



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:59 AM GMT

PDB ID : 3OS3
Title : Mitogen-activated protein kinase kinase 1 (MEK1) in complex with CH4858061 and MgATP
Authors : Lukacs, C.M.; Janson, C.; Schuck, V.; Belunis, C.
Deposited on : 2010-09-08
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

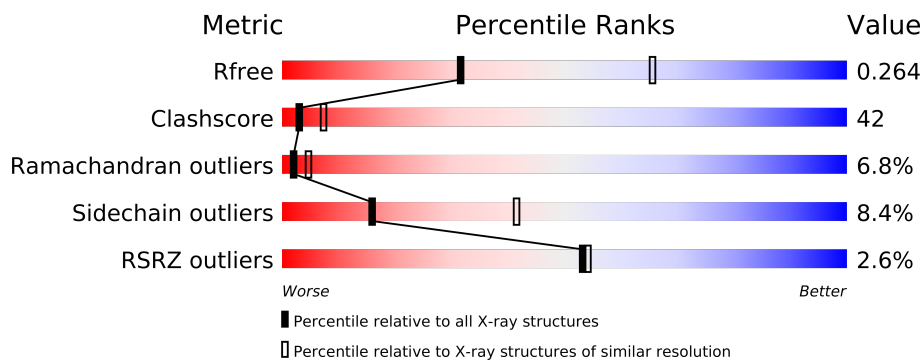
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	307	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	3OS	A	400	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 2203 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

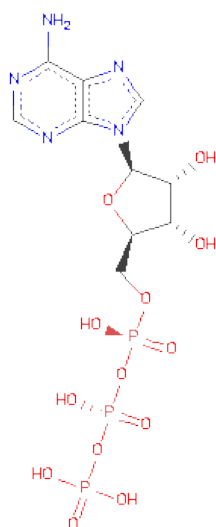
- Molecule 1 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2137	1367	363	392	15	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

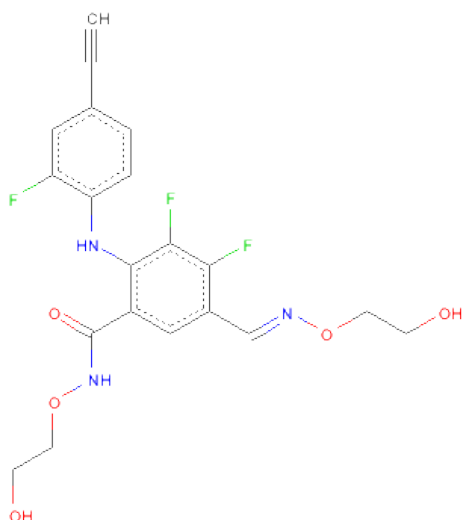
Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MET	-	EXPRESSION TAG	UNP Q02750
A	394	HIS	-	EXPRESSION TAG	UNP Q02750
A	395	HIS	-	EXPRESSION TAG	UNP Q02750
A	396	HIS	-	EXPRESSION TAG	UNP Q02750
A	397	HIS	-	EXPRESSION TAG	UNP Q02750
A	398	HIS	-	EXPRESSION TAG	UNP Q02750
A	399	HIS	-	EXPRESSION TAG	UNP Q02750

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 2-[(4-ETHYNYL-2-FLUOROPHENYL)AMINO]-3,4-DIFLUORO-N-(2-HYDROXYETHOXY)-5-[[[(2-HYDROXYETHOXY)IMINO]METHYL}BENZAMIDE (three-letter code: 3OS) (formula: C₂₀H₁₈F₃N₃O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			31	20	3	3	5		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

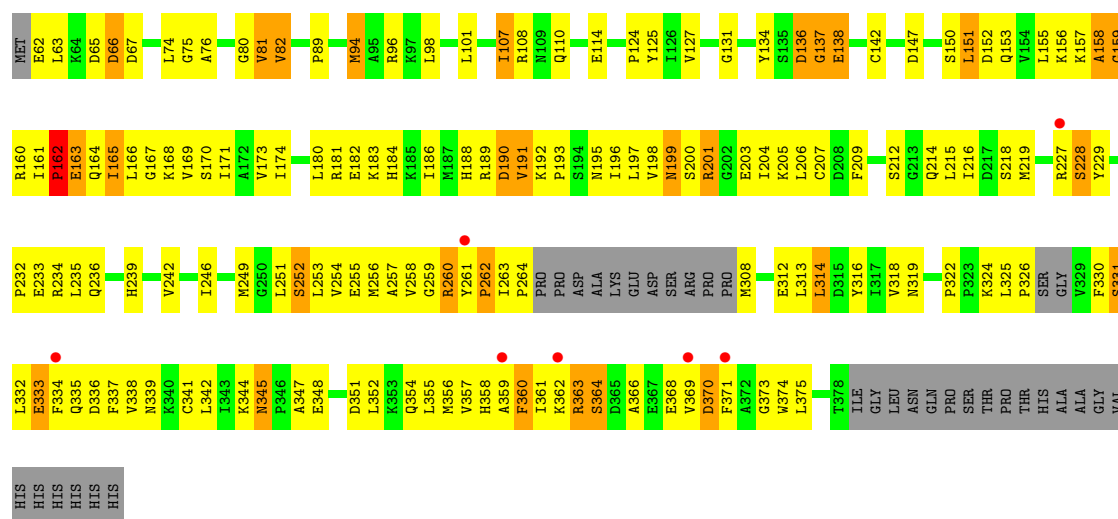
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.00Å 73.00Å 131.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.57 – 2.80 45.57 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.57-2.80) 99.1 (45.57-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.24 (at 2.77Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.268 , 0.356 0.273 , 0.264	Depositor DCC
R_{free} test set	519 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	1.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.4	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 10724 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2203	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3OS, ATP

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	0.44	0/2179	0.69	0/2934

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2137	0	2161	184	0
2	A	31	0	12	2	0
3	A	31	0	18	2	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
All	All	2203	0	2191	184	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

All (184) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:ARG:HD3	1:A:261:TYR:H	1.08	1.13
1:A:260:ARG:HD3	1:A:261:TYR:N	1.79	0.96
1:A:164:GLN:HB3	1:A:369:VAL:HG21	1.48	0.95
1:A:199:ASN:HD21	1:A:203:GLU:H	1.16	0.93
1:A:358:HIS:O	1:A:362:LYS:HG2	1.70	0.91
1:A:108:ARG:HD2	1:A:134:TYR:CD1	2.07	0.89
1:A:162:PRO:HB2	1:A:165:ILE:HB	1.61	0.83
1:A:165:ILE:HD12	1:A:369:VAL:HG11	1.61	0.81
1:A:188:HIS:O	1:A:189:ARG:HB3	1.82	0.79
1:A:362:LYS:HE2	1:A:362:LYS:HA	1.66	0.77
1:A:184:HIS:O	1:A:186:ILE:HG23	1.84	0.77
1:A:355:LEU:H	1:A:355:LEU:HD12	1.50	0.77
1:A:333:GLU:HB3	1:A:360:PHE:HB2	1.68	0.74
1:A:182:GLU:O	1:A:183:LYS:HD2	1.88	0.73
1:A:164:GLN:HB3	1:A:369:VAL:CG2	2.19	0.72
1:A:260:ARG:NH1	1:A:260:ARG:HA	2.05	0.72
1:A:199:ASN:HD21	1:A:203:GLU:N	1.85	0.72
1:A:192:LYS:HB2	1:A:193:PRO:HD2	1.73	0.71
1:A:108:ARG:HD2	1:A:134:TYR:CE1	2.25	0.71
1:A:308:MET:HE2	1:A:312:GLU:HG2	1.72	0.71
1:A:75:GLY:HA3	2:A:1:ATP:H4'	1.73	0.71
1:A:324:LYS:O	1:A:325:LEU:HG	1.90	0.70
1:A:345:ASN:HD22	1:A:348:GLU:H	1.41	0.69
1:A:354:GLN:O	1:A:357:VAL:HG22	1.94	0.68
1:A:199:ASN:ND2	1:A:203:GLU:H	1.91	0.68
1:A:333:GLU:CB	1:A:360:PHE:HB2	2.24	0.67
1:A:333:GLU:C	1:A:335:GLN:H	1.97	0.67
1:A:158:ALA:O	1:A:160:ARG:N	2.26	0.66
1:A:150:SER:C	1:A:152:ASP:H	2.01	0.64
1:A:227:ARG:NH1	1:A:261:TYR:HB2	2.13	0.64
1:A:165:ILE:HG22	1:A:166:LEU:N	2.11	0.63
1:A:74:LEU:HB2	1:A:82:VAL:HG23	1.81	0.62
1:A:63:LEU:HD12	1:A:131:GLY:HA3	1.79	0.62
1:A:345:ASN:ND2	1:A:348:GLU:H	1.97	0.62
1:A:359:ALA:HA	1:A:362:LYS:CG	2.31	0.61
1:A:74:LEU:HB2	1:A:82:VAL:CG2	2.30	0.61
1:A:368:GLU:HG3	1:A:368:GLU:O	1.99	0.61
1:A:318:VAL:HG23	1:A:319:ASN:ND2	2.16	0.60
1:A:254:VAL:HG23	1:A:338:VAL:HG22	1.83	0.60
1:A:351:ASP:O	1:A:355:LEU:HD12	2.02	0.60
1:A:110:GLN:O	1:A:114:GLU:HG3	2.02	0.60
1:A:173:VAL:HG22	1:A:206:LEU:HD21	1.82	0.60
1:A:359:ALA:HA	1:A:362:LYS:HG3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:322:PRO:HB2	1:A:342:LEU:HB3	1.83	0.60
1:A:333:GLU:O	1:A:335:GLN:N	2.34	0.59
1:A:199:ASN:ND2	1:A:203:GLU:HB2	2.18	0.58
1:A:308:MET:CE	1:A:312:GLU:HG2	2.32	0.58
1:A:254:VAL:O	1:A:258:VAL:HG22	2.04	0.58
1:A:199:ASN:ND2	1:A:203:GLU:N	2.51	0.57
1:A:155:LEU:O	1:A:157:LYS:N	2.38	0.57
1:A:370:ASP:OD2	1:A:373:GLY:N	2.31	0.57
1:A:198:VAL:HG12	1:A:204:ILE:HG12	1.87	0.57
1:A:263:ILE:HG21	1:A:313:LEU:HD11	1.86	0.57
1:A:215:LEU:O	1:A:219:MET:HG2	2.04	0.57
1:A:161:ILE:HG22	1:A:165:ILE:HG21	1.87	0.56
1:A:337:PHE:HD1	1:A:358:HIS:CD2	2.23	0.56
1:A:333:GLU:H	1:A:333:GLU:CD	2.08	0.56
1:A:232:PRO:O	1:A:236:GLN:HG3	2.06	0.56
1:A:161:ILE:HG22	1:A:162:PRO:HD2	1.87	0.55
1:A:333:GLU:HG3	1:A:359:ALA:HB3	1.88	0.55
1:A:159:GLY:O	1:A:160:ARG:HG3	2.06	0.55
1:A:260:ARG:HA	1:A:260:ARG:CZ	2.36	0.54
1:A:107:ILE:HD12	1:A:214:GLN:OE1	2.07	0.54
1:A:227:ARG:O	1:A:228:SER:HB2	2.08	0.54
1:A:192:LYS:O	1:A:196:ILE:HG13	2.07	0.54
1:A:80:GLY:HA3	3:A:400:3OS:O31	2.07	0.54
1:A:107:ILE:HD11	1:A:218:SER:OG	2.08	0.54
1:A:67:ASP:HB3	1:A:89:PRO:CD	2.38	0.53
1:A:171:ILE:HD11	1:A:361:ILE:HG23	1.89	0.53
1:A:313:LEU:O	1:A:313:LEU:HD12	2.08	0.53
1:A:167:GLY:CA	1:A:360:PHE:HE1	2.22	0.53
1:A:339:ASN:C	1:A:341:CYS:H	2.10	0.53
1:A:161:ILE:CG2	1:A:162:PRO:HD2	2.39	0.52
1:A:333:GLU:C	1:A:335:GLN:N	2.63	0.52
1:A:136:ASP:O	1:A:138:GLU:N	2.42	0.52
1:A:161:ILE:CG2	1:A:165:ILE:HG21	2.40	0.52
1:A:161:ILE:HD12	1:A:256:MET:HB3	1.92	0.52
1:A:180:LEU:HD22	1:A:186:ILE:HD11	1.92	0.52
1:A:81:VAL:O	1:A:81:VAL:HG13	2.10	0.51
1:A:227:ARG:HH11	1:A:261:TYR:HB2	1.75	0.51
1:A:124:PRO:O	1:A:205:LYS:HG2	2.11	0.51
1:A:199:ASN:HD21	1:A:203:GLU:HB2	1.76	0.51
1:A:167:GLY:O	1:A:171:ILE:HG12	2.10	0.51
1:A:229:TYR:N	1:A:229:TYR:CD1	2.79	0.51
1:A:254:VAL:HG12	1:A:262:PRO:CG	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:VAL:HG12	1:A:204:ILE:HA	1.93	0.50
1:A:67:ASP:HB3	1:A:89:PRO:HG3	1.94	0.50
1:A:254:VAL:HG23	1:A:338:VAL:CG2	2.42	0.50
1:A:174:ILE:HG13	1:A:356:MET:CE	2.41	0.50
1:A:127:VAL:HG21	1:A:207:CYS:HB3	1.92	0.50
1:A:345:ASN:C	1:A:345:ASN:HD22	2.15	0.50
1:A:186:ILE:O	1:A:186:ILE:HG13	2.11	0.50
1:A:150:SER:C	1:A:152:ASP:N	2.65	0.50
1:A:150:SER:O	1:A:152:ASP:N	2.44	0.50
1:A:263:ILE:CG2	1:A:313:LEU:HD11	2.42	0.50
1:A:251:LEU:O	1:A:251:LEU:HG	2.12	0.49
1:A:127:VAL:HG21	1:A:197:LEU:HD12	1.95	0.49
1:A:363:ARG:O	1:A:363:ARG:HG3	2.12	0.49
1:A:345:ASN:ND2	1:A:347:ALA:H	2.10	0.49
1:A:235:LEU:HD22	1:A:314:LEU:HG	1.95	0.49
1:A:362:LYS:CE	1:A:362:LYS:HA	2.41	0.48
1:A:308:MET:HG3	1:A:312:GLU:HB3	1.95	0.48
1:A:254:VAL:HG12	1:A:262:PRO:HG2	1.94	0.48
1:A:360:PHE:CD1	1:A:360:PHE:C	2.87	0.48
1:A:161:ILE:HG23	1:A:374:TRP:CH2	2.48	0.48
1:A:171:ILE:CD1	1:A:361:ILE:HG23	2.43	0.48
1:A:159:GLY:C	1:A:160:ARG:HG3	2.34	0.48
1:A:333:GLU:HG2	1:A:360:PHE:N	2.28	0.48
1:A:345:ASN:ND2	1:A:347:ALA:N	2.62	0.47
1:A:199:ASN:C	1:A:199:ASN:HD22	2.17	0.47
1:A:246:ILE:HD11	1:A:352:LEU:CD2	2.45	0.47
1:A:339:ASN:C	1:A:341:CYS:N	2.66	0.47
1:A:246:ILE:HD11	1:A:352:LEU:HD23	1.95	0.47
1:A:359:ALA:O	1:A:362:LYS:HB2	2.15	0.47
1:A:191:VAL:O	1:A:191:VAL:HG22	2.14	0.47
1:A:67:ASP:HB3	1:A:89:PRO:CG	2.45	0.47
1:A:333:GLU:N	1:A:333:GLU:OE1	2.48	0.46
1:A:322:PRO:HD3	1:A:344:LYS:CD	2.45	0.46
1:A:147:ASP:OD2	1:A:200:SER:HB3	2.16	0.46
1:A:167:GLY:HA2	1:A:360:PHE:HE1	1.81	0.45
1:A:150:SER:OG	1:A:153:GLN:HG3	2.16	0.45
1:A:181:ARG:O	1:A:181:ARG:HD2	2.16	0.45
1:A:181:ARG:NH1	1:A:182:GLU:HG2	2.31	0.45
1:A:151:LEU:HD21	1:A:169:VAL:CG2	2.47	0.45
1:A:163:GLU:C	1:A:165:ILE:N	2.68	0.45
1:A:147:ASP:N	1:A:147:ASP:OD1	2.49	0.45
1:A:316:TYR:C	1:A:316:TYR:CD1	2.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:VAL:HG11	1:A:249:MET:SD	2.57	0.45
1:A:335:GLN:O	1:A:339:ASN:HB2	2.17	0.45
1:A:94:MET:CE	1:A:142:CYS:HB3	2.47	0.45
1:A:253:LEU:CD1	1:A:337:PHE:HE2	2.30	0.45
1:A:163:GLU:OE1	1:A:331:SER:HB3	2.17	0.44
1:A:199:ASN:OD1	1:A:201:ARG:HD3	2.17	0.44
1:A:333:GLU:N	1:A:333:GLU:CD	2.71	0.44
1:A:364:SER:C	1:A:366:ALA:N	2.71	0.44
1:A:62:GLU:HG3	1:A:62:GLU:O	2.16	0.44
1:A:65:ASP:OD1	1:A:96:ARG:NH2	2.46	0.44
1:A:370:ASP:O	1:A:371:PHE:HB3	2.17	0.44
1:A:355:LEU:C	1:A:357:VAL:H	2.21	0.44
1:A:171:ILE:CD1	1:A:361:ILE:HD12	2.48	0.44
1:A:125:TYR:N	1:A:125:TYR:CD1	2.86	0.44
1:A:326:PRO:HD2	1:A:330:PHE:CE2	2.54	0.43
1:A:66:ASP:N	1:A:66:ASP:OD1	2.48	0.43
1:A:261:TYR:C	1:A:263:ILE:H	2.22	0.43
1:A:255:GLU:HB2	1:A:262:PRO:HD3	2.00	0.43
1:A:94:MET:HE3	1:A:142:CYS:HB3	2.00	0.43
1:A:341:CYS:C	1:A:342:LEU:HD23	2.38	0.43
1:A:127:VAL:O	3:A:400:3OS:H15	2.19	0.43
1:A:76:ALA:HA	1:A:81:VAL:HA	2.01	0.43
1:A:345:ASN:C	1:A:345:ASN:ND2	2.72	0.43
1:A:168:LYS:HE3	1:A:369:VAL:HB	1.99	0.43
1:A:98:LEU:HD13	1:A:138:GLU:HG2	2.01	0.42
1:A:337:PHE:O	1:A:338:VAL:C	2.56	0.42
1:A:261:TYR:O	1:A:263:ILE:N	2.50	0.42
1:A:345:ASN:ND2	1:A:348:GLU:N	2.66	0.42
1:A:342:LEU:HD23	1:A:342:LEU:N	2.35	0.42
1:A:360:PHE:HD1	1:A:360:PHE:C	2.23	0.42
1:A:167:GLY:HA2	1:A:360:PHE:CE1	2.55	0.42
1:A:233:GLU:HG2	1:A:234:ARG:N	2.35	0.42
1:A:363:ARG:O	1:A:364:SER:HB2	2.20	0.42
1:A:190:ASP:OD2	1:A:195:ASN:ND2	2.53	0.42
1:A:251:LEU:HD21	1:A:261:TYR:CE1	2.54	0.42
1:A:193:PRO:HD3	1:A:252:SER:OG	2.19	0.42
1:A:263:ILE:HA	1:A:264:PRO:C	2.40	0.41
1:A:358:HIS:C	1:A:362:LYS:HG2	2.38	0.41
1:A:259:GLY:O	1:A:260:ARG:HB2	2.20	0.41
1:A:165:ILE:O	1:A:168:LYS:N	2.48	0.41
1:A:199:ASN:HD21	1:A:203:GLU:CB	2.33	0.41
1:A:258:VAL:HG21	1:A:262:PRO:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:336:ASP:OD2	1:A:358:HIS:HE1	2.03	0.41
1:A:212:SER:O	1:A:216:ILE:HG13	2.20	0.41
1:A:165:ILE:CD1	1:A:369:VAL:HG11	2.42	0.41
1:A:255:GLU:HB2	1:A:262:PRO:CD	2.49	0.41
1:A:167:GLY:HA3	1:A:360:PHE:HE1	1.86	0.41
1:A:257:ALA:O	1:A:330:PHE:HZ	2.04	0.41
1:A:260:ARG:HH11	1:A:261:TYR:H	1.66	0.41
1:A:170:SER:OG	1:A:253:LEU:HD21	2.21	0.41
1:A:358:HIS:CG	1:A:359:ALA:N	2.89	0.40
1:A:333:GLU:HB2	1:A:360:PHE:HB2	2.00	0.40
1:A:260:ARG:HH11	1:A:261:TYR:N	2.19	0.40
1:A:134:TYR:OH	1:A:137:GLY:HA2	2.21	0.40
1:A:188:HIS:CD2	1:A:209:PHE:HB3	2.57	0.40
1:A:74:LEU:HD13	2:A:1:ATP:C2	2.56	0.40
1:A:360:PHE:CD1	1:A:360:PHE:O	2.74	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	266/307 (87%)	203 (76%)	45 (17%)	18 (7%)	2 5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	156	LYS
1	A	158	ALA
1	A	162	PRO
1	A	163	GLU
1	A	331	SER
1	A	334	PHE
1	A	101	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	137	GLY
1	A	151	LEU
1	A	159	GLY
1	A	332	LEU
1	A	364	SER
1	A	136	ASP
1	A	228	SER
1	A	262	PRO
1	A	190	ASP
1	A	242	VAL

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	237/266 (89%)	217 (92%)	20 (8%)	16	41

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	82	VAL
1	A	94	MET
1	A	107	ILE
1	A	138	GLU
1	A	162	PRO
1	A	165	ILE
1	A	191	VAL
1	A	199	ASN
1	A	201	ARG
1	A	239	HIS
1	A	252	SER
1	A	260	ARG
1	A	314	LEU
1	A	333	GLU
1	A	345	ASN
1	A	360	PHE
1	A	363	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	ASP
1	A	375	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	110	GLN
1	A	116	GLN
1	A	164	GLN
1	A	199	ASN
1	A	319	ASN
1	A	335	GLN
1	A	345	ASN
1	A	358	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	ATP	A	1	4	33,33,33	1.08	3 (9%)	52,52,52	2.25	13 (25%)
3	3OS	A	400	-	32,32,32	1.47	6 (18%)	42,42,42	1.30	5 (11%)

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	ATP	A	1	4	-	0/22/38/38	0/1/3/3
3	3OS	A	400	-	-	0/21/21/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	3OS	C25-N27	3.49	1.39	1.34
2	A	1	ATP	C2-N3	3.05	1.38	1.32
3	A	400	3OS	C3-C17	2.83	1.42	1.38
3	A	400	3OS	C1-C9	2.68	1.43	1.39
3	A	400	3OS	C5-C4	2.62	1.44	1.39
2	A	1	ATP	C4-N3	2.34	1.39	1.35
3	A	400	3OS	C16-C17	2.21	1.41	1.37
3	A	400	3OS	C4-C1	2.06	1.44	1.41
2	A	1	ATP	PB-O3B	-2.03	1.56	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ATP	N3-C2-N1	-10.45	119.97	128.71
2	A	1	ATP	O4'-C1'-N9	-5.33	103.48	108.44
2	A	1	ATP	C4-C5-N7	-5.28	105.00	109.52
3	A	400	3OS	C1-N2-C3	4.05	132.69	123.48
3	A	400	3OS	C4-C25-N27	3.32	119.75	115.08
2	A	1	ATP	N3-C4-N9	2.85	130.57	125.43
2	A	1	ATP	N6-C6-N1	-2.81	113.84	119.36
2	A	1	ATP	C8-N7-C5	2.76	112.12	103.58
2	A	1	ATP	C5-C6-N6	2.60	126.60	120.72
2	A	1	ATP	C2'-C1'-N9	2.59	119.91	113.27
2	A	1	ATP	N7-C8-N9	-2.54	107.18	114.36
3	A	400	3OS	C7-C6-C19	-2.52	119.14	120.90
2	A	1	ATP	O3A-PB-O3B	2.46	106.66	101.66
3	A	400	3OS	C5-C6-C7	2.37	119.53	115.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	3OS	C6-C19-N20	2.13	124.11	121.07
2	A	1	ATP	O2B-PB-O3B	2.10	115.11	105.14
2	A	1	ATP	O2'-C2'-C3'	2.06	118.53	111.83
2	A	1	ATP	C2-N3-C4	2.01	119.74	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/307 (88%)	-0.00	7 (2%) 53 54	42, 64, 81, 89	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	PHE	4.3
1	A	334	PHE	3.6
1	A	359	ALA	2.7
1	A	261	TYR	2.3
1	A	227	ARG	2.3
1	A	369	VAL	2.1
1	A	362	LYS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	3OS	A	400	31/31	0.27	2.23	41,57,74,78	0
4	MG	A	401	1/1	0.18	0.24	40,40,40,40	0
2	ATP	A	1	31/31	0.16	-0.53	64,68,70,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.