



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:07 AM GMT

PDB ID : 3EQF
Title : X-ray structure of the human mitogen-activated protein kinase kinase 1 (MEK1) in a binary complex with K252A and MG2P
Authors : Fischmann, T.O.
Deposited on : 2008-09-30
Resolution : 2.70 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>

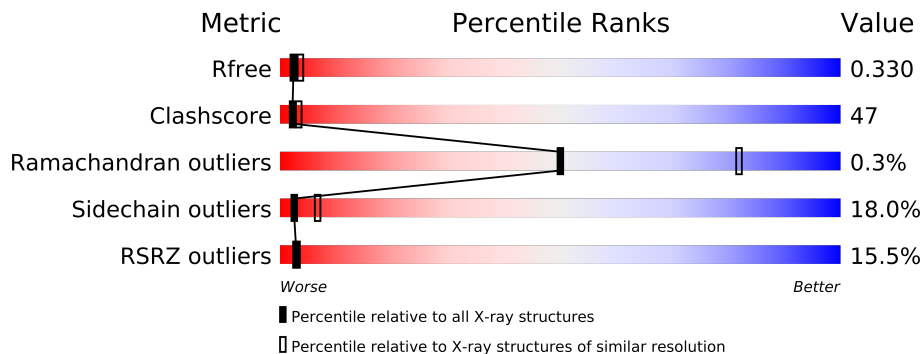
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	360	

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	MG	A	3	-	X
5	NA	A	6	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 2508 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.

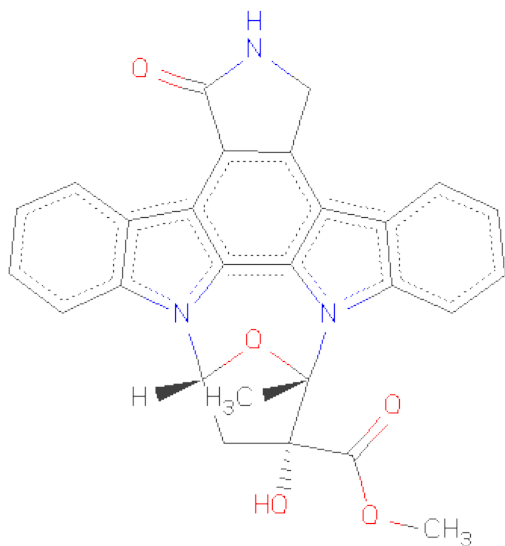
- Molecule 1 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2462	1573	419	454	16	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q02750
A	298	ASN	SER	engineered	UNP Q02750
A	299	LYS	SER	engineered	UNP Q02750
A	300	PHE	TYR	engineered	UNP Q02750

- Molecule 2 is K-252A (three-letter code: KSA) (formula: C₂₇H₂₁N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	35	27	3	5	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is water.

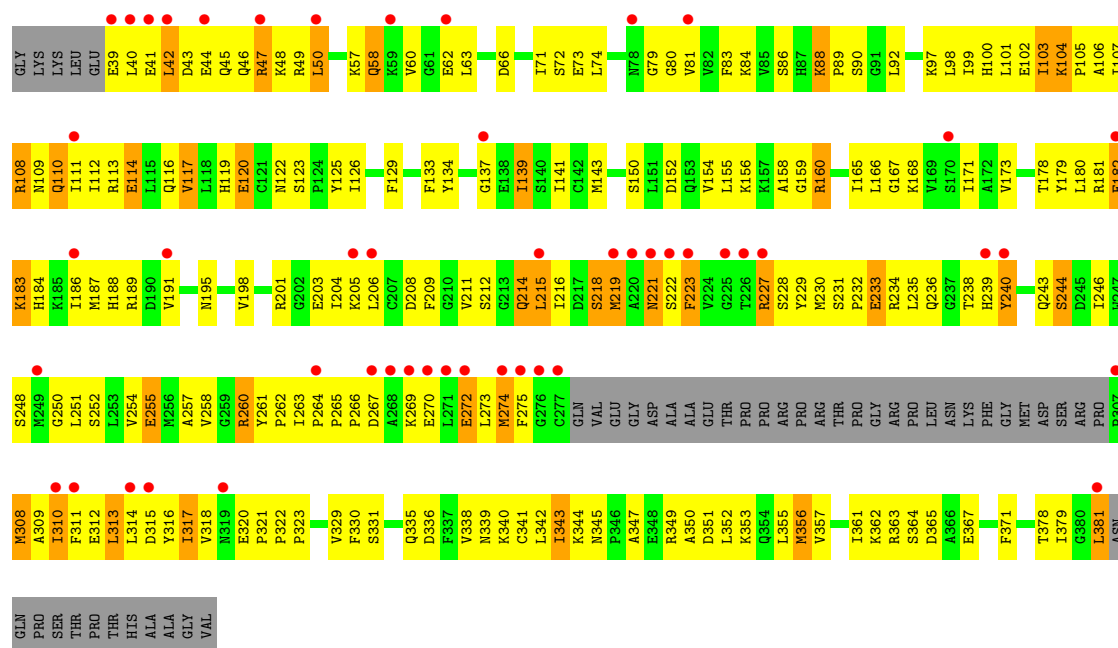
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		

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 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.16Å 78.16Å 222.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 26.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	5.0 (50.00-2.70) 99.0 (26.96-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.72Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.254 , (Not available) 0.260 , 0.330	Depositor DCC
R_{free} test set	577 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 11672 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2508	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: NA, CA, KSA, MG

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	0.26	0/2510	0.37	0/3378

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	2462	0	2496	235	1
2	A	35	0	21	3	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	8	0	0	0	0
All	All	2508	0	2517	237	1

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 47.

All (237) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:GLU:HG3	1:A:356:MET:HE2	1.35	1.03
1:A:71:ILE:HD11	1:A:86:SER:HB2	1.54	0.87
1:A:261:TYR:CE2	1:A:313:LEU:HD11	2.11	0.86
1:A:323:PRO:HD2	1:A:342:LEU:HD13	1.58	0.85
1:A:309:ALA:HB3	1:A:312:GLU:HG3	1.59	0.84
1:A:195:ASN:ND2	1:A:208:ASP:HB3	1.92	0.84
1:A:263:ILE:HG21	1:A:313:LEU:HD21	1.60	0.82
1:A:134:TYR:HD2	1:A:139:ILE:HG12	1.45	0.80
1:A:158:ALA:HB2	1:A:378:THR:HG21	1.64	0.80
1:A:184:HIS:O	1:A:186:ILE:HG13	1.82	0.79
1:A:43:ASP:HB3	1:A:46:GLN:HB2	1.63	0.79
1:A:173:VAL:HG22	1:A:206:LEU:HD21	1.63	0.78
1:A:246:ILE:HD11	1:A:352:LEU:HD23	1.68	0.76
1:A:322:PRO:HD3	1:A:344:LYS:HD3	1.69	0.74
1:A:254:VAL:O	1:A:258:VAL:HG13	1.87	0.74
1:A:250:GLY:O	1:A:254:VAL:HG23	1.87	0.74
1:A:100:HIS:CE1	1:A:102:GLU:HG2	2.23	0.74
1:A:270:GLU:O	1:A:274:MET:HG3	1.88	0.74
1:A:238:THR:HG22	1:A:239:HIS:H	1.51	0.74
1:A:90:SER:OG	1:A:92:LEU:HD12	1.87	0.73
1:A:261:TYR:CE2	1:A:263:ILE:HB	2.24	0.73
1:A:150:SER:O	1:A:154:VAL:HG23	1.87	0.73
1:A:233:GLU:HG3	1:A:239:HIS:O	1.87	0.73
1:A:39:GLU:CG	1:A:356:MET:HE2	2.15	0.72
2:A:1:KSA:H11	2:A:1:KSA:H252	1.70	0.72
1:A:322:PRO:HG3	1:A:344:LYS:HD3	1.72	0.72
1:A:179:TYR:CD2	1:A:183:LYS:HG3	2.25	0.71
1:A:79:GLY:HA2	1:A:223:PHE:HD2	1.55	0.71
1:A:234:ARG:HG3	1:A:240:TYR:HB2	1.73	0.71
1:A:57:LYS:HE3	1:A:129:PHE:O	1.92	0.70
1:A:308:MET:HG2	1:A:312:GLU:CB	2.21	0.70
1:A:316:TYR:O	1:A:320:GLU:HB2	1.92	0.69
1:A:40:LEU:HD13	1:A:183:LYS:CE	2.23	0.68
1:A:322:PRO:CD	1:A:344:LYS:HD3	2.24	0.68
1:A:340:LYS:HA	1:A:343:ILE:HD12	1.76	0.67
1:A:234:ARG:HG3	1:A:240:TYR:CB	2.24	0.67
1:A:251:LEU:CD1	1:A:262:PRO:HG2	2.26	0.66
1:A:187:MET:HE2	1:A:189:ARG:HG2	1.77	0.66
1:A:79:GLY:HA2	1:A:223:PHE:CD2	2.31	0.66
1:A:322:PRO:CG	1:A:344:LYS:HD3	2.26	0.65
1:A:261:TYR:HE2	1:A:313:LEU:HD11	1.59	0.65
1:A:218:SER:O	1:A:221:ASN:ND2	2.30	0.65
1:A:320:GLU:OE2	1:A:321:PRO:HD3	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:188:HIS:CD2	1:A:209:PHE:HB3	2.32	0.65
1:A:40:LEU:HD13	1:A:183:LYS:HE2	1.80	0.64
1:A:73:GLU:HA	1:A:83:PHE:HD2	1.62	0.64
1:A:320:GLU:O	1:A:344:LYS:NZ	2.30	0.64
1:A:39:GLU:HB2	1:A:356:MET:HE3	1.79	0.64
1:A:110:GLN:OE1	1:A:214:GLN:HG2	1.98	0.64
1:A:117:VAL:HG12	1:A:211:VAL:HG11	1.79	0.64
1:A:178:THR:OG1	1:A:352:LEU:HD13	1.98	0.63
1:A:215:LEU:HD12	1:A:215:LEU:O	1.98	0.63
1:A:215:LEU:CD1	1:A:219:MET:HG3	2.29	0.63
1:A:308:MET:CE	1:A:312:GLU:HB3	2.29	0.63
1:A:267:ASP:N	1:A:270:GLU:OE2	2.32	0.62
1:A:158:ALA:HB2	1:A:378:THR:CG2	2.30	0.61
1:A:108:ARG:HG2	1:A:109:ASN:N	2.15	0.61
1:A:308:MET:HE2	1:A:312:GLU:HB3	1.81	0.61
1:A:212:SER:O	1:A:216:ILE:HG13	2.01	0.61
1:A:272:GLU:HG2	1:A:272:GLU:O	1.99	0.61
1:A:233:GLU:HG2	1:A:234:ARG:N	2.17	0.60
1:A:235:LEU:HD13	1:A:314:LEU:HD22	1.84	0.60
1:A:320:GLU:HB3	1:A:321:PRO:HD2	1.84	0.60
1:A:60:VAL:HG22	1:A:92:LEU:CD1	2.32	0.59
1:A:379:ILE:CD1	1:A:381:LEU:HD12	2.32	0.59
1:A:261:TYR:CZ	1:A:313:LEU:HD11	2.36	0.59
1:A:112:ILE:O	1:A:116:GLN:HG2	2.02	0.59
1:A:179:TYR:CE2	1:A:183:LYS:HG3	2.35	0.59
1:A:42:LEU:HD23	1:A:47:ARG:HA	1.84	0.59
1:A:350:ALA:HB3	1:A:355:LEU:HD21	1.85	0.59
1:A:308:MET:HE1	1:A:316:TYR:HB2	1.84	0.59
1:A:112:ILE:HD11	1:A:139:ILE:HD13	1.85	0.59
1:A:231:SER:OG	1:A:244:SER:HB3	2.03	0.59
1:A:363:ARG:O	1:A:367:GLU:HG3	2.03	0.58
1:A:39:GLU:HB2	1:A:356:MET:CE	2.34	0.58
1:A:260:ARG:HG3	1:A:261:TYR:N	2.17	0.58
1:A:71:ILE:HB	1:A:84:LYS:O	2.03	0.58
1:A:263:ILE:CG2	1:A:313:LEU:HD21	2.31	0.57
1:A:43:ASP:OD2	1:A:45:GLN:N	2.38	0.57
1:A:42:LEU:HD23	1:A:47:ARG:CB	2.34	0.57
1:A:310:ILE:O	1:A:310:ILE:HG13	2.03	0.57
1:A:150:SER:OG	1:A:152:ASP:HB3	2.06	0.56
1:A:79:GLY:O	1:A:99:ILE:HG23	2.04	0.56
1:A:269:LYS:O	1:A:273:LEU:HG	2.06	0.56
1:A:323:PRO:HD2	1:A:342:LEU:CD1	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:PRO:O	1:A:263:ILE:HG12	2.05	0.56
1:A:195:ASN:HD21	1:A:208:ASP:HB3	1.66	0.56
1:A:179:TYR:CE1	1:A:184:HIS:HD2	2.24	0.56
1:A:103:ILE:HG21	1:A:107:ILE:HG21	1.86	0.56
1:A:40:LEU:CD1	1:A:183:LYS:HE2	2.36	0.55
1:A:117:VAL:HA	1:A:120:GLU:OE2	2.06	0.55
1:A:88:LYS:HB2	1:A:89:PRO:HD3	1.87	0.55
1:A:228:SER:HB2	1:A:313:LEU:HD13	1.87	0.55
1:A:232:PRO:HB3	1:A:318:VAL:HG22	1.89	0.55
1:A:251:LEU:HD11	1:A:262:PRO:HG2	1.88	0.55
1:A:112:ILE:HD12	1:A:112:ILE:N	2.22	0.55
1:A:102:GLU:HA	1:A:102:GLU:OE2	2.06	0.55
1:A:379:ILE:HG13	1:A:381:LEU:HD12	1.88	0.55
1:A:227:ARG:HG2	1:A:230:MET:CE	2.37	0.55
1:A:42:LEU:HD23	1:A:47:ARG:CA	2.36	0.54
1:A:338:VAL:O	1:A:341:CYS:HB2	2.07	0.54
1:A:308:MET:HG2	1:A:312:GLU:HB3	1.88	0.54
1:A:215:LEU:HD12	1:A:219:MET:HG3	1.89	0.54
1:A:117:VAL:CG1	1:A:211:VAL:HG11	2.37	0.54
1:A:255:GLU:HB2	1:A:262:PRO:HD3	1.88	0.54
1:A:50:LEU:HD11	1:A:122:ASN:HB3	1.89	0.53
1:A:313:LEU:CD2	1:A:317:ILE:HG13	2.38	0.53
1:A:134:TYR:OH	1:A:137:GLY:HA2	2.09	0.53
1:A:103:ILE:CG2	1:A:107:ILE:HG21	2.38	0.53
1:A:320:GLU:HB3	1:A:321:PRO:CD	2.39	0.53
1:A:308:MET:HG2	1:A:312:GLU:OE1	2.09	0.53
1:A:40:LEU:HD11	1:A:182:GLU:HB3	1.90	0.53
1:A:71:ILE:O	1:A:72:SER:HB3	2.08	0.53
1:A:105:PRO:HA	1:A:108:ARG:CZ	2.39	0.53
1:A:49:ARG:HG2	1:A:201:ARG:NH2	2.24	0.53
1:A:160:ARG:HG3	1:A:160:ARG:O	2.08	0.53
1:A:263:ILE:HG21	1:A:313:LEU:CD2	2.36	0.52
1:A:58:GLN:N	1:A:58:GLN:HE21	2.07	0.52
1:A:379:ILE:HD11	1:A:381:LEU:CD1	2.40	0.52
1:A:166:LEU:CD1	1:A:257:ALA:HB2	2.40	0.52
1:A:108:ARG:HD2	1:A:134:TYR:CG	2.45	0.51
1:A:234:ARG:C	1:A:236:GLN:H	2.14	0.51
1:A:261:TYR:OH	1:A:313:LEU:HD11	2.10	0.51
1:A:231:SER:HB2	1:A:233:GLU:OE1	2.10	0.51
1:A:108:ARG:HD2	1:A:134:TYR:HB3	1.93	0.51
1:A:308:MET:HG2	1:A:312:GLU:HB2	1.91	0.51
1:A:179:TYR:CE1	1:A:184:HIS:CD2	2.98	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:LEU:HD13	2:A:1:KSA:C21	2.42	0.50
1:A:364:SER:HA	1:A:367:GLU:OE1	2.11	0.50
1:A:58:GLN:CA	1:A:58:GLN:HE21	2.24	0.50
1:A:74:LEU:HD21	1:A:84:LYS:HB2	1.93	0.50
1:A:270:GLU:HA	1:A:273:LEU:HB2	1.94	0.50
1:A:119:HIS:CD2	1:A:129:PHE:HE2	2.30	0.50
1:A:108:ARG:HD2	1:A:134:TYR:CB	2.42	0.49
1:A:103:ILE:HG22	1:A:107:ILE:HD12	1.93	0.49
1:A:97:LYS:HB3	1:A:141:ILE:HB	1.93	0.49
1:A:258:VAL:HA	1:A:275:PHE:HZ	1.77	0.49
1:A:105:PRO:HB3	1:A:108:ARG:NH2	2.28	0.49
1:A:343:ILE:HG22	1:A:343:ILE:O	2.13	0.49
1:A:322:PRO:HG3	1:A:344:LYS:CD	2.42	0.49
1:A:251:LEU:HD12	1:A:262:PRO:HG2	1.95	0.49
1:A:335:GLN:O	1:A:338:VAL:HG22	2.13	0.49
1:A:343:ILE:HG21	1:A:349:ARG:N	2.28	0.48
1:A:208:ASP:OD1	1:A:208:ASP:O	2.32	0.48
1:A:215:LEU:HD11	1:A:219:MET:HG3	1.94	0.48
1:A:316:TYR:CE1	1:A:320:GLU:HG3	2.48	0.48
1:A:112:ILE:CD1	1:A:139:ILE:HD13	2.42	0.48
1:A:187:MET:HE1	1:A:240:TYR:CD2	2.48	0.48
1:A:167:GLY:O	1:A:171:ILE:HD12	2.14	0.48
1:A:126:ILE:HD13	1:A:180:LEU:HD21	1.95	0.48
1:A:345:ASN:HD21	1:A:347:ALA:HB3	1.78	0.48
1:A:258:VAL:HG23	1:A:260:ARG:H	1.77	0.48
1:A:49:ARG:HG2	1:A:201:ARG:HH22	1.78	0.48
1:A:155:LEU:O	1:A:159:GLY:N	2.40	0.48
1:A:214:GLN:OE1	1:A:214:GLN:O	2.32	0.48
1:A:191:VAL:HB	1:A:248:SER:CB	2.44	0.48
1:A:361:ILE:O	1:A:365:ASP:HB2	2.13	0.47
1:A:100:HIS:NE2	1:A:102:GLU:HG2	2.29	0.47
1:A:308:MET:CE	1:A:316:TYR:HB2	2.44	0.47
1:A:198:VAL:HA	1:A:203:GLU:O	2.15	0.47
1:A:229:TYR:OH	1:A:255:GLU:OE1	2.32	0.47
1:A:274:MET:HG3	1:A:274:MET:H	1.54	0.47
1:A:101:LEU:HD21	1:A:223:PHE:CE1	2.50	0.47
1:A:323:PRO:CD	1:A:342:LEU:HD13	2.38	0.47
1:A:223:PHE:CD1	1:A:223:PHE:N	2.79	0.47
1:A:43:ASP:OD2	1:A:44:GLU:N	2.48	0.46
1:A:353:LYS:O	1:A:357:VAL:HG22	2.14	0.46
1:A:106:ALA:O	1:A:110:GLN:HB2	2.14	0.46
1:A:336:ASP:O	1:A:340:LYS:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:ILE:N	1:A:205:LYS:HB3	2.31	0.46
1:A:255:GLU:HA	1:A:260:ARG:O	2.16	0.46
1:A:108:ARG:CD	1:A:134:TYR:CD1	2.99	0.46
1:A:379:ILE:CG1	1:A:381:LEU:HD12	2.46	0.46
1:A:80:GLY:HA3	1:A:98:LEU:O	2.16	0.46
1:A:179:TYR:CD2	1:A:183:LYS:HE3	2.51	0.46
1:A:108:ARG:CD	1:A:134:TYR:CG	2.99	0.46
1:A:345:ASN:ND2	1:A:347:ALA:HB3	2.31	0.45
1:A:379:ILE:HD11	1:A:381:LEU:HD12	1.98	0.45
1:A:198:VAL:HG12	1:A:204:ILE:HG12	1.98	0.45
1:A:243:GLN:HE22	1:A:349:ARG:HG2	1.81	0.45
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.80	0.45
1:A:338:VAL:HG23	1:A:339:ASN:N	2.30	0.45
1:A:264:PRO:HB3	1:A:316:TYR:CZ	2.52	0.45
1:A:309:ALA:HB1	1:A:311:PHE:CE2	2.52	0.45
1:A:110:GLN:NE2	1:A:114:GLU:OE2	2.49	0.45
1:A:101:LEU:CD2	1:A:223:PHE:CZ	3.00	0.45
2:A:1:KSA:C11	2:A:1:KSA:H252	2.42	0.45
1:A:308:MET:HE3	1:A:316:TYR:HD2	1.82	0.45
1:A:187:MET:HE1	1:A:240:TYR:HD2	1.83	0.44
1:A:104:LYS:HG3	1:A:107:ILE:HD12	2.00	0.44
1:A:126:ILE:CD1	1:A:180:LEU:HD21	2.47	0.44
1:A:195:ASN:CG	1:A:208:ASP:HB3	2.37	0.44
1:A:112:ILE:CD1	1:A:112:ILE:N	2.80	0.44
1:A:110:GLN:HG2	1:A:113:ARG:HH12	1.82	0.44
1:A:108:ARG:CG	1:A:109:ASN:N	2.79	0.44
1:A:234:ARG:HG3	1:A:240:TYR:HB3	1.99	0.44
1:A:134:TYR:CD2	1:A:139:ILE:HG12	2.37	0.44
1:A:309:ALA:CB	1:A:312:GLU:HG3	2.38	0.44
1:A:215:LEU:HD12	1:A:215:LEU:C	2.35	0.44
1:A:123:SER:C	1:A:125:TYR:H	2.22	0.43
1:A:165:ILE:HD12	1:A:371:PHE:HD1	1.84	0.43
1:A:102:GLU:C	1:A:103:ILE:HG12	2.36	0.43
1:A:63:LEU:HB3	1:A:133:PHE:CE1	2.53	0.43
1:A:186:ILE:HG23	1:A:189:ARG:HH21	1.83	0.43
1:A:343:ILE:CG2	1:A:349:ARG:N	2.82	0.42
1:A:227:ARG:HG2	1:A:230:MET:HE3	2.00	0.42
1:A:111:ILE:HG23	1:A:215:LEU:HB2	2.02	0.42
1:A:39:GLU:CB	1:A:356:MET:HE2	2.49	0.42
1:A:43:ASP:O	1:A:47:ARG:HB2	2.20	0.42
1:A:73:GLU:HA	1:A:83:PHE:CD2	2.49	0.42
1:A:39:GLU:HG3	1:A:356:MET:CE	2.26	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:GLY:HA2	1:A:223:PHE:HB3	2.01	0.42
1:A:345:ASN:OD1	1:A:347:ALA:HB3	2.20	0.42
1:A:112:ILE:CD1	1:A:112:ILE:H	2.33	0.41
1:A:234:ARG:CG	1:A:240:TYR:HB2	2.48	0.41
1:A:42:LEU:HD23	1:A:47:ARG:CG	2.50	0.41
1:A:101:LEU:HD21	1:A:223:PHE:CZ	2.55	0.41
1:A:379:ILE:HD11	1:A:381:LEU:HD13	2.02	0.41
1:A:191:VAL:HB	1:A:248:SER:HB2	2.02	0.41
1:A:111:ILE:HA	1:A:114:GLU:HG3	2.01	0.41
1:A:108:ARG:HD3	1:A:134:TYR:CD1	2.55	0.41
1:A:73:GLU:OE2	1:A:81:VAL:HG13	2.20	0.41
1:A:338:VAL:CG2	1:A:339:ASN:N	2.83	0.41
1:A:329:VAL:HG23	1:A:330:PHE:CD2	2.55	0.41
1:A:108:ARG:HD2	1:A:134:TYR:CD1	2.55	0.41
1:A:233:GLU:HG2	1:A:234:ARG:H	1.85	0.41
1:A:227:ARG:HG2	1:A:230:MET:HE1	2.02	0.41
1:A:106:ALA:HA	1:A:109:ASN:HD22	1.85	0.41
1:A:110:GLN:CG	1:A:113:ARG:HH12	2.34	0.41
1:A:60:VAL:HG22	1:A:92:LEU:HD11	2.02	0.41
1:A:126:ILE:CA	1:A:205:LYS:HB3	2.50	0.41
1:A:114:GLU:HB2	1:A:212:SER:HB2	2.02	0.41
1:A:263:ILE:HA	1:A:264:PRO:HA	1.74	0.40
1:A:265:PRO:HA	1:A:266:PRO:HD2	1.77	0.40
1:A:45:GLN:HB2	1:A:45:GLN:HE21	1.73	0.40
1:A:274:MET:HE2	1:A:274:MET:HB2	1.89	0.40
1:A:60:VAL:CG2	1:A:92:LEU:CD1	3.00	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	Distance(Å)	Clash(Å)
1:A:66:ASP:OD1	1:A:66:ASP:OD1[11.555]	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	310/360 (86%)	284 (92%)	25 (8%)	1 (0%)	50 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASN

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	272/310 (88%)	223 (82%)	49 (18%)	2 7

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	42	LEU
1	A	47	ARG
1	A	48	LYS
1	A	50	LEU
1	A	58	GLN
1	A	62	GLU
1	A	88	LYS
1	A	103	ILE
1	A	104	LYS
1	A	108	ARG
1	A	110	GLN
1	A	114	GLU
1	A	117	VAL
1	A	120	GLU
1	A	139	ILE
1	A	143	MET
1	A	156	LYS
1	A	160	ARG
1	A	168	LYS
1	A	181	ARG
1	A	182	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	LYS
1	A	214	GLN
1	A	215	LEU
1	A	218	SER
1	A	219	MET
1	A	222	SER
1	A	223	PHE
1	A	227	ARG
1	A	233	GLU
1	A	240	TYR
1	A	244	SER
1	A	252	SER
1	A	255	GLU
1	A	260	ARG
1	A	272	GLU
1	A	274	MET
1	A	308	MET
1	A	310	ILE
1	A	313	LEU
1	A	315	ASP
1	A	317	ILE
1	A	331	SER
1	A	343	ILE
1	A	351	ASP
1	A	356	MET
1	A	362	LYS
1	A	381	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	100	HIS
1	A	109	ASN
1	A	145	HIS
1	A	243	GLN

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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	KSA	A	1	-	40,42,42	1.75	11 (27%)	64,70,70	1.65	13 (20%)

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	KSA	A	1	-	-	0/8/46/46	0/0/8/8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	KSA	O1-C24	-4.03	1.38	1.43
2	A	1	KSA	C3-N1	3.76	1.43	1.39
2	A	1	KSA	C8-C3	-3.24	1.38	1.42
2	A	1	KSA	C5-C4	-2.79	1.39	1.42
2	A	1	KSA	C1-C22	2.72	1.56	1.54
2	A	1	KSA	C1-C2	-2.68	1.53	1.57
2	A	1	KSA	C13-C14	2.35	1.42	1.36
2	A	1	KSA	C23-N3	2.12	1.47	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	KSA	O3-C22	2.10	1.25	1.20
2	A	1	KSA	C19-C18	2.08	1.41	1.36
2	A	1	KSA	C4-N2	2.00	1.41	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	KSA	C1-C2-N1	4.95	112.53	110.06
2	A	1	KSA	C6-C5-C4	-4.37	115.26	121.81
2	A	1	KSA	C16-C17-N2	-4.00	104.95	108.91
2	A	1	KSA	C8-C9-C10	4.00	110.74	106.37
2	A	1	KSA	C5-C16-C17	3.59	110.30	106.37
2	A	1	KSA	C9-C10-N1	-2.98	105.42	109.40
2	A	1	KSA	O1-C2-C1	2.97	106.58	100.76
2	A	1	KSA	C27-C24-N2	-2.91	108.29	112.76
2	A	1	KSA	C5-C4-C3	2.84	123.60	121.20
2	A	1	KSA	C5-C6-C15	2.43	130.82	128.93
2	A	1	KSA	C6-C5-C16	2.13	138.59	133.51
2	A	1	KSA	C11-C10-N1	2.05	134.45	130.55
2	A	1	KSA	C14-C9-C8	-2.04	129.37	135.38

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	314/360 (87%)	0.77	49 (15%) 3 3	48, 71, 112, 128	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	HIS	11.1
1	A	40	LEU	8.3
1	A	277	CYS	8.1
1	A	223	PHE	6.8
1	A	276	GLY	6.5
1	A	271	LEU	5.0
1	A	222	SER	4.9
1	A	270	GLU	4.9
1	A	240	TYR	4.8
1	A	314	LEU	4.7
1	A	267	ASP	4.0
1	A	310	ILE	4.0
1	A	275	PHE	4.0
1	A	41	GLU	3.7
1	A	221	ASN	3.6
1	A	381	LEU	3.5
1	A	225	GLY	3.4
1	A	62	GLU	3.4
1	A	42	LEU	3.4
1	A	269	LYS	3.3
1	A	264	PRO	3.3
1	A	39	GLU	3.3
1	A	219	MET	3.2
1	A	311	PHE	3.2
1	A	44	GLU	3.1
1	A	272	GLU	3.1
1	A	268	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	ASN	2.9
1	A	215	LEU	2.8
1	A	137	GLY	2.8
1	A	170	SER	2.7
1	A	220	ALA	2.7
1	A	59	LYS	2.5
1	A	307	PRO	2.4
1	A	78	ASN	2.4
1	A	205	LYS	2.4
1	A	226	THR	2.4
1	A	186	ILE	2.4
1	A	81	VAL	2.3
1	A	47	ARG	2.3
1	A	206	LEU	2.3
1	A	111	ILE	2.2
1	A	191	VAL	2.2
1	A	315	ASP	2.2
1	A	50	LEU	2.1
1	A	249	MET	2.1
1	A	274	MET	2.1
1	A	227	ARG	2.0
1	A	182	GLU	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
5	NA	A	6	1/1	0.58	12.88	44,44,44,44	0
3	MG	A	3	1/1	0.37	2.62	47,47,47,47	0
4	CA	A	5	1/1	0.18	0.01	55,55,55,55	1
2	KSA	A	1	35/35	0.16	-0.21	55,58,61,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.