Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:15 pm GMT

PDB ID	:	4M69
Title	:	Crystal structure of the mouse RIP3-MLKL complex
Authors	:	Xie, T.; Peng, W.; Yan, C.; Wu, J.; Shi, Y.
Deposited on	:	2013-08-09
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949
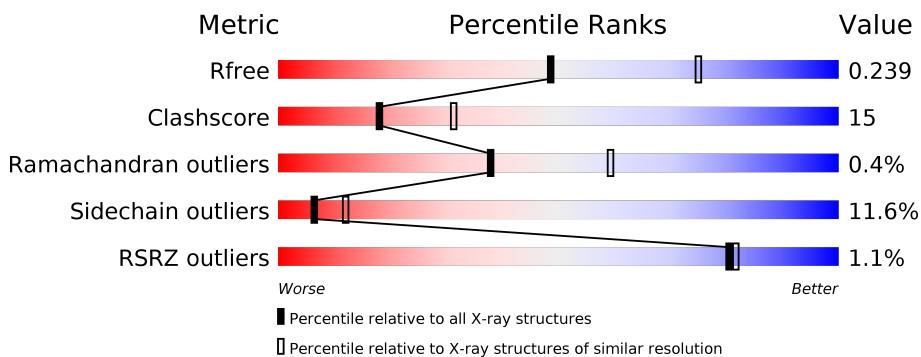
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
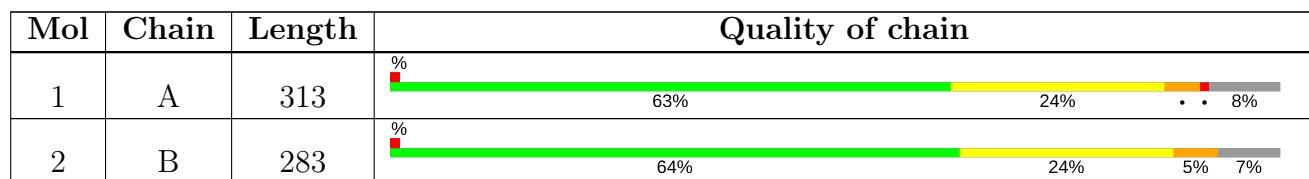
The reported resolution of this entry is 2.50 Å.

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		0.239
Clashscore		15
Ramachandran outliers		0.4%
Sidechain outliers		11.6%
RSRZ outliers		1.1%

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	63% 24% · · 8%
2	B	283	64% 24% 5% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	402	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 4613 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.
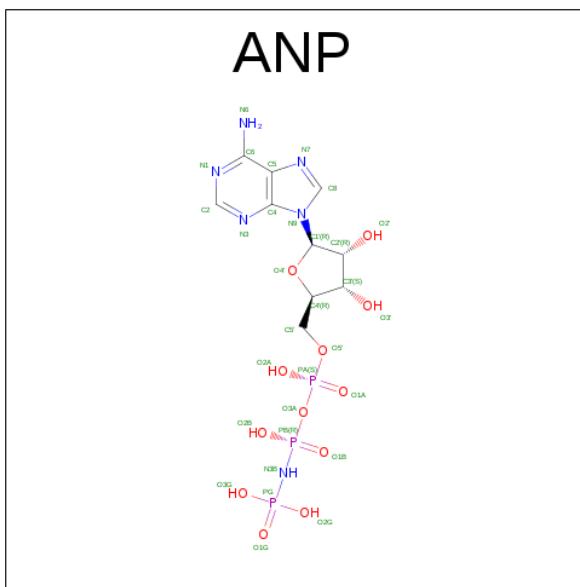
- Molecule 1 is a protein called Receptor-interacting serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total 2284	C 1454	N 390	O 427	P 3	S 10	0	1	0

- Molecule 2 is a protein called Mixed lineage kinase domain-like protein.
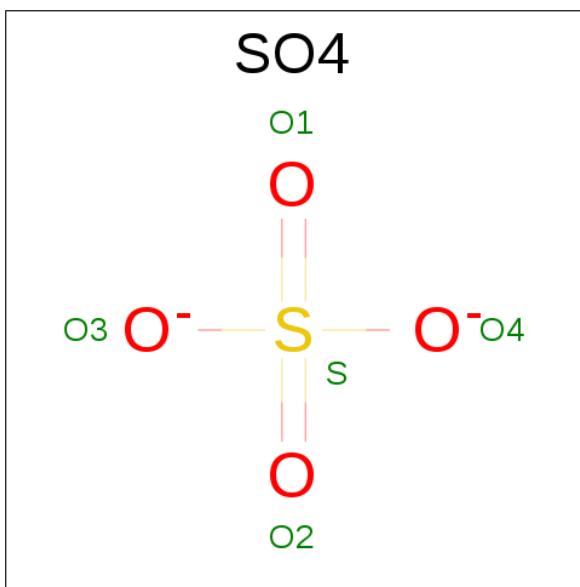
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total 2118	C 1347	N 365	O 396	S 10	0	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Cl 2	0	0
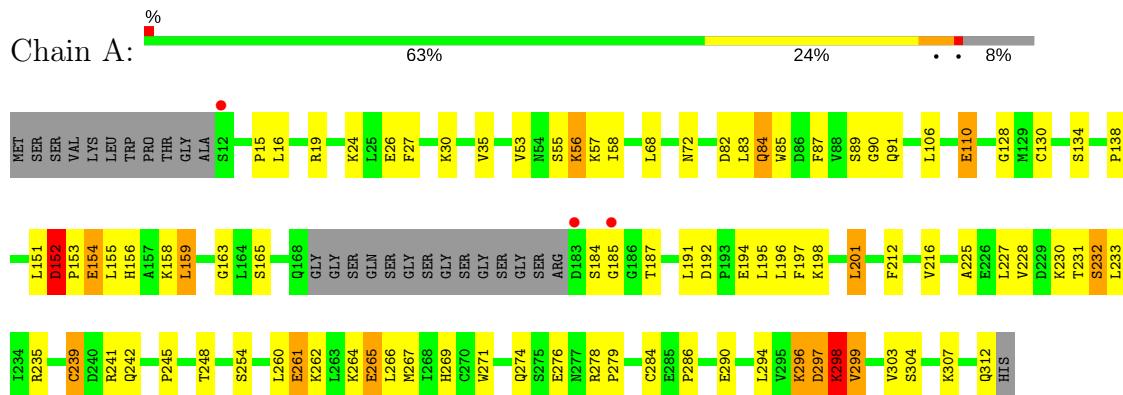
- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	109	Total 109	O 109	0	0
7	B	58	Total 58	O 58	0	0

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 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: Receptor-interacting serine/threonine-protein kinase 3

• Molecule 2: Mixed lineage kinase domain-like protein

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	106.44Å 141.95Å 107.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 2.50 39.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.57-2.50) 95.7 (39.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.220 , 0.246 0.212 , 0.239	Depositor DCC
R_{free} test set	1440 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4613	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: MG, CL, TPO, SEP, ANP, 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	0.47	4/2303 (0.2%)	0.58	2/3123 (0.1%)
2	B	0.41	2/2160 (0.1%)	0.53	2/2913 (0.1%)
All	All	0.44	6/4463 (0.1%)	0.55	4/6036 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	PRO	N-CD	5.36	1.55	1.47
1	A	153	PRO	N-CD	5.31	1.55	1.47
1	A	15	PRO	N-CD	5.28	1.55	1.47
2	B	224	PRO	N-CD	5.22	1.55	1.47
1	A	138	PRO	N-CD	5.16	1.55	1.47
2	B	372	PRO	N-CD	5.07	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	371	ASN	C-N-CD	5.71	140.40	128.40
2	B	223	ASN	C-N-CD	5.57	140.10	128.40
1	A	152	ASP	C-N-CD	5.54	140.04	128.40
1	A	278	ARG	C-N-CD	5.52	139.99	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	TPO	Mainchain
1	A	232	SEP	Mainchain

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	2284	0	2287	69	0
2	B	2118	0	2150	72	0
3	A	31	0	13	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	109	0	0	8	0
7	B	58	0	0	5	0
All	All	4613	0	4450	134	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 15.

All (134) 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)
2:B:202:LYS:HG2	2:B:203:MET:HG2	1.36	1.07
1:A:228:VAL:HG21	1:A:233:LEU:HD23	1.35	1.03
2:B:202:LYS:HD3	2:B:203:MET:H	1.21	1.02
2:B:359:SER:O	2:B:362:ILE:HG12	1.65	0.95
1:A:197:PHE:HD2	1:A:239:CYS:SG	1.96	0.89
1:A:197:PHE:CE2	1:A:239:CYS:HB2	2.08	0.88
2:B:202:LYS:CD	2:B:203:MET:H	1.87	0.86
1:A:297:ASP:C	1:A:298:LYS:HG2	1.94	0.85
1:A:197:PHE:HD2	1:A:239:CYS:HG	0.84	0.82
1:A:286:PRO:O	1:A:290:GLU:HG3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:VAL:CG2	1:A:233:LEU:HD23	2.12	0.79
2:B:202:LYS:HG2	2:B:203:MET:CG	2.13	0.79
1:A:197:PHE:CD2	1:A:239:CYS:SG	2.73	0.78
2:B:202:LYS:CG	2:B:203:MET:HG2	2.13	0.78
1:A:265:GLU:OE2	1:A:269[B]:HIS:CD2	2.39	0.76
1:A:163:GLY:HA2	7:A:585:HOH:O	1.86	0.75
1:A:154:GLU:O	1:A:155:LEU:HB2	1.88	0.74
2:B:183:ILE:HG13	2:B:184:LYS:H	1.51	0.74
1:A:228:VAL:HG21	1:A:233:LEU:CD2	2.13	0.73
1:A:228:VAL:HG22	2:B:372:PRO:HB3	1.70	0.73
1:A:184:SEP:O	1:A:187:THR:HG22	1.88	0.72
1:A:197:PHE:HE2	1:A:239:CYS:HB2	1.51	0.72
2:B:291:THR:HG23	7:B:608:HOH:O	1.88	0.71
2:B:183:ILE:HG23	2:B:184:LYS:N	2.04	0.71
1:A:53:VAL:CG1	1:A:55:SER:OG	2.38	0.70
1:A:194:GLU:O	1:A:198:LYS:HB2	1.93	0.69
2:B:202:LYS:HD3	2:B:203:MET:N	2.03	0.69
2:B:288:LYS:N	2:B:288:LYS:HD2	2.09	0.68
1:A:84:GLN:HG2	1:A:89:SER:HB3	1.76	0.68
1:A:30:LYS:HE3	7:A:571:HOH:O	1.94	0.68
1:A:296:LYS:O	1:A:299:VAL:HG22	1.95	0.67
1:A:265:GLU:OE2	1:A:269[B]:HIS:HD2	1.77	0.67
1:A:297:ASP:O	1:A:298:LYS:HG2	1.94	0.67
2:B:202:LYS:CD	2:B:203:MET:N	2.59	0.65
2:B:279:THR:HG22	2:B:282:GLU:H	1.62	0.65
1:A:227:LEU:CD2	2:B:372:PRO:HB2	2.27	0.65
1:A:72:ASN:ND2	7:A:505:HOH:O	2.21	0.61
2:B:202:LYS:HD2	2:B:202:LYS:N	2.15	0.61
2:B:281:ARG:HH11	2:B:281:ARG:HA	1.66	0.61
1:A:261:GLU:CD	1:A:261:GLU:H	2.04	0.60
2:B:368:ARG:HH21	2:B:368:ARG:CG	2.15	0.59
1:A:227:LEU:HD22	2:B:372:PRO:HB2	1.85	0.58
1:A:297:ASP:O	1:A:298:LYS:CG	2.51	0.58
2:B:288:LYS:CB	7:B:645:HOH:O	2.51	0.58
1:A:296:LYS:NZ	7:A:578:HOH:O	2.36	0.58
2:B:281:ARG:HH12	2:B:284:LEU:HB2	1.69	0.58
2:B:202:LYS:CG	2:B:203:MET:N	2.67	0.57
2:B:225:GLN:O	2:B:226:ALA:HB3	2.05	0.56
2:B:316:HIS:O	2:B:317:ARG:HB2	2.05	0.56
2:B:235:THR:HG22	2:B:338:GLU:HG2	1.88	0.55
2:B:368:ARG:NH2	2:B:374:CYS:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ARG:NH1	2:B:284:LEU:HB2	2.20	0.55
1:A:184:SEP:O	1:A:187:THR:N	2.39	0.55
2:B:375:LEU:HD22	2:B:376:TYR:N	2.21	0.55
2:B:368:ARG:NH1	7:B:619:HOH:O	2.40	0.55
1:A:56:LYS:HA	1:A:90:GLY:HA3	1.88	0.54
1:A:19:ARG:HB3	1:A:83:LEU:CD2	2.38	0.54
1:A:56:LYS:CD	1:A:89:SER:O	2.56	0.54
2:B:242:THR:O	2:B:245:LYS:HB3	2.08	0.53
1:A:184:SEP:N	1:A:187:THR:HG22	2.22	0.53
1:A:198:LYS:HB3	1:A:201:LEU:HB2	1.90	0.53
2:B:361:THR:HG22	2:B:369:LEU:HD21	1.91	0.52
1:A:260:LEU:HG	1:A:264:LYS:HE3	1.92	0.52
1:A:197:PHE:CE2	1:A:239:CYS:CB	2.90	0.52
1:A:197:PHE:CZ	1:A:235:ARG:HA	2.43	0.52
1:A:192:ASP:HB3	1:A:195:LEU:HD12	1.90	0.52
2:B:288:LYS:H	2:B:288:LYS:CD	2.23	0.52
1:A:228:VAL:HG12	2:B:368:ARG:NE	2.25	0.52
2:B:264:LYS:HD2	2:B:265:PRO:HA	1.91	0.51
1:A:56:LYS:HD3	1:A:89:SER:O	2.11	0.51
1:A:58:ILE:HG12	1:A:91:GLN:HB2	1.92	0.51
2:B:364:VAL:CG1	2:B:368:ARG:HB3	2.41	0.51
2:B:368:ARG:CG	2:B:368:ARG:NH2	2.73	0.51
2:B:399:PHE:HB3	2:B:402:CYS:HB2	1.94	0.50
1:A:254:SER:HB3	7:A:519:HOH:O	2.11	0.50
2:B:368:ARG:HG2	2:B:368:ARG:NH2	2.26	0.50
2:B:367:GLU:HG2	2:B:368:ARG:N	2.27	0.49
2:B:229:VAL:HG11	2:B:266:PRO:O	2.13	0.49
1:A:241:ARG:NH1	7:A:563:HOH:O	2.46	0.49
2:B:246:PHE:HA	2:B:308:ARG:NH1	2.27	0.49
2:B:399:PHE:O	2:B:402:CYS:HB2	2.12	0.49
2:B:331:GLN:HB3	7:B:628:HOH:O	2.12	0.48
1:A:228:VAL:O	1:A:228:VAL:HG23	2.14	0.48
2:B:183:ILE:HG23	2:B:184:LYS:H	1.78	0.48
2:B:299:VAL:HG23	2:B:392:ILE:HG21	1.96	0.48
1:A:212:PHE:O	1:A:216:VAL:HG23	2.13	0.48
1:A:266:LEU:HD11	1:A:284:CYS:SG	2.54	0.47
1:A:185:GLY:HA3	1:A:227:LEU:O	2.14	0.47
1:A:24:LYS:HB2	1:A:85:TRP:CZ3	2.49	0.47
2:B:224:PRO:HD2	2:B:225:GLN:OE1	2.15	0.47
2:B:420:VAL:HG12	2:B:421:GLY:H	1.80	0.47
1:A:53:VAL:HG12	1:A:55:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:LYS:HG2	2:B:203:MET:N	2.30	0.46
2:B:389:LEU:HA	2:B:389:LEU:HD23	1.72	0.46
1:A:56:LYS:HD2	1:A:89:SER:O	2.16	0.46
2:B:281:ARG:HH11	2:B:281:ARG:CA	2.27	0.46
2:B:430:GLU:O	2:B:434:GLU:HG3	2.15	0.46
1:A:128:GLY:HA3	1:A:159:LEU:HD22	1.98	0.45
2:B:279:THR:HG22	2:B:281:ARG:N	2.32	0.45
2:B:288:LYS:H	2:B:288:LYS:HD2	1.79	0.45
1:A:53:VAL:HG11	1:A:55:SER:OG	2.15	0.45
1:A:297:ASP:O	1:A:298:LYS:CB	2.65	0.45
1:A:110:GLU:HB2	7:A:568:HOH:O	2.15	0.45
1:A:232:SEP:O2P	2:B:404:SER:OG	2.21	0.44
1:A:19:ARG:HB3	1:A:83:LEU:HD23	2.00	0.44
1:A:276:GLU:CD	1:A:276:GLU:H	2.21	0.44
1:A:27:PHE:HE1	1:A:35:VAL:HG13	1.83	0.44
2:B:277:LEU:O	2:B:286:ARG:NH2	2.51	0.44
2:B:281:ARG:O	2:B:281:ARG:NH1	2.51	0.44
1:A:24:LYS:HB3	1:A:85:TRP:CZ2	2.53	0.43
2:B:235:THR:CG2	2:B:338:GLU:HG2	2.47	0.43
2:B:202:LYS:H	2:B:202:LYS:HD2	1.81	0.43
1:A:152:ASP:OD1	1:A:156:HIS:N	2.44	0.43
2:B:183:ILE:HG13	2:B:184:LYS:N	2.25	0.43
2:B:387:ILE:O	2:B:391:GLU:HG3	2.18	0.43
1:A:87:PHE:O	2:B:228:SER:HB3	2.18	0.43
2:B:279:THR:HG23	2:B:322:SER:HA	1.99	0.43
1:A:158:LYS:NZ	4:A:402:SO4:O2	2.51	0.42
2:B:375:LEU:HD13	2:B:377:ASP:HB3	2.01	0.42
1:A:154:GLU:O	1:A:155:LEU:CB	2.62	0.42
2:B:324:PHE:CE2	2:B:334:LEU:HD13	2.54	0.42
1:A:225:ALA:HA	7:A:503:HOH:O	2.18	0.42
1:A:303:VAL:HG12	1:A:307:LYS:HD3	2.02	0.42
2:B:246:PHE:HB3	2:B:308:ARG:CG	2.50	0.42
2:B:394:THR:HB	2:B:396:LYS:HG3	2.02	0.42
2:B:397:ILE:HB	2:B:400:GLU:HG3	2.02	0.42
1:A:130:CYS:O	1:A:134:SER:HB3	2.20	0.41
2:B:428:LEU:HA	2:B:428:LEU:HD23	1.84	0.41
1:A:245:PRO:HG3	2:B:373:PHE:CD1	2.56	0.41
2:B:290:LEU:HA	7:B:608:HOH:O	2.21	0.41
2:B:185:GLU:HG2	2:B:257:ILE:HD11	2.02	0.41
1:A:191:LEU:HD23	1:A:196:LEU:HG	2.03	0.40
2:B:225:GLN:CD	2:B:225:GLN:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG12	1:A:267:MET:HE2	2.04	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	281/313 (90%)	259 (92%)	21 (8%)	1 (0%)	38	59
2	B	260/283 (92%)	247 (95%)	12 (5%)	1 (0%)	38	59
All	All	541/596 (91%)	506 (94%)	33 (6%)	2 (0%)	38	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	LYS
2	B	183	ILE

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	252/269 (94%)	221 (88%)	31 (12%)	5	10
2	B	240/257 (93%)	214 (89%)	26 (11%)	7	14
All	All	492/526 (94%)	435 (88%)	57 (12%)	6	12

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	26	GLU
1	A	56	LYS
1	A	57	LYS
1	A	68	LEU
1	A	82	ASP
1	A	84	GLN
1	A	106	LEU
1	A	110	GLU
1	A	151	LEU
1	A	152	ASP
1	A	154	GLU
1	A	159	LEU
1	A	165	SER
1	A	201	LEU
1	A	230	LYS
1	A	239	CYS
1	A	242	GLN
1	A	248	THR
1	A	261	GLU
1	A	262	LYS
1	A	265	GLU
1	A	271	TRP
1	A	274	GLN
1	A	294	LEU
1	A	296	LYS
1	A	297	ASP
1	A	298	LYS
1	A	299	VAL
1	A	304	SER
1	A	312	GLN
2	B	182	GLN
2	B	184	LYS
2	B	189	GLU
2	B	199	LYS
2	B	200	THR
2	B	202	LYS
2	B	225	GLN
2	B	244	LYS
2	B	269	SER
2	B	281	ARG
2	B	287	GLU

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Mol	Chain	Res	Type
2	B	288	LYS
2	B	291	THR
2	B	308	ARG
2	B	339	LEU
2	B	344	ASN
2	B	358	SER
2	B	360	SER
2	B	366	PRO
2	B	368	ARG
2	B	375	LEU
2	B	416	LYS
2	B	422	GLN
2	B	428	LEU
2	B	430	GLU
2	B	453	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	B	182	GLN
2	B	331	GLN
2	B	422	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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
1	SEP	A	184	1	9,9,10	0.69	0	9,12,14	1.24	0
1	TPO	A	231	1	9,10,11	0.77	0	10,14,16	1.49	1 (10%)
1	SEP	A	232	1	9,9,10	0.68	0	9,12,14	1.50	2 (22%)

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
1	SEP	A	184	1	-	0/5/8/10	0/0/0/0
1	TPO	A	231	1	-	0/8/11/13	0/0/0/0
1	SEP	A	232	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	TPO	O-C-CA	-3.12	117.86	125.15
1	A	232	SEP	O-C-CA	-2.33	118.57	125.02
1	A	232	SEP	OG-CB-CA	2.56	110.69	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	184	SEP	3	0
1	A	232	SEP	1	0

5.5　Carbohydrates　ⓘ

There are no carbohydrates in this entry.

5.6　Ligand geometry　ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	#$|Z| > 2$
3	ANP	A	401	5	29,33,33	1.98	8 (27%)	28,52,52	2.03	7 (25%)
4	SO4	A	402	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	B	501	-	4,4,4	0.40	0	6,6,6	0.06	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
3	ANP	A	401	5	-	0/13/38/38	0/3/3/3
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	SO4	B	501	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ANP	PG-O3G	-2.13	1.50	1.56
3	A	401	ANP	PB-O2B	-2.12	1.50	1.56
3	A	401	ANP	PG-O2G	-2.05	1.51	1.56
3	A	401	ANP	C5-C4	3.03	1.47	1.40
3	A	401	ANP	PG-O1G	4.23	1.50	1.46
3	A	401	ANP	PB-O1B	4.40	1.51	1.46
3	A	401	ANP	PG-N3B	4.43	1.75	1.63
3	A	401	ANP	PB-N3B	4.46	1.75	1.63

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ANP	N3-C2-N1	-5.90	123.72	128.86
3	A	401	ANP	O1G-PG-N3B	-4.98	104.35	111.79
3	A	401	ANP	C4-C5-N7	-2.95	106.56	109.41
3	A	401	ANP	PA-O3A-PB	-2.56	123.33	132.38
3	A	401	ANP	O1B-PB-N3B	-2.10	108.65	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ANP	O3G-PG-O2G	2.21	113.87	107.69
3	A	401	ANP	O2B-PB-O1B	4.00	118.19	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	SO4	1	0

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	284/313 (90%)	-0.18	3 (1%)	80	81	24, 44, 78, 124	0
2	B	264/283 (93%)	-0.14	3 (1%)	80	81	32, 51, 84, 123	0
All	All	548/596 (91%)	-0.16	6 (1%)	80	81	24, 48, 82, 124	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	SER	3.4
2	B	458	GLU	2.7
1	A	185	GLY	2.7
1	A	183	ASP	2.4
2	B	456	VAL	2.3
2	B	200	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	A	184	10/11	0.88	0.17	-	122,125,126,126	0
1	TPO	A	231	11/12	0.85	0.22	-	99,99,100,100	0
1	SEP	A	232	10/11	0.94	0.12	-	66,67,67,67	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	402	5/5	0.75	0.35	5.51	106,106,107,107	0
3	ANP	A	401	31/31	0.97	0.15	0.08	30,31,34,35	0
4	SO4	B	501	5/5	0.89	0.16	-0.28	97,97,97,97	0
6	CL	A	404	1/1	0.92	0.13	-	75,75,75,75	0
6	CL	A	405	1/1	0.72	0.09	-	81,81,81,81	0
5	MG	A	403	1/1	0.96	0.07	-	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.