



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:21 AM UTC

PDB ID : 4U3Z / pdb_00004u3z
Title : APO MAP4K4 T181E Phosphomimetic Mutant
Authors : Harris, S.F.; Wu, P.; Coons, M.
Deposited on : 2014-07-23
Resolution : 2.09 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

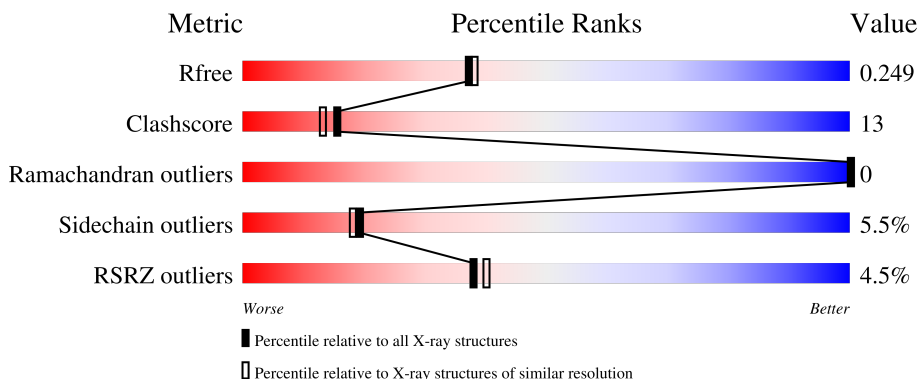
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	332	5% 61% 22% • 15%
1	B	332	3% 68% 19% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5145 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.

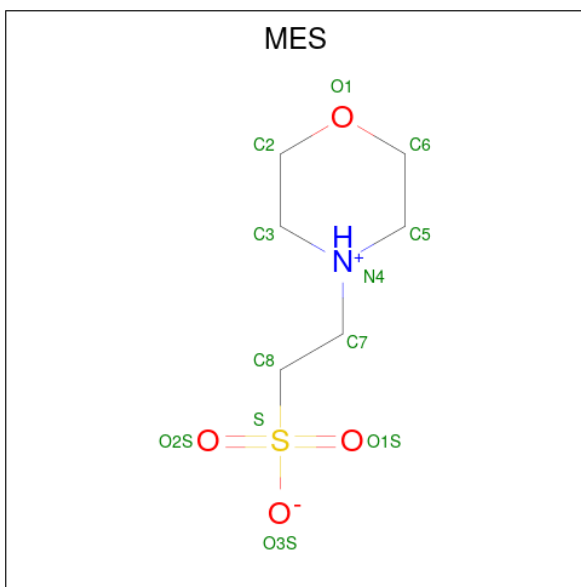
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	294	Total	C	N	O	S	0	3	0
			2414	1536	428	436	14			
1	A	282	Total	C	N	O	S	0	1	0
			2295	1465	409	407	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP O95819
B	1	SER	-	expression tag	UNP O95819
B	181	GLU	THR	engineered mutation	UNP O95819
B	329	GLY	-	expression tag	UNP O95819
B	330	ASN	-	expression tag	UNP O95819
B	331	SER	-	expression tag	UNP O95819
A	0	GLY	-	expression tag	UNP O95819
A	1	SER	-	expression tag	UNP O95819
A	181	GLU	THR	engineered mutation	UNP O95819
A	329	GLY	-	expression tag	UNP O95819
A	330	ASN	-	expression tag	UNP O95819
A	331	SER	-	expression tag	UNP O95819

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	210	Total	O	0	0
			210	210		
4	A	201	Total	O	0	0
			201	201		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.72Å 80.90Å 92.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.41 – 2.09 60.41 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (60.41-2.09) 99.9 (60.41-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.183 , 0.249 (Not available) , 0.249	Depositor DCC
R_{free} test set	1824 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5145	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: MES, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/2347	0.83	4/3168 (0.1%)
1	B	0.49	0/2472	0.79	4/3340 (0.1%)
All	All	0.48	0/4819	0.81	8/6508 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	TYR	N-CA-C	5.58	118.13	111.71
1	B	292	GLN	CA-C-N	5.30	125.01	119.82
1	B	292	GLN	C-N-CA	5.30	125.01	119.82
1	A	237	HIS	CA-C-N	5.28	124.73	119.24
1	A	237	HIS	C-N-CA	5.28	124.73	119.24
1	A	286	HIS	CA-C-N	5.11	125.14	119.32
1	A	286	HIS	C-N-CA	5.11	125.14	119.32
1	B	45	VAL	N-CA-C	5.01	115.73	110.67

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	2295	0	2316	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2414	0	2404	67	0
2	A	24	0	24	0	0
3	A	1	0	0	0	0
4	A	201	0	0	20	0
4	B	210	0	0	14	0
All	All	5145	0	4744	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:SER:HB3	4:A:697:HOH:O	1.39	1.19
1:A:57:ASP:HB2	1:A:185:ARG:HD3	1.26	1.16
1:A:92:LYS:HB3	1:A:93:SER:HB3	1.35	1.08
1:A:290:ARG:HB3	4:A:679:HOH:O	1.51	1.06
1:A:287:PRO:HA	4:A:679:HOH:O	1.59	1.02
1:A:236:MET:HE1	1:A:244:LEU:HD12	1.41	1.02
1:A:92:LYS:CB	1:A:93:SER:HB3	1.97	0.94
1:A:105:MET:HE1	1:A:170:VAL:HG13	1.53	0.90
1:B:179:ASP:HB2	4:B:595:HOH:O	1.74	0.86
1:A:57:ASP:CB	1:A:185:ARG:HD3	2.05	0.86
1:A:94:PRO:HA	1:A:95:PRO:C	2.01	0.84
1:A:210:TYR:HB2	4:A:697:HOH:O	1.78	0.83
1:A:69:GLU:HG3	1:A:177:GLN:HG2	1.60	0.82
1:B:211:ASP:OD1	1:B:213:ARG:HD3	1.85	0.76
1:B:212[B]:TYR:CE2	1:B:213:ARG:HD2	2.21	0.76
1:A:79:HIS:HD2	1:A:81:ASN:H	1.34	0.74
1:A:57:ASP:HB2	1:A:185:ARG:CD	2.13	0.74
1:B:237:HIS:HD2	1:B:239[B]:MET:H	1.36	0.73
1:A:236:MET:CE	1:A:244:LEU:HD12	2.17	0.73
1:A:75:LYS:HG3	4:A:683:HOH:O	1.87	0.73
1:B:143:HIS:HD2	4:B:559:HOH:O	1.71	0.72
1:A:92:LYS:HB3	1:A:93:SER:CB	2.18	0.72
1:B:236:MET:HE3	1:B:240:ARG:HG2	1.72	0.71
1:B:239[A]:MET:HE1	4:A:620:HOH:O	1.91	0.70
1:B:237:HIS:HD2	1:B:239[A]:MET:H	1.37	0.70
1:B:239[A]:MET:O	1:B:239[A]:MET:HE3	1.92	0.69
1:B:212[B]:TYR:CZ	1:B:213:ARG:HD2	2.28	0.69
1:B:44[A]:HIS:CE1	4:B:474:HOH:O	2.44	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:PRO:HA	4:B:580:HOH:O	1.92	0.68
1:A:236:MET:HE1	1:A:244:LEU:CD1	2.22	0.68
1:B:160:LEU:HD21	1:B:178:LEU:HD22	1.76	0.67
1:A:113:ILE:O	1:A:117:VAL:HG23	1.95	0.67
1:A:79:HIS:CD2	1:A:81:ASN:H	2.12	0.67
1:A:187:THR:HG22	1:A:188:PHE:CD2	2.31	0.66
1:B:35:THR:HG21	1:B:180:ARG:NH1	2.11	0.65
1:B:239[A]:MET:CG	4:A:645:HOH:O	2.44	0.65
1:B:237:HIS:CD2	1:B:239[B]:MET:H	2.15	0.64
1:B:237:HIS:CD2	1:B:239[A]:MET:H	2.16	0.64
1:B:311:LYS:HG2	4:B:448:HOH:O	1.98	0.63
1:A:57:ASP:HB2	1:A:185:ARG:HH11	1.63	0.63
1:B:91:LYS:HE2	4:B:584:HOH:O	2.00	0.61
1:B:178:LEU:HD23	4:B:567:HOH:O	1.99	0.61
1:A:291:ASP:HB2	4:A:700:HOH:O	2.03	0.59
1:A:60:GLU:OE1	1:A:94:PRO:HG2	2.04	0.58
1:A:135:ARG:HH22	1:A:295:GLU:CD	2.13	0.56
1:A:27:LEU:HG	1:A:102:TRP:CH2	2.40	0.56
1:B:29:GLU:O	1:B:29:GLU:HG3	2.07	0.55
1:B:38:GLN:HB3	1:B:40:TYR:CE2	2.42	0.55
1:B:302:LEU:O	1:B:306:ILE:HG13	2.06	0.54
1:A:132:TYR:HA	1:A:292:GLN:HE22	1.72	0.54
1:A:19:ARG:HB3	4:A:681:HOH:O	2.07	0.54
1:B:237:HIS:CD2	1:B:238:PRO:HD2	2.43	0.54
1:B:294:ASN:O	1:B:298:VAL:HG23	2.08	0.53
1:B:267:GLU:HG3	4:B:467:HOH:O	2.09	0.53
1:B:38:GLN:NE2	1:B:180:ARG:NH2	2.57	0.53
1:B:236:MET:HE3	1:B:240:ARG:CG	2.40	0.53
1:A:222:THR:O	1:A:225:GLU:HB3	2.08	0.52
1:B:79:HIS:HE1	1:B:81:ASN:HD22	1.57	0.52
1:A:57:ASP:HB2	1:A:185:ARG:NH1	2.25	0.52
1:A:204:GLU:H	1:A:204:GLU:CD	2.16	0.52
1:B:29:GLU:O	1:B:30:VAL:C	2.53	0.51
1:B:237:HIS:HB2	4:A:623:HOH:O	2.08	0.51
1:A:39:VAL:N	4:A:662:HOH:O	2.44	0.51
1:B:239[A]:MET:HG3	4:A:645:HOH:O	2.08	0.51
1:B:59:THR:O	1:B:63:GLU:HG3	2.12	0.50
1:B:201:ALA:HB1	1:A:243:PHE:HB2	1.93	0.50
1:B:143:HIS:O	1:B:146:ILE:HG22	2.12	0.50
1:A:185:ARG:O	1:A:185:ARG:HG3	2.12	0.49
1:B:157:GLN:HG2	4:B:500:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LYS:NZ	4:A:700:HOH:O	2.41	0.49
1:A:178:LEU:HG	4:A:688:HOH:O	2.13	0.49
1:B:35:THR:HB	1:B:38:GLN:HB2	1.95	0.48
1:B:203:ASP:OD2	1:A:203:ASP:OD2	2.30	0.48
1:B:239[A]:MET:CE	4:A:620:HOH:O	2.56	0.48
1:B:237:HIS:HE1	1:A:179:ASP:OD1	1.96	0.48
1:A:85:TYR:CZ	1:A:87:GLY:HA2	2.48	0.48
1:B:77:SER:O	1:B:143:HIS:HE1	1.96	0.48
1:B:297:GLN:O	1:B:301:GLN:HG3	2.14	0.48
1:B:56:MET:HE3	1:B:101:LEU:HD23	1.96	0.47
1:A:89:PHE:C	1:A:90:ILE:HD12	2.39	0.47
1:B:25:PHE:CZ	1:B:44[A]:HIS:HD2	2.33	0.47
1:B:151:HIS:O	1:B:152:ARG:HB2	2.13	0.47
1:B:236:MET:HE3	1:B:240:ARG:CD	2.45	0.47
1:A:141:LEU:CD1	1:A:219[B]:CYS:SG	3.03	0.47
1:A:257:LYS:HE3	4:A:689:HOH:O	2.14	0.47
1:A:304:ASP:O	1:A:308:ARG:HG2	2.15	0.46
1:A:236:MET:HE3	1:A:240:ARG:HG2	1.98	0.46
1:B:35:THR:HG21	1:B:180:ARG:HH11	1.78	0.46
1:B:308:ARG:HB3	1:B:308:ARG:CZ	2.45	0.46
1:A:47:THR:OG1	1:A:49:GLN:HG3	2.16	0.46
1:B:217:TRP:C	1:B:217:TRP:CD1	2.94	0.45
1:B:175:SER:HB2	4:B:606:HOH:O	2.16	0.45
1:A:44:HIS:CE1	1:A:47:THR:HG23	2.52	0.45
1:A:160:LEU:HG	1:A:170:VAL:CG2	2.48	0.44
1:B:121:LYS:C	1:B:121:LYS:HD3	2.43	0.44
1:A:179:ASP:O	1:A:179:ASP:CG	2.60	0.44
1:A:269:CYS:O	1:A:277:ARG:HD3	2.17	0.44
1:B:201:ALA:CB	1:A:243:PHE:HB2	2.48	0.44
1:A:60:GLU:HB3	4:A:694:HOH:O	2.18	0.44
1:B:227:ALA:HB1	1:B:258:TRP:CZ2	2.53	0.43
1:A:64:GLU:HG3	1:A:65:GLU:N	2.34	0.43
1:A:207:ASP:O	1:A:208:ALA:C	2.60	0.43
1:B:237:HIS:CG	1:B:238:PRO:HD2	2.53	0.43
1:A:104:VAL:C	1:A:105:MET:HG3	2.43	0.43
1:B:14:ASP:HA	4:B:538:HOH:O	2.18	0.43
1:B:236:MET:HE2	1:B:244:LEU:HD11	2.01	0.43
1:A:92:LYS:CG	1:A:93:SER:HB3	2.46	0.43
1:B:299:ARG:HB2	4:B:599:HOH:O	2.17	0.42
1:B:277:ARG:HG2	1:B:278:PRO:HD2	2.01	0.42
1:A:57:ASP:C	1:A:185:ARG:HG2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PHE:CE2	1:A:109:GLY:HA2	2.55	0.42
1:B:91:LYS:HB3	1:B:100:GLN:HB2	2.02	0.42
1:A:153:ASP:HB2	4:A:609:HOH:O	2.20	0.42
1:B:60:GLU:CD	1:B:60:GLU:H	2.28	0.41
1:A:39:VAL:HA	4:A:662:HOH:O	2.20	0.41
1:A:236:MET:HE3	1:A:236:MET:HB3	1.72	0.41
1:B:38:GLN:HE22	1:B:180:ARG:HH21	1.67	0.41
1:B:62:GLU:HA	1:B:65:GLU:OE1	2.21	0.41
1:A:27:LEU:HD22	1:A:40:TYR:CB	2.51	0.41
1:B:256:LYS:HB2	4:B:545:HOH:O	2.20	0.41
1:A:105:MET:HE3	1:A:105:MET:HB2	1.88	0.41
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.78	0.40
1:A:132:TYR:CA	1:A:292:GLN:HE22	2.33	0.40
1:B:91:LYS:HA	1:B:91:LYS:HD3	1.94	0.40
1:A:201:ALA:N	4:A:645:HOH:O	2.42	0.40
1:B:38:GLN:NE2	1:B:180:ARG:CZ	2.85	0.40
1:B:204:GLU:CD	4:B:577:HOH:O	2.64	0.40

There are no symmetry-related clashes.

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	275/332 (83%)	264 (96%)	11 (4%)	0	100	100
1	B	293/332 (88%)	286 (98%)	7 (2%)	0	100	100
All	All	568/664 (86%)	550 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	251/290 (87%)	231 (92%)	20 (8%)	11	8
1	B	263/290 (91%)	255 (97%)	8 (3%)	36	41
All	All	514/580 (89%)	486 (95%)	28 (5%)	19	18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	THR
1	B	60	GLU
1	B	121	LYS
1	B	164	ASN
1	B	189	ILE
1	B	199	VAL
1	B	204	GLU
1	B	213	ARG
1	A	29	GLU
1	A	31	VAL
1	A	39	VAL
1	A	59	THR
1	A	68	LEU
1	A	126	LYS
1	A	146	ILE
1	A	163	GLU
1	A	179	ASP
1	A	182	VAL
1	A	185	ARG
1	A	187	THR
1	A	199	VAL
1	A	203	ASP
1	A	204	GLU
1	A	240	ARG
1	A	260	LYS
1	A	280	THR
1	A	308	ARG

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Mol	Chain	Res	Type
1	A	309	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	81	ASN
1	B	143	HIS
1	B	237	HIS
1	B	294	ASN
1	B	305	HIS
1	A	71	ASN
1	A	79	HIS
1	A	81	ASN
1	A	123	ASN
1	A	148	HIS
1	A	164	ASN
1	A	186	ASN
1	A	292	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	MES	A	401	-	12,12,12	1.37	1 (8%)	15,16,16	1.69	5 (33%)
2	MES	A	402	-	12,12,12	1.38	3 (25%)	15,16,16	1.82	5 (33%)

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	MES	A	401	-	-	0/6/14/14	0/1/1/1
2	MES	A	402	-	-	5/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	MES	C8-S	-2.51	1.74	1.77
2	A	402	MES	O1S-S	2.35	1.51	1.45
2	A	402	MES	C5-N4	-2.12	1.41	1.46
2	A	402	MES	C7-C8	2.06	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	MES	C7-N4-C3	3.26	119.91	111.24
2	A	402	MES	O1S-S-C8	3.20	111.56	106.73
2	A	401	MES	O2S-S-C8	2.97	111.22	106.73
2	A	402	MES	O2S-S-C8	2.71	110.83	106.73
2	A	401	MES	O1S-S-C8	2.47	110.45	106.73
2	A	401	MES	C2-C3-N4	2.41	113.79	110.12
2	A	402	MES	C7-N4-C5	2.39	117.60	111.24
2	A	401	MES	C6-C5-N4	2.38	113.74	110.12
2	A	401	MES	C7-N4-C3	2.15	116.98	111.24
2	A	402	MES	O2S-S-O1S	-2.14	106.87	113.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	MES	C8-C7-N4-C3
2	A	402	MES	C8-C7-N4-C5
2	A	402	MES	C7-C8-S-O3S
2	A	402	MES	C7-C8-S-O1S
2	A	402	MES	C7-C8-S-O2S

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	282/332 (84%)	0.15	17 (6%)	27 29	11, 34, 67, 108	1 (0%)
1	B	294/332 (88%)	-0.05	9 (3%)	51 54	12, 31, 56, 79	3 (1%)
All	All	576/664 (86%)	0.05	26 (4%)	38 40	11, 33, 63, 108	4 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	VAL	4.2
1	B	212[A]	TYR	3.8
1	B	30	VAL	3.6
1	B	17	SER	3.4
1	B	16	SER	3.3
1	A	31	VAL	3.3
1	B	176	ALA	3.1
1	A	95	PRO	2.9
1	A	68	LEU	2.8
1	B	209	THR	2.8
1	A	23	GLY	2.7
1	A	107	PHE	2.5
1	A	66	ILE	2.4
1	A	94	PRO	2.4
1	B	182	VAL	2.3
1	A	22	ALA	2.2
1	A	59	THR	2.2
1	B	35	THR	2.2
1	A	57	ASP	2.2
1	A	18	LEU	2.2
1	A	29	GLU	2.1
1	A	39	VAL	2.1
1	A	58	VAL	2.1
1	A	99	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	19	ARG	2.1
1	B	18	LEU	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	MES	A	402	12/12	0.83	0.14	36,50,56,60	0
3	NA	A	403	1/1	0.91	0.10	42,42,42,42	0
2	MES	A	401	12/12	0.98	0.05	22,25,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.