



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:27 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

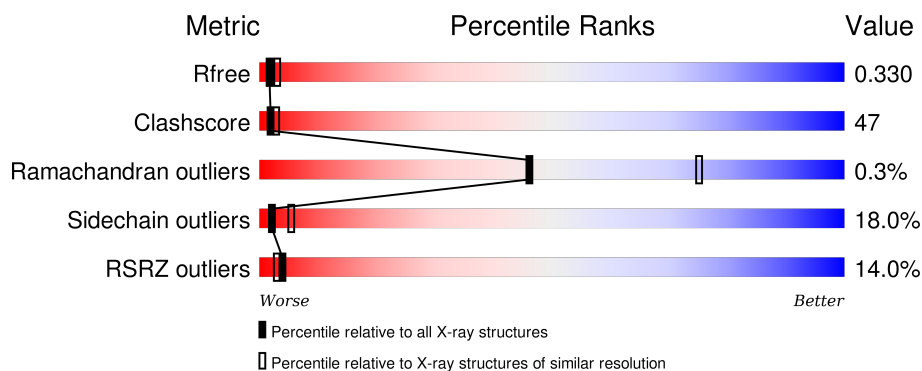
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	360	

## 2 Entry composition [i](#)

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

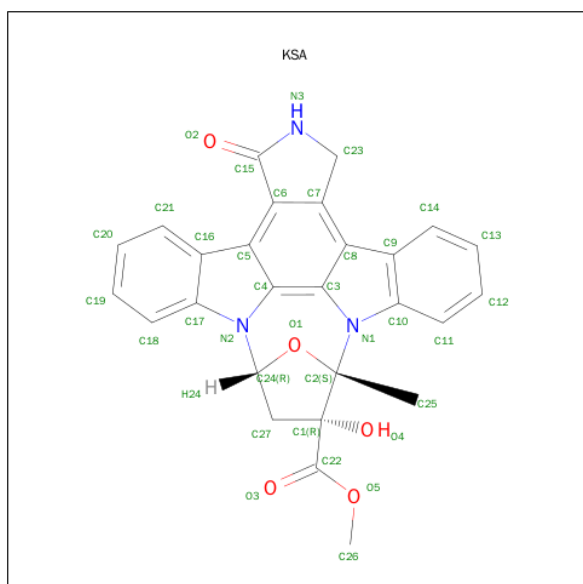
- Molecule 1 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

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

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:  $C_{27}H_{21}N_3O_5$ ).



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

- 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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.16 Å 78.16 Å 222.99 Å 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) 99.1 (26.96-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.72 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.254 , (Not available) 0.259 , 0.330	Depositor DCC
$R_{free}$ test set	577 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 66.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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

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 47.

All (237) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLU:OE2	1:A:321:PRO:HD3	1.97	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASP:OD1	1:A:66:ASP:OD1[11_555]	2.14	0.06

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	46 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASN

### 5.3.2 Protein sidechains [i](#)

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 5

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

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Mol	Chain	Res	Type
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
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 [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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	-	30,42,42	1.66	8 (26%)	28,70,70	1.47	3 (10%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	KSA	O1-C24	-3.95	1.38	1.43
2	A	1	KSA	C8-C3	-3.10	1.38	1.42
2	A	1	KSA	C5-C4	-2.68	1.39	1.42
2	A	1	KSA	C19-C18	2.06	1.41	1.36
2	A	1	KSA	O3-C22	2.12	1.25	1.20
2	A	1	KSA	C25-C2	2.14	1.55	1.52
2	A	1	KSA	C13-C14	2.33	1.42	1.36
2	A	1	KSA	C1-C22	2.83	1.56	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	KSA	C5-C16-C17	3.59	110.30	106.37
2	A	1	KSA	O1-C2-C1	3.68	106.58	100.22
2	A	1	KSA	C8-C9-C10	4.00	110.74	106.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	KSA	3	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	314/360 (87%)	0.69	44 (14%) 4 3	48, 71, 112, 128	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	HIS	13.0
1	A	277	CYS	9.0
1	A	40	LEU	6.0
1	A	223	PHE	6.0
1	A	276	GLY	5.6
1	A	240	TYR	5.5
1	A	222	SER	4.7
1	A	314	LEU	4.7
1	A	221	ASN	4.0
1	A	270	GLU	3.9
1	A	41	GLU	3.5
1	A	267	ASP	3.4
1	A	170	SER	3.4
1	A	311	PHE	3.3
1	A	275	PHE	3.3
1	A	310	ILE	3.3
1	A	264	PRO	3.1
1	A	44	GLU	3.0
1	A	271	LEU	3.0
1	A	62	GLU	2.9
1	A	381	LEU	2.9
1	A	137	GLY	2.9
1	A	220	ALA	2.9
1	A	272	GLU	2.8
1	A	269	LYS	2.8
1	A	315	ASP	2.7
1	A	219	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	2.7
1	A	42	LEU	2.6
1	A	225	GLY	2.6
1	A	307	PRO	2.6
1	A	47	ARG	2.5
1	A	253	LEU	2.5
1	A	317	ILE	2.5
1	A	249	MET	2.5
1	A	50	LEU	2.4
1	A	313	LEU	2.3
1	A	319	ASN	2.2
1	A	102	GLU	2.2
1	A	328	GLY	2.1
1	A	81	VAL	2.1
1	A	169	VAL	2.1
1	A	191	VAL	2.0
1	A	348	GLU	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	KSA	A	1	35/35	0.93	0.16	-0.18	55,58,61,62	0
5	NA	A	6	1/1	0.93	0.58	-	44,44,44,44	0
4	CA	A	5	1/1	0.98	0.20	-	55,55,55,55	1
3	MG	A	3	1/1	0.91	0.35	-	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.