



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:43 AM UTC

PDB ID : 1W2F / pdb_00001w2f
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

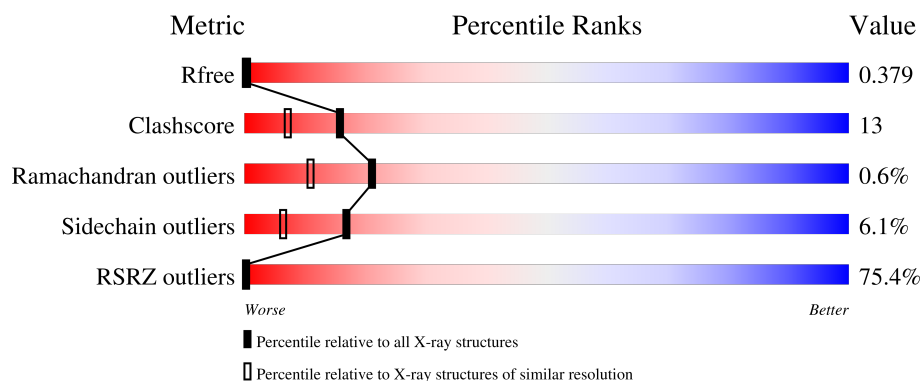
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 of 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 $\leq 5\%$. 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	276	75% 71% 24% .
1	B	276	72% 65% 30% ..

2 Entry composition [i](#)

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.

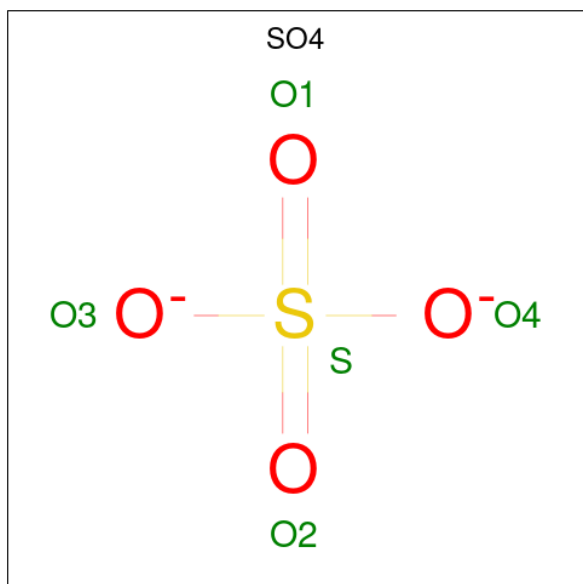
- Molecule 1 is a protein called INOSITOL-TRISPHOSPHATE 3-KINASE A.

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 (CCD ID: SO4) (formula: O₄S).



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	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		

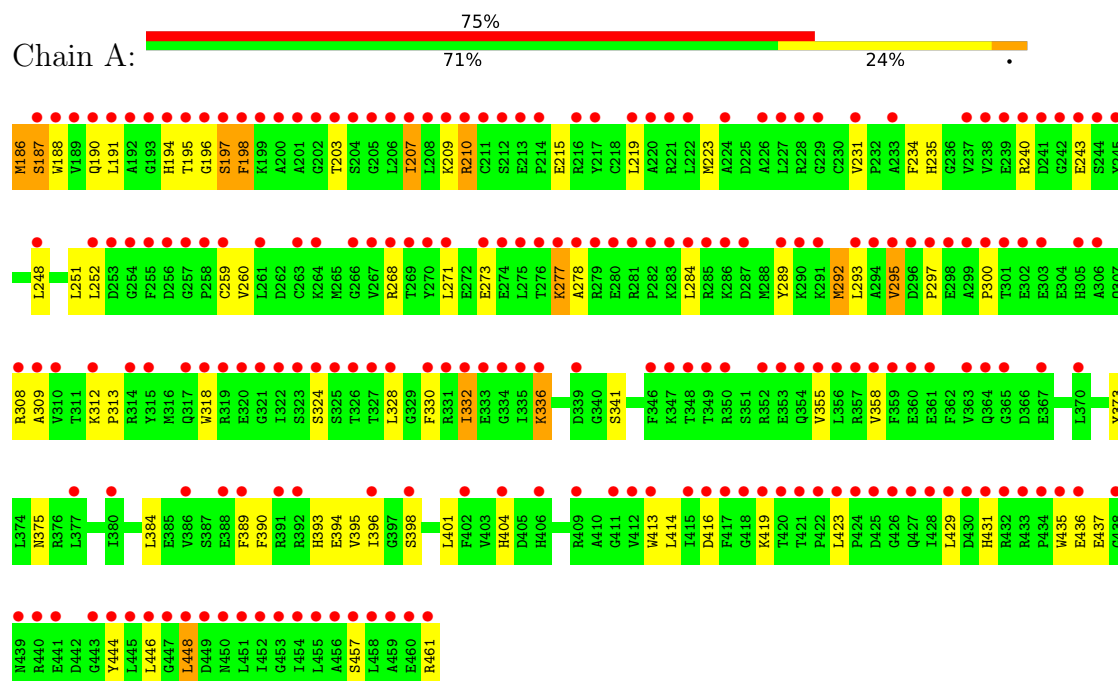
- Molecule 3 is water.

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

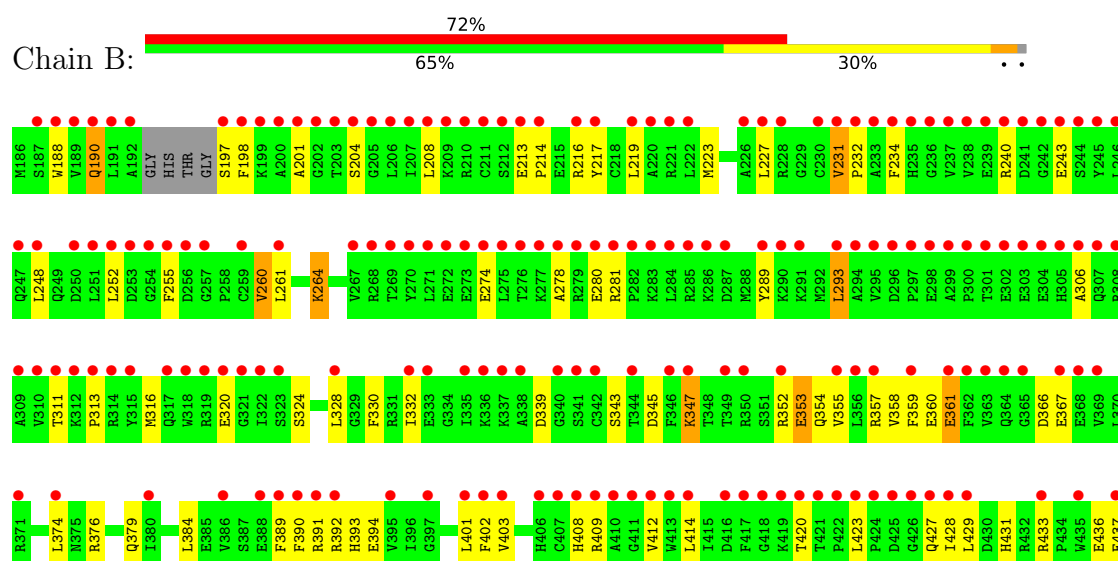
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



• Molecule 1: INOSITOL-TRISPHOSPHATE 3-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 45.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.5 (45.17-1.80) 100.0 (45.17-1.80)	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 0.347 , 0.379	Depositor DCC
R_{free} test set	4887 reflections (1.44%)	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)	0.37 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	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.

²Theoretical 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: 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	1.44	5/2253 (0.2%)	1.07	2/3025 (0.1%)
1	B	1.33	7/2226 (0.3%)	1.02	1/2987 (0.0%)
All	All	1.39	12/4479 (0.3%)	1.05	3/6012 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	VAL	CA-C	-6.99	1.46	1.52
1	B	402	PHE	CA-C	-6.45	1.44	1.52
1	A	332	ILE	CA-CB	-6.19	1.46	1.54
1	B	343	SER	N-CA	-5.84	1.39	1.46
1	B	450	ASN	CA-C	-5.55	1.45	1.52
1	B	403	VAL	CA-C	-5.51	1.45	1.52
1	B	260	VAL	CA-C	-5.45	1.45	1.52
1	A	375	ASN	C-O	-5.36	1.17	1.24
1	B	353	GLU	C-O	-5.31	1.17	1.24
1	A	259	CYS	CA-C	-5.23	1.46	1.52
1	A	395	VAL	CA-CB	-5.08	1.47	1.53
1	A	292	MSE	SE-CE	-5.07	1.80	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	VAL	CB-CA-C	-5.51	104.81	112.02
1	A	457	SER	N-CA-C	-5.38	105.50	111.36
1	B	457	SER	N-CA-C	-5.31	105.41	111.14

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	2215	0	2190	58	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	4	0
3	B	120	0	0	1	1
All	All	4690	0	4359	117	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 (117) 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:A:436:GLU:O	1:A:437:GLU:C	2.42	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:460:GLU:O	1:B:461:ARG:C	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:PHE:CD1	1:A:393:HIS:CE1	2.93	0.56
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:444:TYR:CD2	1:B:444:TYR:C	2.84	0.56
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:A:332:ILE:HD13	1:A:358:VAL:CG1	2.42	0.49
1:A:209:LYS:HZ3	1:A:215:GLU:CD	2.21	0.49
1:A:268:ARG:HE	1:A:435:TRP:CD1	2.29	0.49
1:A:390:PHE:CZ	1:A:431:HIS:CD2	3.00	0.49
1:B:436:GLU:O	1:B:437:GLU:C	2.55	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: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:A:190:GLN:HG2	1:A:198:PHE:CZ	2.49	0.47
1:A:194:HIS:HE2	1:A:416:ASP:CG	2.23	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:261:LEU:C	1:B:261:LEU:HD23	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:394:GLU:HG2	1:A:396:ILE:HG12	1.99	0.45
1:A:260:VAL:CG1	1:A:401:LEU:HD11	2.47	0.44
1:A:398:SER:HA	1:A:416:ASP:O	2.18	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:A:444:TYR:C	1:A:444:TYR:CD2	2.94	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:A:197:SER:O	1:A:198:PHE:C	2.60	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:260:VAL:CG1	1:B:401:LEU:HD11	2.47	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: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:A:419:LYS:NZ	3:A:2125:HOH:O	2.44	0.43
1:B:354:GLN:O	1:B:358:VAL:HG23	2.19	0.43
1:A:330:PHE:CD1	1:A:330:PHE:C	2.97	0.42
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:223:MSE:SE	1:A:234:PHE:H	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:341:SER:HB2	1:B:345:ASP:HA	2.03	0.41
1:A:187:SER:H	1:A:190:GLN:CD	2.29	0.40
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%)	30	19
1	B	268/276 (97%)	258 (96%)	8 (3%)	2 (1%)	18	8
All	All	542/552 (98%)	525 (97%)	14 (3%)	3 (1%)	21	11

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%)	222 (94%)	15 (6%)	16	6
1	B	235/231 (102%)	221 (94%)	14 (6%)	17	7
All	All	472/462 (102%)	443 (94%)	29 (6%)	17	6

All (29) 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	243	GLU
1	A	277	LYS
1	A	308	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

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Mol	Chain	Res	Type
1	B	264	LYS
1	B	281	ARG
1	B	293	LEU
1	B	311	THR
1	B	347	LYS
1	B	361	GLU
1	B	367	GLU
1	B	461	ARG

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

Mol	Chain	Res	Type
1	A	190	GLN
1	A	235	HIS
1	A	404	HIS
1	A	427	GLN
1	A	450	ASN
1	B	235	HIS
1	B	379	GLN
1	B	393	HIS
1	B	406	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 oligosaccharides 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	1463	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	A	1464	-	4,4,4	0.27	0	6,6,6	0.37	0
2	SO4	A	1462	-	4,4,4	0.35	0	6,6,6	0.23	0
2	SO4	B	1462	-	4,4,4	0.25	0	6,6,6	0.24	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 [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	270/276 (97%)	3.29	206 (76%) 0 0	8, 18, 59, 73	0
1	B	266/276 (96%)	3.69	198 (74%) 0 0	7, 20, 61, 76	0
All	All	536/552 (97%)	3.49	404 (75%) 0 0	7, 19, 61, 76	0

All (404) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	13.8
1	B	284	LEU	11.7
1	A	198	PHE	11.6
1	B	192	ALA	11.5
1	B	297	PRO	11.0
1	B	189	VAL	10.7
1	A	195	THR	10.6
1	B	313	PRO	9.9
1	B	198	PHE	9.8
1	A	187	SER	9.6
1	A	192	ALA	9.5
1	A	191	LEU	9.4
1	A	202	GLY	9.3
1	B	295	VAL	9.3
1	A	200	ALA	9.2
1	B	278	ALA	9.2
1	A	203	THR	9.2
1	B	310	VAL	9.2
1	B	307	GLN	9.2
1	A	194	HIS	9.0
1	A	189	VAL	9.0
1	B	306	ALA	9.0
1	B	300	PRO	9.0
1	B	197	SER	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	193	GLY	8.9
1	B	289	TYR	8.9
1	B	187	SER	8.7
1	B	299	ALA	8.5
1	B	188	TRP	8.4
1	B	309	ALA	8.4
1	B	311	THR	8.4
1	A	188	TRP	8.3
1	B	290	LYS	8.2
1	A	197	SER	8.2
1	B	308	ARG	8.1
1	B	293	LEU	8.0
1	B	286	LYS	8.0
1	B	275	LEU	7.9
1	B	301	THR	7.9
1	A	196	GLY	7.9
1	A	201	ALA	7.8
1	B	282	PRO	7.6
1	B	294	ALA	7.5
1	B	204	SER	7.5
1	A	206	LEU	7.3
1	B	202	GLY	7.2
1	B	283	LYS	7.2
1	A	293	LEU	7.2
1	B	190	GLN	7.2
1	B	199	LYS	7.1
1	B	305	HIS	7.1
1	B	287	ASP	6.9
1	A	199	LYS	6.8
1	B	276	THR	6.6
1	A	435	TRP	6.6
1	B	291	LYS	6.5
1	B	205	GLY	6.5
1	B	273	GLU	6.5
1	B	285	ARG	6.5
1	A	205	GLY	6.4
1	A	455	LEU	6.4
1	A	426	GLY	6.3
1	B	277	LYS	6.3
1	B	302	GLU	6.2
1	B	281	ARG	6.2
1	B	318	TRP	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	204	SER	6.2
1	B	461	ARG	6.1
1	B	200	ALA	6.1
1	A	190	GLN	6.0
1	A	428	ILE	6.0
1	B	203	THR	6.0
1	A	290	LYS	6.0
1	B	279	ARG	6.0
1	B	304	GLU	5.9
1	A	295	VAL	5.8
1	B	201	ALA	5.8
1	A	207	ILE	5.7
1	B	242	GLY	5.6
1	B	303	GLU	5.6
1	A	424	PRO	5.6
1	B	207	ILE	5.6
1	A	275	LEU	5.5
1	B	206	LEU	5.4
1	B	426	GLY	5.4
1	B	238	VAL	5.4
1	B	254	GLY	5.3
1	B	255	PHE	5.3
1	A	318	TRP	5.2
1	B	460	GLU	5.2
1	B	298	GLU	5.1
1	B	245	TYR	5.1
1	B	296	ASP	5.1
1	B	274	GLU	5.1
1	B	280	GLU	5.0
1	A	241	ASP	5.0
1	A	423	LEU	5.0
1	B	312	LYS	5.0
1	A	322	ILE	5.0
1	B	315	TYR	4.9
1	A	458	LEU	4.8
1	B	369	VAL	4.8
1	A	454	ILE	4.8
1	A	392	ARG	4.8
1	A	425	ASP	4.8
1	A	461	ARG	4.7
1	B	214	PRO	4.7
1	A	294	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	237	VAL	4.6
1	A	284	LEU	4.6
1	B	392	ARG	4.6
1	A	356	LEU	4.6
1	B	208	LEU	4.6
1	A	319	ARG	4.5
1	B	241	ASP	4.5
1	B	320	GLU	4.5
1	A	289	TYR	4.5
1	A	240	ARG	4.5
1	B	338	ALA	4.5
1	A	210	ARG	4.5
1	A	283	LYS	4.4
1	A	350	ARG	4.4
1	A	436	GLU	4.4
1	A	326	THR	4.4
1	B	314	ARG	4.4
1	B	340	GLY	4.3
1	B	252	LEU	4.3
1	A	263	CYS	4.3
1	B	317	GLN	4.3
1	A	270	TYR	4.3
1	B	271	LEU	4.2
1	A	460	GLU	4.2
1	A	269	THR	4.2
1	B	458	LEU	4.2
1	B	319	ARG	4.2
1	A	242	GLY	4.1
1	A	279	ARG	4.1
1	B	240	ARG	4.1
1	B	428	ILE	4.1
1	B	210	ARG	4.1
1	A	253	ASP	4.1
1	B	333	GLU	4.1
1	A	208	LEU	4.1
1	B	322	ILE	4.0
1	A	450	ASN	4.0
1	A	456	ALA	4.0
1	A	447	GLY	4.0
1	B	335	ILE	4.0
1	B	244	SER	4.0
1	A	443	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	330	PHE	4.0
1	A	296	ASP	3.9
1	A	360	GLU	3.9
1	B	221	ARG	3.9
1	A	267	VAL	3.9
1	B	246	LEU	3.9
1	A	238	VAL	3.9
1	B	243	GLU	3.8
1	A	226	ALA	3.8
1	A	438	GLY	3.8
1	A	271	LEU	3.8
1	A	451	LEU	3.8
1	B	391	ARG	3.8
1	A	430	ASP	3.7
1	A	429	LEU	3.7
1	A	346	PHE	3.7
1	B	421	THR	3.7
1	A	459	ALA	3.7
1	A	281	ARG	3.7
1	A	391	ARG	3.7
1	B	433	ARG	3.7
1	A	389	PHE	3.7
1	B	256	ASP	3.7
1	A	365	GLY	3.7
1	B	209	LYS	3.7
1	B	424	PRO	3.7
1	B	323	SER	3.6
1	A	298	GLU	3.6
1	A	355	VAL	3.6
1	B	272	GLU	3.6
1	A	433	ARG	3.6
1	A	257	GLY	3.5
1	A	327	THR	3.5
1	A	409	ARG	3.5
1	A	359	PHE	3.5
1	A	278	ALA	3.5
1	B	236	GLY	3.5
1	A	452	ILE	3.5
1	A	252	LEU	3.5
1	A	448	LEU	3.5
1	B	220	ALA	3.5
1	B	257	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	365	GLY	3.5
1	A	441	GLU	3.4
1	A	315	TYR	3.4
1	A	282	PRO	3.4
1	A	363	VAL	3.4
1	A	213	GLU	3.4
1	A	287	ASP	3.4
1	B	270	TYR	3.4
1	A	349	THR	3.4
1	B	344	THR	3.4
1	A	237	VAL	3.3
1	A	224	ALA	3.3
1	B	455	LEU	3.3
1	B	435	TRP	3.3
1	B	356	LEU	3.3
1	A	367	GLU	3.3
1	A	297	PRO	3.3
1	B	425	ASP	3.3
1	B	454	ILE	3.2
1	A	248	LEU	3.2
1	A	432	ARG	3.2
1	B	448	LEU	3.2
1	B	361	GLU	3.2
1	A	354	GLN	3.2
1	A	332	ILE	3.2
1	A	220	ALA	3.2
1	A	323	SER	3.2
1	A	310	VAL	3.2
1	B	406	HIS	3.2
1	A	273	GLU	3.2
1	A	219	LEU	3.1
1	B	457	SER	3.1
1	A	321	GLY	3.1
1	A	216	ARG	3.1
1	A	434	PRO	3.1
1	B	409	ARG	3.1
1	A	305	HIS	3.1
1	A	211	CYS	3.1
1	B	259	CYS	3.1
1	A	299	ALA	3.1
1	A	422	PRO	3.1
1	A	444	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	423	LEU	3.1
1	A	277	LYS	3.1
1	A	286	LYS	3.1
1	B	359	PHE	3.1
1	A	361	GLU	3.1
1	B	239	GLU	3.1
1	B	386	VAL	3.0
1	A	446	LEU	3.0
1	A	386	VAL	3.0
1	B	346	PHE	3.0
1	B	390	PHE	3.0
1	A	258	PRO	3.0
1	B	251	LEU	3.0
1	A	325	SER	3.0
1	B	212	SER	3.0
1	B	211	CYS	3.0
1	B	230	CYS	3.0
1	A	406	HIS	2.9
1	B	250	ASP	2.9
1	A	357	ARG	2.9
1	B	216	ARG	2.9
1	B	336	LYS	2.9
1	A	308	ARG	2.9
1	B	429	LEU	2.9
1	A	243	GLU	2.9
1	A	411	GLY	2.9
1	A	300	PRO	2.9
1	B	228	ARG	2.9
1	B	419	LYS	2.9
1	A	261	LEU	2.9
1	A	335	ILE	2.9
1	A	396	ILE	2.9
1	B	452	ILE	2.9
1	B	253	ASP	2.8
1	A	352	ARG	2.8
1	A	291	LYS	2.8
1	B	438	GLY	2.8
1	B	349	THR	2.8
1	B	233	ALA	2.8
1	A	427	GLN	2.8
1	A	254	GLY	2.8
1	A	245	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	217	TYR	2.7
1	B	247	GLN	2.7
1	A	255	PHE	2.7
1	A	259	CYS	2.7
1	A	348	THR	2.7
1	A	285	ARG	2.7
1	B	231	VAL	2.7
1	B	269	THR	2.7
1	A	364	GLN	2.7
1	A	347	LYS	2.7
1	B	355	VAL	2.7
1	B	410	ALA	2.7
1	B	234	PHE	2.7
1	A	244	SER	2.7
1	A	239	GLU	2.7
1	A	266	GLY	2.6
1	B	418	GLY	2.6
1	A	314	ARG	2.6
1	A	276	THR	2.6
1	A	312	LYS	2.6
1	A	420	THR	2.6
1	A	421	THR	2.6
1	B	232	PRO	2.6
1	B	408	HIS	2.6
1	A	353	GLU	2.6
1	B	267	VAL	2.6
1	B	403	VAL	2.6
1	B	341	SER	2.6
1	A	431	HIS	2.6
1	B	427	GLN	2.6
1	B	367	GLU	2.6
1	A	212	SER	2.6
1	B	422	PRO	2.5
1	A	417	PHE	2.5
1	A	280	GLU	2.5
1	A	320	GLU	2.5
1	B	413	TRP	2.5
1	A	264	LYS	2.5
1	A	231	VAL	2.5
1	A	358	VAL	2.5
1	A	214	PRO	2.5
1	B	416	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	2.5
1	B	364	GLN	2.5
1	A	416	ASP	2.5
1	A	328	LEU	2.5
1	B	321	GLY	2.5
1	A	221	ARG	2.5
1	B	437	GLU	2.5
1	A	301	THR	2.5
1	B	407	CYS	2.4
1	A	227	LEU	2.4
1	A	377	LEU	2.4
1	B	235	HIS	2.4
1	B	328	LEU	2.4
1	A	317	GLN	2.4
1	B	420	THR	2.4
1	B	456	ALA	2.4
1	B	412	VAL	2.4
1	A	324	SER	2.4
1	A	445	LEU	2.4
1	B	374	LEU	2.4
1	B	268	ARG	2.4
1	B	388	GLU	2.4
1	B	451	LEU	2.4
1	B	332	ILE	2.4
1	A	306	ALA	2.4
1	B	397	GLY	2.4
1	B	347	LYS	2.4
1	B	357	ARG	2.3
1	A	217	TYR	2.3
1	B	362	PHE	2.3
1	B	389	PHE	2.3
1	A	309	ALA	2.3
1	A	415	ILE	2.3
1	B	439	ASN	2.3
1	B	395	VAL	2.3
1	A	413	TRP	2.3
1	A	333	GLU	2.3
1	B	401	LEU	2.3
1	B	459	ALA	2.3
1	B	352	ARG	2.3
1	B	368	GLU	2.3
1	A	439	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	402	PHE	2.3
1	B	402	PHE	2.3
1	A	440	ARG	2.3
1	A	388	GLU	2.3
1	B	342	CYS	2.3
1	B	222	LEU	2.3
1	B	227	LEU	2.3
1	A	229	GLY	2.2
1	A	274	GLU	2.2
1	A	256	ASP	2.2
1	A	404	HIS	2.2
1	B	350	ARG	2.2
1	A	222	LEU	2.2
1	A	370	LEU	2.2
1	A	398	SER	2.2
1	A	453	GLY	2.2
1	B	226	ALA	2.2
1	B	219	LEU	2.2
1	B	261	LEU	2.2
1	A	418	GLY	2.2
1	B	411	GLY	2.2
1	B	447	GLY	2.2
1	A	334	GLY	2.2
1	B	248	LEU	2.2
1	A	268	ARG	2.2
1	B	337	LYS	2.2
1	A	302	GLU	2.1
1	B	213	GLU	2.1
1	B	380	ILE	2.1
1	A	412	VAL	2.1
1	A	457	SER	2.1
1	B	414	LEU	2.1
1	A	303	GLU	2.1
1	A	380	ILE	2.1
1	A	339	ASP	2.1
1	A	336	LYS	2.1
1	A	331	ARG	2.1
1	A	209	LYS	2.1
1	A	419	LYS	2.1
1	B	363	VAL	2.1
1	A	449	ASP	2.0
1	B	417	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	228	ARG	2.0
1	B	371	ARG	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1462	5/5	0.35	0.27	82,83,83,84	0
2	SO4	A	1464	5/5	0.53	0.27	73,75,75,76	0
2	SO4	A	1462	5/5	0.66	0.24	65,65,68,68	0
2	SO4	A	1463	5/5	0.70	0.21	70,71,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.