WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2024 – 03:53 pm 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 (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	Percentile Ranks	Value
Rfree		0.379
Clashscore		13
Ramachandran outliers		0.6%
Sidechain outliers		6.6%
RSRZ outliers		72.8%

Worse → *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
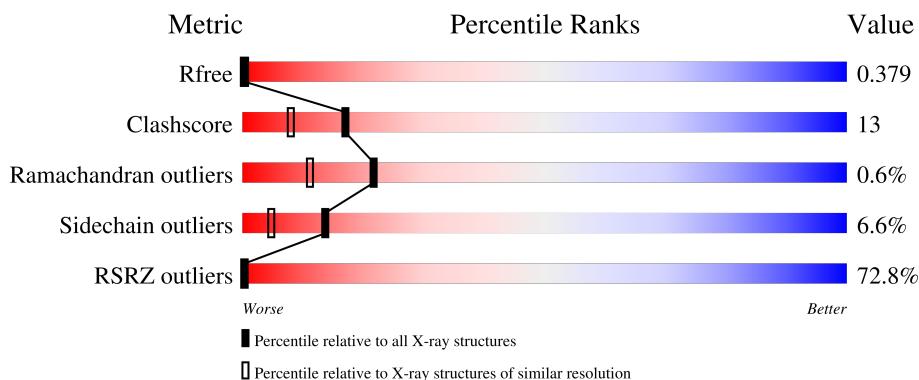
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	276	71% / 73% 24% •
1	B	276	70% / 66% 30% ••
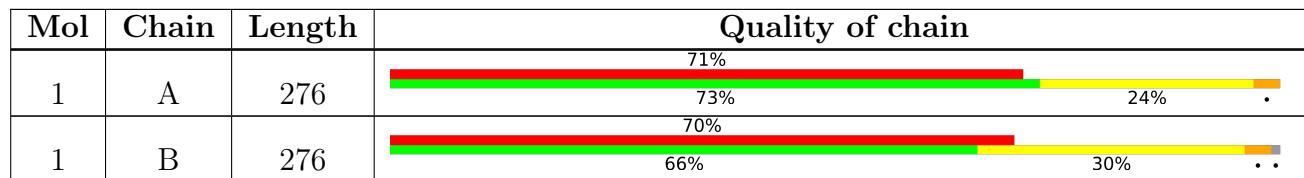
2 Entry composition (i)

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 2215	C 1386	N 403	O 413	S 7	Se 6	0	0	0
1	B	272	Total 2190	C 1372	N 397	O 408	S 7	Se 6	0	0	0

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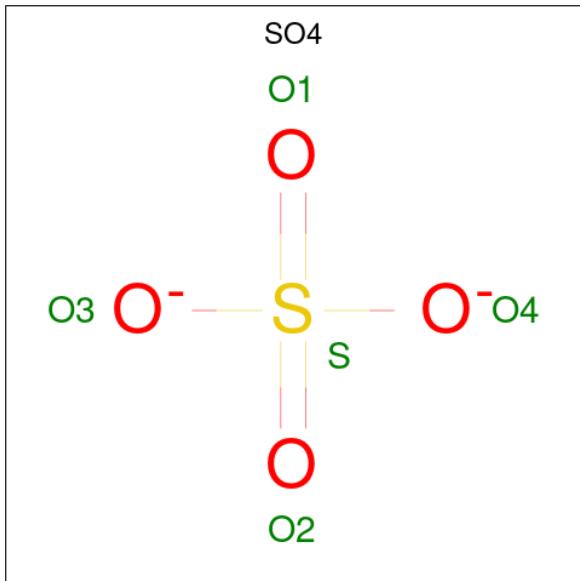
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0

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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	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

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

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. 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. 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
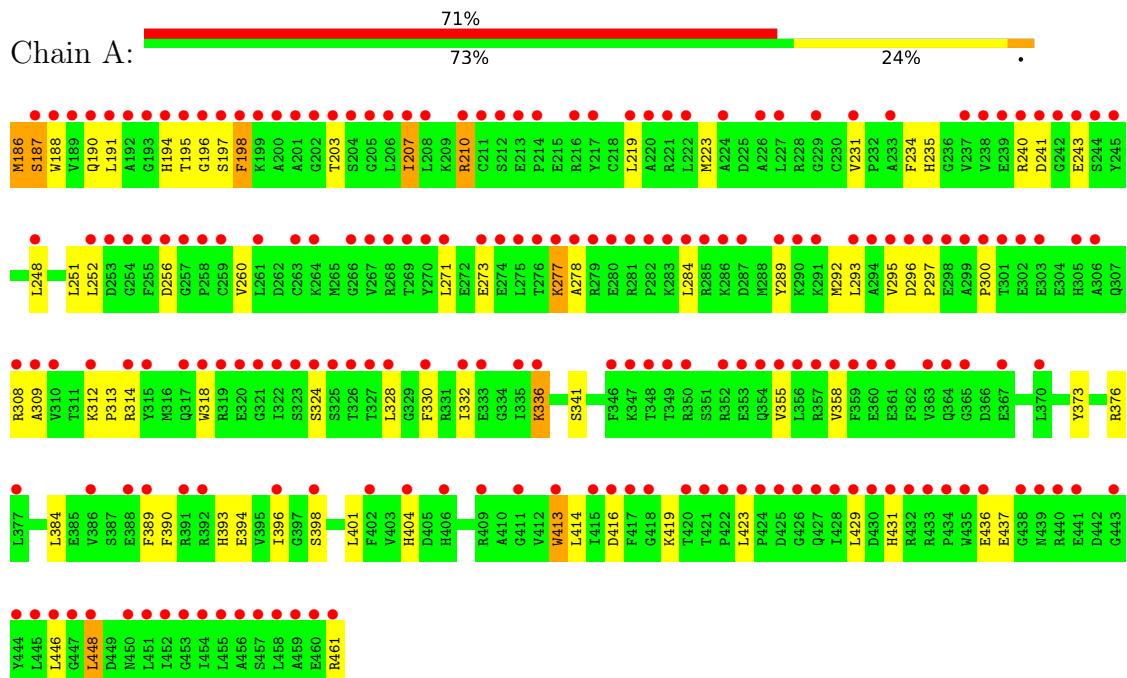
- Molecule 1: INOSITOL-TRISPHOSPHATE 3-KINASE A
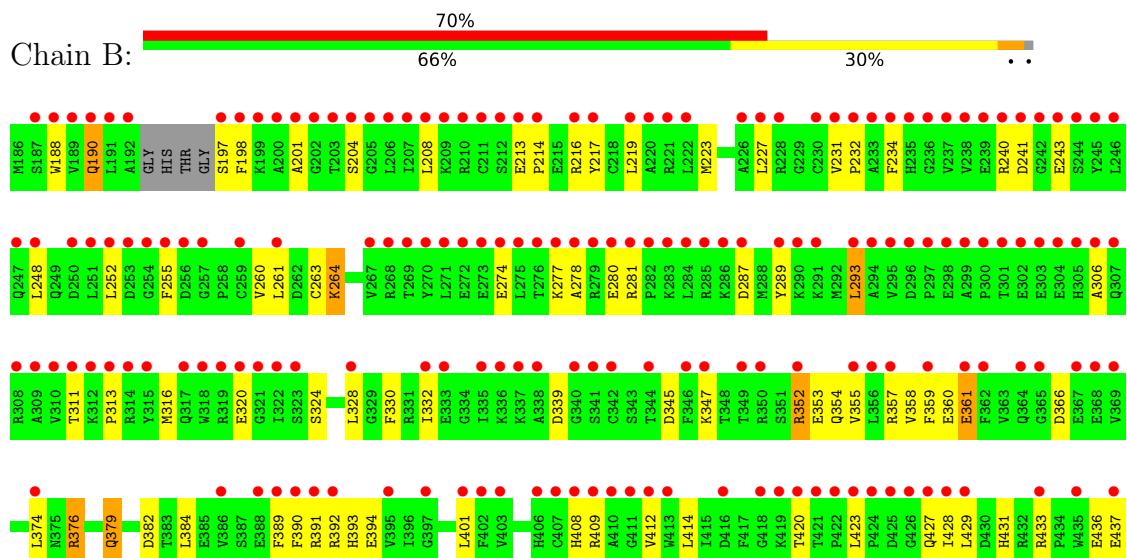
4 Data and refinement statistics (i)

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	Depositor
	45.17 – 1.80	EDS
% Data completeness	91.5 (45.17-1.80)	Depositor
(in resolution range)	100.0 (45.17-1.80)	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	Depositor
	0.347 , 0.379	DCC
R_{free} test set	609 reflections (1.09%)	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]	$< |L| > = 0.45$, $< L^2 > = 0.28$	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.*

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[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 ⓘ

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:CD2	1:B:444:TYR:C	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: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: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

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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: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: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: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: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 ⓘ

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%)	30	19
1	B	268/276 (97%)	258 (96%)	8 (3%)	2 (1%)	19	9
All	All	542/552 (98%)	525 (97%)	14 (3%)	3 (1%)	22	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 ⓘ

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%)	12	4
1	B	235/231 (102%)	221 (94%)	14 (6%)	16	6
All	All	472/462 (102%)	441 (93%)	31 (7%)	14	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

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

Warning: The R factor obtained from EDS is 0.3816,which does not match the depositor's R factor of 0.203. Please interpret the results in this section carefully.

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%)	3.13	197 (72%)	0	0	8, 18, 59, 73	0
1	B	266/276 (96%)	3.54	193 (72%)	0	0	7, 20, 61, 76	0
All	All	536/552 (97%)	3.33	390 (72%)	0	0	7, 19, 61, 76	0

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	13.3
1	B	284	LEU	11.3
1	A	198	PHE	11.2
1	B	192	ALA	11.0
1	B	297	PRO	10.7
1	A	195	THR	10.3
1	B	189	VAL	10.3
1	B	313	PRO	9.6
1	B	198	PHE	9.5
1	A	187	SER	9.4
1	A	192	ALA	9.1
1	A	191	LEU	9.1
1	B	307	GLN	9.0
1	A	203	THR	9.0
1	B	295	VAL	8.9
1	A	202	GLY	8.9
1	A	200	ALA	8.8
1	B	278	ALA	8.8
1	B	310	VAL	8.8
1	A	194	HIS	8.8
1	B	197	SER	8.7
1	A	189	VAL	8.7

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Mol	Chain	Res	Type	RSRZ
1	B	300	PRO	8.7
1	B	289	TYR	8.6
1	B	306	ALA	8.6
1	A	193	GLY	8.5
1	B	187	SER	8.5
1	B	290	LYS	8.2
1	B	311	THR	8.1
1	B	299	ALA	8.1
1	B	309	ALA	8.0
1	B	308	ARG	8.0
1	A	197	SER	8.0
1	B	188	TRP	8.0
1	B	286	LYS	7.9
1	A	188	TRP	7.9
1	B	293	LEU	7.7
1	B	301	THR	7.7
1	B	275	LEU	7.7
1	A	196	GLY	7.6
1	A	201	ALA	7.5
1	B	282	PRO	7.4
1	B	204	SER	7.3
1	B	283	LYS	7.1
1	B	294	ALA	7.1
1	B	199	LYS	7.1
1	B	190	GLN	7.0
1	A	206	LEU	7.0
1	B	202	GLY	6.9
1	A	293	LEU	6.9
1	B	305	HIS	6.9
1	B	287	ASP	6.8
1	A	199	LYS	6.7
1	B	291	LYS	6.5
1	B	276	THR	6.4
1	B	273	GLU	6.4
1	B	285	ARG	6.4
1	A	435	TRP	6.2
1	B	205	GLY	6.2
1	B	277	LYS	6.2
1	B	302	GLU	6.1
1	A	205	GLY	6.1
1	A	455	LEU	6.1
1	B	281	ARG	6.1

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

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Mol	Chain	Res	Type	RSRZ
1	B	392	ARG	4.5
1	B	214	PRO	4.5
1	B	320	GLU	4.5
1	A	319	ARG	4.4
1	A	284	LEU	4.4
1	B	237	VAL	4.4
1	B	241	ASP	4.4
1	A	240	ARG	4.4
1	A	294	ALA	4.4
1	A	283	LYS	4.4
1	A	210	ARG	4.4
1	A	356	LEU	4.4
1	B	208	LEU	4.4
1	A	436	GLU	4.3
1	A	289	TYR	4.3
1	A	350	ARG	4.3
1	B	314	ARG	4.3
1	B	338	ALA	4.2
1	A	326	THR	4.2
1	B	317	GLN	4.2
1	A	263	CYS	4.1
1	B	252	LEU	4.1
1	A	460	GLU	4.1
1	B	340	GLY	4.1
1	A	270	TYR	4.1
1	B	319	ARG	4.1
1	A	279	ARG	4.0
1	B	240	ARG	4.0
1	B	271	LEU	4.0
1	A	269	THR	4.0
1	B	210	ARG	4.0
1	B	333	GLU	4.0
1	B	458	LEU	4.0
1	A	253	ASP	3.9
1	A	242	GLY	3.9
1	B	428	ILE	3.9
1	A	450	ASN	3.9
1	A	360	GLU	3.9
1	A	208	LEU	3.9
1	B	322	ILE	3.9
1	B	244	SER	3.8
1	B	221	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	296	ASP	3.8
1	B	335	ILE	3.8
1	A	447	GLY	3.8
1	A	456	ALA	3.8
1	A	330	PHE	3.8
1	B	243	GLU	3.8
1	A	443	GLY	3.8
1	A	267	VAL	3.7
1	B	246	LEU	3.7
1	A	238	VAL	3.7
1	B	391	ARG	3.7
1	A	430	ASP	3.6
1	A	438	GLY	3.6
1	A	271	LEU	3.6
1	A	451	LEU	3.6
1	A	226	ALA	3.6
1	A	281	ARG	3.6
1	A	391	ARG	3.6
1	B	433	ARG	3.6
1	B	209	LYS	3.6
1	A	298	GLU	3.6
1	A	429	LEU	3.5
1	B	421	THR	3.5
1	A	346	PHE	3.5
1	B	256	ASP	3.5
1	A	389	PHE	3.5
1	B	323	SER	3.5
1	B	272	GLU	3.5
1	A	459	ALA	3.5
1	B	424	PRO	3.5
1	A	433	ARG	3.5
1	A	365	GLY	3.5
1	A	409	ARG	3.4
1	A	355	VAL	3.4
1	A	327	THR	3.4
1	A	441	GLU	3.4
1	A	359	PHE	3.3
1	A	257	GLY	3.3
1	A	452	ILE	3.3
1	A	213	GLU	3.3
1	B	236	GLY	3.3
1	A	278	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	252	LEU	3.3
1	A	448	LEU	3.3
1	B	220	ALA	3.3
1	A	287	ASP	3.3
1	A	315	TYR	3.3
1	B	257	GLY	3.3
1	B	365	GLY	3.3
1	A	282	PRO	3.2
1	A	363	VAL	3.2
1	A	349	THR	3.2
1	B	344	THR	3.2
1	A	367	GLU	3.2
1	B	270	TYR	3.2
1	A	237	VAL	3.1
1	B	455	LEU	3.1
1	B	361	GLU	3.1
1	B	425	ASP	3.1
1	A	432	ARG	3.1
1	A	224	ALA	3.1
1	B	356	LEU	3.1
1	A	354	GLN	3.1
1	B	435	TRP	3.1
1	A	297	PRO	3.1
1	A	273	GLU	3.1
1	B	454	ILE	3.1
1	A	248	LEU	3.1
1	A	323	SER	3.1
1	B	448	LEU	3.1
1	A	216	ARG	3.0
1	A	332	ILE	3.0
1	B	406	HIS	3.0
1	B	409	ARG	3.0
1	A	220	ALA	3.0
1	B	457	SER	3.0
1	A	310	VAL	3.0
1	A	277	LYS	3.0
1	A	286	LYS	3.0
1	A	361	GLU	3.0
1	B	239	GLU	3.0
1	A	305	HIS	3.0
1	A	219	LEU	3.0
1	A	211	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	259	CYS	3.0
1	A	434	PRO	2.9
1	A	321	GLY	2.9
1	A	422	PRO	2.9
1	A	444	TYR	2.9
1	B	359	PHE	2.9
1	B	423	LEU	2.9
1	A	299	ALA	2.9
1	B	386	VAL	2.9
1	A	357	ARG	2.8
1	A	446	LEU	2.8
1	B	346	PHE	2.8
1	B	390	PHE	2.8
1	A	325	SER	2.8
1	B	212	SER	2.8
1	A	258	PRO	2.8
1	A	386	VAL	2.8
1	B	211	CYS	2.8
1	B	230	CYS	2.8
1	B	250	ASP	2.8
1	B	216	ARG	2.8
1	A	406	HIS	2.8
1	B	251	LEU	2.8
1	B	336	LYS	2.8
1	A	243	GLU	2.8
1	A	308	ARG	2.8
1	B	419	LYS	2.8
1	B	228	ARG	2.8
1	A	291	LYS	2.7
1	A	352	ARG	2.7
1	B	429	LEU	2.7
1	A	300	PRO	2.7
1	B	253	ASP	2.7
1	A	411	GLY	2.7
1	A	335	ILE	2.7
1	A	396	ILE	2.7
1	B	452	ILE	2.7
1	A	261	LEU	2.7
1	A	427	GLN	2.7
1	B	349	THR	2.6
1	B	247	GLN	2.6
1	A	285	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	438	GLY	2.6
1	A	259	CYS	2.6
1	A	347	LYS	2.6
1	A	348	THR	2.6
1	A	254	GLY	2.6
1	A	364	GLN	2.6
1	B	233	ALA	2.6
1	A	255	PHE	2.6
1	A	239	GLU	2.6
1	A	245	TYR	2.6
1	B	217	TYR	2.6
1	B	269	THR	2.6
1	B	231	VAL	2.5
1	A	244	SER	2.5
1	A	312	LYS	2.5
1	A	314	ARG	2.5
1	B	234	PHE	2.5
1	B	355	VAL	2.5
1	A	353	GLU	2.5
1	B	410	ALA	2.5
1	B	367	GLU	2.5
1	A	266	GLY	2.5
1	B	408	HIS	2.5
1	B	418	GLY	2.5
1	A	276	THR	2.5
1	A	420	THR	2.5
1	A	421	THR	2.5
1	B	427	GLN	2.5
1	A	280	GLU	2.5
1	A	320	GLU	2.5
1	B	232	PRO	2.4
1	B	341	SER	2.4
1	A	264	LYS	2.4
1	A	431	HIS	2.4
1	A	212	SER	2.4
1	B	267	VAL	2.4
1	B	403	VAL	2.4
1	B	416	ASP	2.4
1	B	422	PRO	2.4
1	A	417	PHE	2.4
1	B	364	GLN	2.4
1	B	437	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	2.4
1	A	416	ASP	2.4
1	A	214	PRO	2.4
1	A	231	VAL	2.4
1	A	358	VAL	2.4
1	B	413	TRP	2.3
1	A	317	GLN	2.3
1	B	407	CYS	2.3
1	A	301	THR	2.3
1	A	328	LEU	2.3
1	B	235	HIS	2.3
1	A	233	ALA	2.3
1	B	388	GLU	2.3
1	B	321	GLY	2.3
1	B	268	ARG	2.3
1	B	420	THR	2.3
1	A	227	LEU	2.3
1	A	377	LEU	2.3
1	B	328	LEU	2.3
1	A	324	SER	2.3
1	B	347	LYS	2.3
1	B	412	VAL	2.3
1	A	445	LEU	2.3
1	B	374	LEU	2.3
1	B	456	ALA	2.2
1	B	357	ARG	2.2
1	A	333	GLU	2.2
1	B	451	LEU	2.2
1	B	332	ILE	2.2
1	B	439	ASN	2.2
1	B	368	GLU	2.2
1	B	352	ARG	2.2
1	B	362	PHE	2.2
1	B	389	PHE	2.2
1	A	306	ALA	2.2
1	B	397	GLY	2.2
1	A	217	TYR	2.2
1	A	415	ILE	2.2
1	A	388	GLU	2.2
1	A	440	ARG	2.2
1	B	395	VAL	2.2
1	A	439	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	309	ALA	2.2
1	B	401	LEU	2.2
1	A	274	GLU	2.2
1	B	342	CYS	2.1
1	A	402	PHE	2.1
1	B	402	PHE	2.1
1	B	459	ALA	2.1
1	A	413	TRP	2.1
1	B	350	ARG	2.1
1	A	256	ASP	2.1
1	A	404	HIS	2.1
1	B	222	LEU	2.1
1	B	227	LEU	2.1
1	A	398	SER	2.1
1	A	229	GLY	2.1
1	A	222	LEU	2.1
1	A	370	LEU	2.1
1	B	337	LYS	2.1
1	A	302	GLU	2.1
1	B	213	GLU	2.1
1	A	268	ARG	2.1
1	A	453	GLY	2.1
1	B	226	ALA	2.0
1	B	219	LEU	2.0
1	B	261	LEU	2.0
1	A	303	GLU	2.0
1	A	418	GLY	2.0
1	B	411	GLY	2.0
1	B	447	GLY	2.0
1	A	336	LYS	2.0
1	A	457	SER	2.0
1	B	248	LEU	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 monosaccharides 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(Å^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.