



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2017 – 06:06 PM EDT

PDB ID : 3FYJ  
Title : Crystal structure of an optimzied benzothiophene inhibitor bound to MAP-KAP Kinase-2 (MK-2)  
Authors : Kurumbail, R.G.; Caspers, N.  
Deposited on : unknown  
Resolution : 3.80 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
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) : rb-20030345

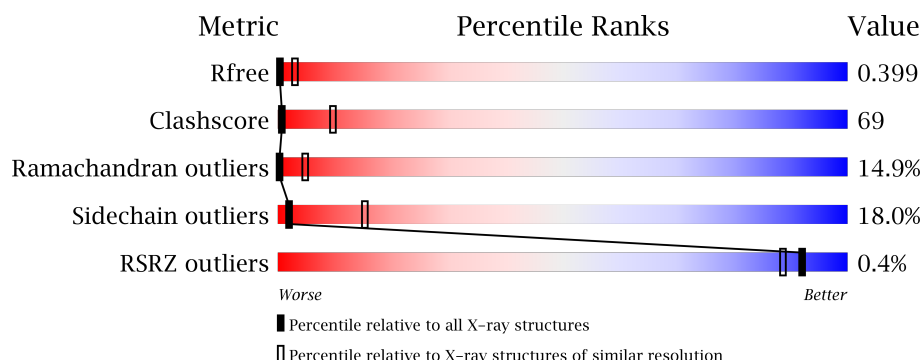
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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	X	327	<div> <div>16%</div> <div>50%</div> <div>20%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

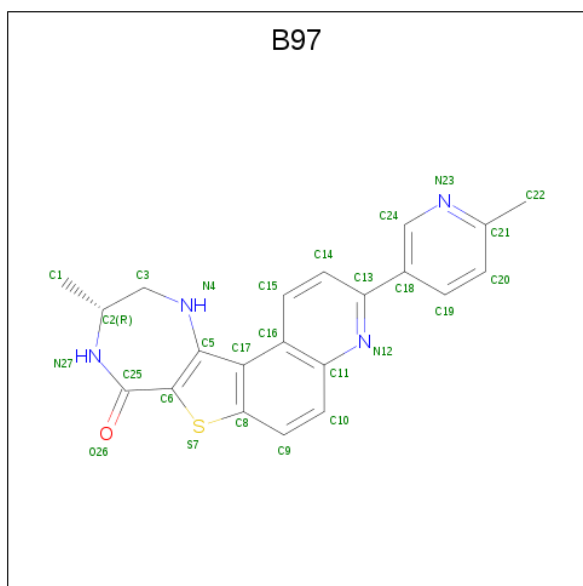
There are 2 unique types of molecules in this entry. The entry contains 2325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	282	Total	C	N	O	S	0	0	0
			2298	1462	396	423	17			

- Molecule 2 is (10R)-10-methyl-3-(6-methylpyridin-3-yl)-9,10,11,12-tetrahydro-8H-[1,4]diazepino[5',6':4,5]thieno[3,2-f]quinolin-8-one (three-letter code: B97) (formula: C<sub>21</sub>H<sub>18</sub>N<sub>4</sub>OS).





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.55Å 255.55Å 255.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 3.80 29.51 – 3.80	Depositor EDS
% Data completeness (in resolution range)	85.1 (29.51-3.80) 85.5 (29.51-3.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 3.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.328 , 0.388 0.327 , 0.399	Depositor DCC
$R_{free}$ test set	294 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	129.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	2325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B97

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	X	0.56	0/2344	0.72	1/3157 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	X	134	LEU	CA-CB-CG	-5.21	103.31	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	2298	0	2315	321	0
2	X	27	0	18	6	0
All	All	2325	0	2333	322	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 69.

All (322) 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:X:108:HIS:CE1	1:X:208:PHE:CD1	2.37	1.11
1:X:196:SER:OG	1:X:198:ARG:HG2	1.60	1.01
1:X:188:LYS:HB3	1:X:190:GLU:OE2	1.60	0.99
1:X:184:HIS:HD2	1:X:205:LEU:HD21	1.25	0.99
1:X:288:ASN:HB2	1:X:289:PRO:HD3	1.43	0.97
1:X:307:LYS:O	1:X:313:ARG:NE	1.99	0.95
1:X:140:CYS:HB2	2:X:372:B97:H19	1.53	0.89
1:X:108:HIS:CE1	1:X:208:PHE:CG	2.62	0.88
1:X:97:ASP:OD2	1:X:132:LYS:HG2	1.73	0.87
1:X:299:LYS:HA	1:X:302:ILE:HD12	1.55	0.87
1:X:65:VAL:HG22	1:X:81:ILE:HD11	1.57	0.86
1:X:144:GLY:C	1:X:193:LEU:HD23	1.99	0.83
1:X:292:SER:OG	1:X:293:GLU:OE1	1.96	0.83
1:X:143:GLY:HA3	1:X:194:TYR:HB2	1.60	0.83
1:X:198:ARG:HG3	1:X:201:ALA:HB2	1.59	0.83
1:X:86:THR:O	1:X:87:GLN:HB2	1.78	0.82
1:X:105:VAL:HG23	1:X:106:GLU:N	1.95	0.82
1:X:108:HIS:ND1	1:X:208:PHE:CG	2.48	0.81
1:X:79:LEU:HD23	1:X:92:LEU:HD23	1.63	0.80
1:X:63:TYR:O	1:X:84:LYS:NZ	2.15	0.79
1:X:184:HIS:C	1:X:184:HIS:HD1	1.85	0.78
1:X:299:LYS:HA	1:X:302:ILE:CD1	2.13	0.78
1:X:254:TYR:CD1	1:X:260:TYR:O	2.37	0.78
1:X:288:ASN:HB2	1:X:289:PRO:CD	2.14	0.77
1:X:198:ARG:O	1:X:201:ALA:HB3	1.86	0.76
1:X:150:ILE:O	1:X:153:ARG:HG3	1.86	0.75
1:X:337:HIS:HB3	1:X:341:VAL:HG23	1.69	0.75
1:X:49:LYS:HG2	1:X:113:GLN:OE1	1.86	0.75
1:X:299:LYS:CA	1:X:302:ILE:HD12	2.16	0.74
1:X:96:GLN:HE22	1:X:131:ARG:HH12	1.31	0.74
1:X:254:TYR:HD1	1:X:260:TYR:O	1.71	0.74
1:X:161:ARG:HH22	1:X:333:GLN:HG3	1.53	0.74
1:X:196:SER:OG	1:X:198:ARG:CG	2.35	0.73
1:X:146:LEU:HD11	1:X:166:ILE:HD13	1.69	0.73
1:X:360:LEU:O	1:X:362:THR:N	2.22	0.73
1:X:136:ILE:HD13	1:X:136:ILE:O	1.89	0.72
1:X:248:SER:O	1:X:252:ILE:HG12	1.90	0.72
1:X:124:TYR:HB3	1:X:126:ASN:HD21	1.54	0.72
1:X:213:GLU:OE1	1:X:215:THR:HB	1.89	0.72
1:X:258:CYS:SG	1:X:259:GLY:N	2.63	0.72
1:X:307:LYS:HB2	1:X:313:ARG:HG2	1.72	0.72
1:X:81:ILE:HG22	1:X:90:PHE:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:96:GLN:HE22	1:X:131:ARG:NH1	1.87	0.72
1:X:105:VAL:HG23	1:X:106:GLU:H	1.53	0.71
1:X:302:ILE:HG22	1:X:306:LEU:HD23	1.71	0.71
1:X:143:GLY:HA3	1:X:194:TYR:CB	2.19	0.71
1:X:108:HIS:ND1	1:X:208:PHE:HB2	2.06	0.70
1:X:146:LEU:HD21	1:X:166:ILE:CG2	2.22	0.70
1:X:136:ILE:HD11	1:X:138:MET:SD	2.31	0.70
1:X:79:LEU:HD23	1:X:92:LEU:CD2	2.21	0.70
1:X:46:PHE:CD2	1:X:46:PHE:C	2.65	0.69
1:X:81:ILE:HG22	1:X:90:PHE:CB	2.22	0.69
1:X:146:LEU:HD21	1:X:166:ILE:HG21	1.74	0.69
1:X:100:LYS:NZ	1:X:104:GLU:OE1	2.25	0.69
1:X:307:LYS:HB2	1:X:313:ARG:CG	2.23	0.69
1:X:185:ARG:CZ	1:X:212:LYS:HD2	2.23	0.69
1:X:184:HIS:ND1	1:X:184:HIS:O	2.23	0.68
1:X:319:PHE:CE1	1:X:325:ILE:HG13	2.29	0.68
2:X:372:B97:HN4	2:X:372:B97:H15	1.59	0.67
1:X:184:HIS:CD2	1:X:205:LEU:HD21	2.18	0.67
1:X:180:ILE:O	1:X:181:ASN:HB2	1.93	0.66
1:X:80:GLN:HG2	1:X:82:PHE:CZ	2.29	0.66
1:X:188:LYS:HD2	1:X:190:GLU:OE1	1.96	0.66
1:X:246:MET:HA	1:X:249:LEU:HD12	1.76	0.66
1:X:112:SER:C	1:X:114:CYS:H	1.99	0.65
1:X:112:SER:CB	1:X:119:ARG:HA	2.27	0.65
1:X:258:CYS:O	1:X:338:THR:HA	1.97	0.64
1:X:337:HIS:CB	1:X:341:VAL:HG23	2.26	0.64
1:X:174:ILE:HB	1:X:316:ILE:HD13	1.79	0.64
1:X:315:THR:O	1:X:318:GLU:HB2	1.98	0.64
1:X:128:TYR:CD2	1:X:129:ALA:N	2.66	0.64
1:X:153:ARG:NH1	1:X:157:ALA:O	2.30	0.63
1:X:316:ILE:HA	1:X:319:PHE:HB3	1.78	0.63
1:X:350:GLU:O	1:X:354:GLU:HB3	1.99	0.62
1:X:353:LYS:HG2	1:X:354:GLU:N	2.14	0.62
1:X:112:SER:O	1:X:114:CYS:N	2.33	0.62
1:X:74:ILE:HD11	1:X:93:LYS:HE3	1.82	0.62
1:X:319:PHE:C	1:X:319:PHE:CD1	2.73	0.61
1:X:297:GLU:O	1:X:300:MET:HB3	2.01	0.61
1:X:181:ASN:O	1:X:213:GLU:HG2	2.01	0.61
1:X:185:ARG:O	1:X:210:PHE:HD2	1.83	0.61
1:X:160:GLU:OE1	1:X:331:VAL:HG13	2.01	0.61
1:X:107:LEU:HB3	1:X:182:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:239:LYS:HB3	1:X:310:PRO:HB2	1.83	0.60
1:X:309:GLU:O	1:X:313:ARG:CZ	2.49	0.60
1:X:298:VAL:HG12	1:X:302:ILE:HD11	1.83	0.60
1:X:214:THR:HG21	1:X:242:LYS:HD3	1.83	0.60
1:X:58:ALA:O	1:X:60:ILE:N	2.35	0.60
1:X:159:THR:HG22	1:X:161:ARG:H	1.67	0.60
1:X:142:ASP:HB3	2:X:372:B97:C21	2.32	0.60
1:X:198:ARG:O	1:X:201:ALA:CB	2.49	0.59
1:X:174:ILE:HA	1:X:177:LEU:HD12	1.85	0.59
1:X:53:GLN:NE2	1:X:53:GLN:H	2.01	0.59
1:X:81:ILE:O	1:X:90:PHE:N	2.36	0.59
1:X:191:ASN:OD1	2:X:372:B97:H1	2.03	0.58
1:X:246:MET:O	1:X:247:TRP:C	2.41	0.58
1:X:246:MET:SD	1:X:316:ILE:HB	2.43	0.58
1:X:83:ASN:OD1	1:X:83:ASN:C	2.40	0.58
1:X:79:LEU:HD22	1:X:79:LEU:N	2.18	0.58
1:X:362:THR:O	1:X:364:ARG:N	2.37	0.58
1:X:105:VAL:CG2	1:X:106:GLU:N	2.64	0.57
1:X:108:HIS:ND1	1:X:208:PHE:CB	2.66	0.57
1:X:307:LYS:O	1:X:313:ARG:CD	2.53	0.57
1:X:188:LYS:NZ	1:X:357:THR:HG23	2.19	0.57
1:X:105:VAL:CG2	1:X:106:GLU:H	2.18	0.57
1:X:188:LYS:HG3	1:X:360:LEU:HD12	1.87	0.57
1:X:109:TRP:O	1:X:112:SER:OG	2.21	0.56
1:X:112:SER:C	1:X:114:CYS:N	2.57	0.56
1:X:182:ILE:HA	1:X:212:LYS:O	2.05	0.56
1:X:181:ASN:O	1:X:213:GLU:HA	2.05	0.56
1:X:304:ASN:HA	1:X:307:LYS:HE2	1.88	0.56
1:X:107:LEU:HD13	1:X:182:ILE:HD13	1.87	0.56
1:X:167:MET:HA	1:X:170:ILE:HD12	1.87	0.56
1:X:174:ILE:CG2	1:X:178:HIS:NE2	2.69	0.56
1:X:107:LEU:HB3	1:X:182:ILE:HD11	1.88	0.56
1:X:296:GLU:HA	1:X:299:LYS:HD2	1.88	0.56
1:X:98:CYS:O	1:X:99:PRO:C	2.44	0.56
1:X:114:CYS:SG	1:X:117:ILE:N	2.78	0.55
1:X:97:ASP:HB3	1:X:132:LYS:O	2.07	0.55
1:X:178:HIS:O	1:X:181:ASN:N	2.33	0.55
1:X:93:LYS:HB3	1:X:136:ILE:HG23	1.88	0.55
1:X:71:GLY:H	1:X:78:VAL:HB	1.72	0.55
1:X:92:LEU:HG	1:X:92:LEU:O	2.04	0.55
1:X:300:MET:O	1:X:303:ARG:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:158:PHE:CZ	1:X:162:GLU:HB3	2.42	0.55
1:X:316:ILE:HG23	1:X:317:THR:H	1.72	0.55
1:X:97:ASP:OD2	1:X:132:LYS:CG	2.50	0.55
1:X:69:VAL:HG12	1:X:70:LEU:N	2.22	0.54
1:X:239:LYS:CB	1:X:310:PRO:HB2	2.37	0.54
1:X:114:CYS:SG	1:X:117:ILE:HG13	2.47	0.54
1:X:164:SER:O	1:X:168:LYS:N	2.35	0.54
1:X:100:LYS:NZ	1:X:104:GLU:CD	2.61	0.54
1:X:112:SER:HB2	1:X:119:ARG:HA	1.90	0.54
1:X:96:GLN:O	1:X:97:ASP:HB3	2.08	0.54
1:X:108:HIS:HB3	1:X:120:ILE:HD12	1.90	0.53
1:X:145:GLU:N	1:X:193:LEU:HD23	2.23	0.53
1:X:162:GLU:HA	1:X:165:GLU:OE2	2.08	0.53
1:X:83:ASN:O	1:X:87:GLN:N	2.40	0.53
1:X:307:LYS:C	1:X:309:GLU:H	2.12	0.53
1:X:316:ILE:O	1:X:317:THR:C	2.45	0.53
1:X:52:LEU:HB2	1:X:109:TRP:CD1	2.44	0.53
1:X:174:ILE:HB	1:X:316:ILE:CD1	2.38	0.53
1:X:103:ARG:HH11	1:X:103:ARG:HB2	1.74	0.53
1:X:143:GLY:CA	1:X:194:TYR:HB2	2.34	0.53
1:X:149:ARG:HD3	1:X:194:TYR:CD2	2.44	0.53
1:X:52:LEU:HD22	1:X:53:GLN:H	1.74	0.53
1:X:167:MET:SD	1:X:170:ILE:HD12	2.50	0.52
1:X:341:VAL:O	1:X:344:GLU:O	2.26	0.52
1:X:196:SER:OG	1:X:201:ALA:HB2	2.09	0.52
1:X:80:GLN:CG	1:X:82:PHE:CZ	2.92	0.52
1:X:306:LEU:O	1:X:307:LYS:C	2.48	0.52
1:X:128:TYR:HD2	1:X:129:ALA:N	2.07	0.52
1:X:80:GLN:CD	1:X:82:PHE:HZ	2.11	0.52
1:X:338:THR:O	1:X:341:VAL:HB	2.09	0.52
1:X:193:LEU:O	1:X:203:LEU:HB2	2.10	0.52
1:X:142:ASP:HB3	2:X:372:B97:C22	2.39	0.52
1:X:81:ILE:CG2	1:X:90:PHE:HB2	2.37	0.52
1:X:349:TRP:C	1:X:351:ASP:N	2.61	0.51
1:X:351:ASP:HB3	1:X:355:GLU:OE2	2.09	0.51
1:X:355:GLU:O	1:X:358:SER:HB2	2.10	0.51
1:X:356:MET:HE1	1:X:360:LEU:HD11	1.92	0.51
1:X:103:ARG:NH1	1:X:103:ARG:HB2	2.26	0.51
1:X:208:PHE:HD1	1:X:208:PHE:N	2.09	0.51
1:X:324:TRP:CD1	1:X:331:VAL:HG22	2.45	0.51
1:X:46:PHE:HD2	1:X:46:PHE:C	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:307:LYS:CB	1:X:313:ARG:HG2	2.39	0.51
1:X:188:LYS:HB3	1:X:190:GLU:CD	2.31	0.51
1:X:116:HIS:O	1:X:204:LYS:HA	2.11	0.50
1:X:131:ARG:O	1:X:132:LYS:C	2.50	0.50
1:X:208:PHE:CD1	1:X:208:PHE:N	2.79	0.50
1:X:349:TRP:O	1:X:353:LYS:N	2.44	0.50
1:X:213:GLU:CD	1:X:215:THR:HB	2.31	0.50
1:X:307:LYS:C	1:X:309:GLU:N	2.64	0.50
1:X:241:ASP:O	1:X:243:SER:N	2.43	0.50
1:X:202:ILE:HG23	1:X:203:LEU:N	2.25	0.50
1:X:350:GLU:HA	1:X:353:LYS:HD2	1.93	0.50
1:X:96:GLN:NE2	1:X:131:ARG:HH12	2.05	0.50
1:X:350:GLU:HA	1:X:353:LYS:CD	2.42	0.50
1:X:108:HIS:CE1	1:X:208:PHE:CE1	2.98	0.49
1:X:58:ALA:C	1:X:60:ILE:N	2.64	0.49
1:X:288:ASN:CB	1:X:289:PRO:CD	2.83	0.49
1:X:61:ASP:O	1:X:84:LYS:HD2	2.13	0.49
1:X:161:ARG:NH1	1:X:331:VAL:O	2.38	0.49
1:X:146:LEU:O	1:X:149:ARG:HB3	2.12	0.49
1:X:153:ARG:NH1	1:X:158:PHE:HD1	2.09	0.49
1:X:323:PRO:HB3	1:X:327:GLN:HE21	1.78	0.49
1:X:194:TYR:CG	1:X:203:LEU:HB3	2.48	0.49
1:X:323:PRO:O	1:X:324:TRP:C	2.51	0.49
1:X:100:LYS:O	1:X:101:ALA:C	2.51	0.49
1:X:198:ARG:CG	1:X:201:ALA:HB2	2.37	0.49
1:X:311:THR:HG22	1:X:312:GLN:N	2.27	0.49
1:X:103:ARG:O	1:X:106:GLU:HB3	2.13	0.48
1:X:188:LYS:HZ3	1:X:357:THR:HG23	1.78	0.48
1:X:164:SER:O	1:X:165:GLU:C	2.51	0.48
1:X:178:HIS:O	1:X:180:ILE:N	2.46	0.48
1:X:324:TRP:HA	1:X:327:GLN:HG2	1.95	0.48
1:X:256:LEU:O	1:X:338:THR:HG21	2.14	0.48
1:X:307:LYS:HB2	1:X:313:ARG:HG3	1.94	0.48
1:X:58:ALA:C	1:X:60:ILE:H	2.15	0.48
1:X:112:SER:HB2	1:X:119:ARG:HG3	1.95	0.48
1:X:158:PHE:HE2	1:X:163:ALA:HA	1.77	0.48
1:X:82:PHE:CE2	1:X:89:LYS:HB3	2.48	0.48
1:X:96:GLN:O	1:X:97:ASP:CB	2.61	0.48
1:X:184:HIS:ND1	1:X:184:HIS:C	2.48	0.48
1:X:169:SER:O	1:X:170:ILE:C	2.52	0.48
1:X:136:ILE:C	1:X:136:ILE:HD13	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:243:SER:HA	1:X:246:MET:HG2	1.95	0.47
1:X:288:ASN:N	1:X:289:PRO:HD2	2.29	0.47
1:X:264:TYR:O	1:X:265:SER:HB2	2.14	0.47
1:X:57:ASN:O	1:X:58:ALA:C	2.53	0.47
1:X:110:ARG:O	1:X:113:GLN:HB2	2.14	0.47
1:X:80:GLN:CD	1:X:82:PHE:CZ	2.87	0.47
1:X:101:ALA:O	1:X:104:GLU:N	2.48	0.47
1:X:120:ILE:CG2	1:X:121:VAL:N	2.78	0.47
1:X:250:GLY:O	1:X:251:VAL:C	2.53	0.47
1:X:112:SER:HB3	1:X:119:ARG:HA	1.95	0.46
1:X:161:ARG:HD2	1:X:329:THR:HA	1.97	0.46
1:X:107:LEU:HD13	1:X:182:ILE:CD1	2.45	0.46
1:X:96:GLN:NE2	1:X:131:ARG:NH1	2.61	0.46
1:X:170:ILE:O	1:X:173:ALA:HB3	2.15	0.46
1:X:324:TRP:HE1	1:X:331:VAL:CG1	2.29	0.46
1:X:293:GLU:O	1:X:295:SER:N	2.48	0.46
1:X:46:PHE:CD2	1:X:47:HIS:N	2.84	0.46
1:X:174:ILE:HG22	1:X:178:HIS:CE1	2.50	0.46
1:X:294:VAL:O	1:X:295:SER:C	2.53	0.46
1:X:188:LYS:HG3	1:X:360:LEU:CD1	2.46	0.46
1:X:174:ILE:CG2	1:X:178:HIS:CE1	2.98	0.46
1:X:186:ASP:O	1:X:188:LYS:N	2.43	0.46
1:X:300:MET:O	1:X:301:LEU:C	2.55	0.45
1:X:356:MET:CE	1:X:360:LEU:HD11	2.45	0.45
1:X:262:PRO:O	1:X:263:PHE:HB2	2.17	0.45
1:X:255:ILE:O	1:X:259:GLY:HA2	2.17	0.45
1:X:60:ILE:O	1:X:84:LYS:NZ	2.37	0.45
1:X:110:ARG:HG3	1:X:110:ARG:H	1.52	0.45
1:X:135:LEU:HD12	1:X:135:LEU:N	2.31	0.45
1:X:337:HIS:C	1:X:341:VAL:HG23	2.37	0.45
1:X:52:LEU:HA	1:X:53:GLN:HE21	1.82	0.45
1:X:82:PHE:HA	1:X:88:GLU:O	2.16	0.45
1:X:323:PRO:O	1:X:325:ILE:N	2.50	0.45
1:X:205:LEU:HG	1:X:206:THR:N	2.32	0.45
1:X:184:HIS:CD2	1:X:205:LEU:HD11	2.52	0.45
1:X:255:ILE:HG13	1:X:255:ILE:H	1.41	0.45
1:X:161:ARG:HD2	1:X:329:THR:HG23	1.99	0.44
1:X:166:ILE:O	1:X:170:ILE:HG13	2.16	0.44
1:X:323:PRO:HA	1:X:326:MET:CE	2.47	0.44
1:X:175:GLN:O	1:X:176:TYR:C	2.54	0.44
1:X:248:SER:O	1:X:251:VAL:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:103:ARG:O	1:X:106:GLU:N	2.50	0.44
1:X:104:GLU:OE2	1:X:209:GLY:HA2	2.18	0.44
1:X:108:HIS:HB3	1:X:120:ILE:CD1	2.48	0.44
1:X:99:PRO:HA	1:X:102:ARG:CZ	2.48	0.44
1:X:166:ILE:O	1:X:167:MET:C	2.55	0.44
1:X:174:ILE:HG22	1:X:178:HIS:NE2	2.32	0.44
1:X:324:TRP:CA	1:X:327:GLN:HG2	2.48	0.44
1:X:101:ALA:O	1:X:105:VAL:HG22	2.18	0.43
1:X:316:ILE:HG23	1:X:317:THR:N	2.32	0.43
1:X:286:PHE:HD1	1:X:291:TRP:CD2	2.35	0.43
1:X:144:GLY:O	1:X:146:LEU:N	2.51	0.43
1:X:174:ILE:O	1:X:175:GLN:C	2.56	0.43
1:X:97:ASP:HB2	1:X:134:LEU:HB2	2.00	0.43
1:X:108:HIS:HE1	1:X:208:PHE:CD1	2.24	0.43
1:X:182:ILE:HA	1:X:213:GLU:HA	1.99	0.43
1:X:183:ALA:N	1:X:212:LYS:O	2.47	0.43
1:X:316:ILE:HD11	1:X:320:MET:HE1	1.99	0.43
1:X:145:GLU:O	1:X:146:LEU:C	2.57	0.43
1:X:149:ARG:HH22	1:X:199:PRO:HA	1.84	0.43
1:X:71:GLY:N	1:X:78:VAL:HB	2.33	0.43
1:X:83:ASN:O	1:X:87:GLN:HA	2.19	0.43
1:X:80:GLN:HG2	1:X:82:PHE:CE1	2.54	0.43
1:X:66:THR:CG2	1:X:82:PHE:HE1	2.33	0.42
1:X:142:ASP:HB3	2:X:372:B97:H22A	2.00	0.42
1:X:118:VAL:HG13	1:X:118:VAL:O	2.18	0.42
1:X:284:TYR:HE1	1:X:286:PHE:HZ	1.66	0.42
1:X:254:TYR:CE2	1:X:291:TRP:CZ2	3.06	0.42
1:X:286:PHE:HA	1:X:291:TRP:CD1	2.53	0.42
1:X:142:ASP:N	1:X:195:THR:O	2.52	0.42
1:X:145:GLU:O	1:X:147:PHE:N	2.52	0.42
1:X:243:SER:O	1:X:246:MET:HB2	2.20	0.42
1:X:65:VAL:HG13	1:X:81:ILE:HD12	2.02	0.42
1:X:100:LYS:NZ	1:X:209:GLY:O	2.53	0.42
1:X:315:THR:HG23	1:X:318:GLU:OE1	2.20	0.42
1:X:324:TRP:HE1	1:X:331:VAL:HG13	1.84	0.42
1:X:142:ASP:C	1:X:195:THR:O	2.59	0.42
1:X:337:HIS:O	1:X:338:THR:C	2.57	0.42
1:X:202:ILE:HG13	1:X:203:LEU:H	1.85	0.42
1:X:354:GLU:C	1:X:356:MET:N	2.73	0.42
1:X:86:THR:OG1	1:X:87:GLN:N	2.52	0.42
1:X:111:ALA:O	1:X:114:CYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:190:GLU:N	1:X:190:GLU:OE2	2.53	0.41
1:X:302:ILE:CG2	1:X:306:LEU:HD23	2.43	0.41
1:X:171:GLY:O	1:X:172:GLU:C	2.59	0.41
1:X:181:ASN:O	1:X:214:THR:N	2.52	0.41
1:X:141:LEU:CD2	1:X:195:THR:HG22	2.51	0.41
1:X:298:VAL:O	1:X:302:ILE:HD12	2.19	0.41
1:X:178:HIS:N	1:X:178:HIS:CD2	2.86	0.41
1:X:349:TRP:O	1:X:352:VAL:N	2.53	0.41
1:X:71:GLY:O	1:X:78:VAL:N	2.53	0.41
1:X:125:GLU:CD	1:X:132:LYS:HE3	2.41	0.41
1:X:264:TYR:HB2	1:X:265:SER:H	1.60	0.41
1:X:53:GLN:NE2	1:X:109:TRP:CH2	2.89	0.41
1:X:155:ASP:OD1	1:X:155:ASP:C	2.59	0.41
1:X:178:HIS:C	1:X:180:ILE:N	2.74	0.41
1:X:200:ASN:O	1:X:201:ALA:C	2.59	0.41
1:X:284:TYR:O	1:X:284:TYR:CD1	2.74	0.41
1:X:53:GLN:CD	1:X:53:GLN:N	2.74	0.41
1:X:158:PHE:CE1	1:X:162:GLU:HB3	2.56	0.41
1:X:178:HIS:CD2	1:X:178:HIS:H	2.38	0.41
1:X:305:LEU:O	1:X:313:ARG:HD3	2.21	0.41
1:X:61:ASP:OD1	1:X:61:ASP:N	2.53	0.41
1:X:284:TYR:CE1	1:X:286:PHE:CZ	3.09	0.41
1:X:323:PRO:CB	1:X:327:GLN:HE21	2.34	0.41
1:X:360:LEU:O	1:X:361:ALA:C	2.60	0.41
1:X:53:GLN:NE2	1:X:53:GLN:N	2.68	0.41
1:X:167:MET:O	1:X:168:LYS:C	2.60	0.40
1:X:86:THR:O	1:X:87:GLN:CB	2.55	0.40
1:X:214:THR:HG21	1:X:242:LYS:HB3	2.03	0.40
1:X:121:VAL:HG12	1:X:137:VAL:O	2.22	0.40
1:X:253:MET:O	1:X:257:LEU:HD22	2.21	0.40
1:X:176:TYR:HA	1:X:179:SER:OG	2.22	0.40
1:X:257:LEU:HD13	1:X:257:LEU:HA	1.91	0.40
1:X:288:ASN:CB	1:X:289:PRO:HD3	2.29	0.40
1:X:325:ILE:HA	1:X:325:ILE:HD13	1.86	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	X	276/327 (84%)	156 (56%)	79 (29%)	41 (15%)	<b>0</b> <b>5</b>

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	74	ILE
1	X	146	LEU
1	X	187	VAL
1	X	262	PRO
1	X	263	PHE
1	X	294	VAL
1	X	361	ALA
1	X	363	MET
1	X	59	ILE
1	X	100	LYS
1	X	113	GLN
1	X	115	PRO
1	X	128	TYR
1	X	129	ALA
1	X	145	GLU
1	X	154	GLY
1	X	156	GLN
1	X	181	ASN
1	X	242	LYS
1	X	258	CYS
1	X	295	SER
1	X	314	MET
1	X	360	LEU
1	X	132	LYS
1	X	166	ILE
1	X	186	ASP
1	X	195	THR
1	X	259	GLY

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Mol	Chain	Res	Type
1	X	310	PRO
1	X	330	LYS
1	X	85	ARG
1	X	97	ASP
1	X	207	ASP
1	X	299	LYS
1	X	302	ILE
1	X	303	ARG
1	X	179	SER
1	X	323	PRO
1	X	338	THR
1	X	352	VAL
1	X	165	GLU

### 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	X	256/296 (86%)	210 (82%)	46 (18%)	2 15

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	45	GLN
1	X	46	PHE
1	X	53	GLN
1	X	64	LYS
1	X	77	LYS
1	X	81	ILE
1	X	89	LYS
1	X	92	LEU
1	X	98	CYS
1	X	103	ARG
1	X	106	GLU
1	X	108	HIS
1	X	114	CYS

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Mol	Chain	Res	Type
1	X	121	VAL
1	X	126	ASN
1	X	128	TYR
1	X	131	ARG
1	X	133	CYS
1	X	134	LEU
1	X	136	ILE
1	X	151	GLN
1	X	155	ASP
1	X	177	LEU
1	X	182	ILE
1	X	203	LEU
1	X	206	THR
1	X	216	SER
1	X	239	LYS
1	X	240	TYR
1	X	242	LYS
1	X	243	SER
1	X	264	TYR
1	X	293	GLU
1	X	296	GLU
1	X	304	ASN
1	X	313	ARG
1	X	315	THR
1	X	316	ILE
1	X	317	THR
1	X	326	MET
1	X	351	ASP
1	X	353	LYS
1	X	354	GLU
1	X	356	MET
1	X	357	THR
1	X	364	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	53	GLN
1	X	57	ASN
1	X	75	ASN
1	X	96	GLN
1	X	126	ASN

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Mol	Chain	Res	Type
1	X	304	ASN
1	X	327	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

1 ligand is 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$
2	B97	X	372	-	26,31,31	1.56	5 (19%)	29,46,46	1.26	4 (13%)

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	B97	X	372	-	-	0/4/17/17	0/4/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	372	B97	C10-C11	-2.80	1.36	1.41
2	X	372	B97	C9-C8	-2.12	1.37	1.40
2	X	372	B97	C18-C13	-2.05	1.45	1.48
2	X	372	B97	C5-C17	2.12	1.44	1.41
2	X	372	B97	C25-N27	4.71	1.37	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	372	B97	C14-C13-C18	-2.05	117.88	121.94
2	X	372	B97	C15-C16-C17	-2.04	120.02	123.18
2	X	372	B97	C18-C13-N12	2.24	120.52	117.15
2	X	372	B97	C17-C16-C11	3.90	123.04	118.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	372	B97	6	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	X	282/327 (86%)	-0.23	1 (0%) 92 88	80, 80, 80, 80	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	239	LYS	2.6

### 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	B97	X	372	27/27	0.83	0.31	0.36	80,80,80,80	0

## 6.5 Other polymers

There are no such residues in this entry.