5/5	0.15	0.99	65,65,68,68	0
2	SO4	B	1462	5/5	0.16	-0.39	82,83,83,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.