



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3M1S  
Title : Structure of Ruthenium Half-Sandwich Complex Bound to Glycogen Synthase Kinase 3  
Authors : Atilla-Gokcumen, G.E.; Di Costanzo, L.; Zimmermann, G.; Meggers, E.  
Deposited on : 2010-03-05  
Resolution : 3.13 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.

---

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

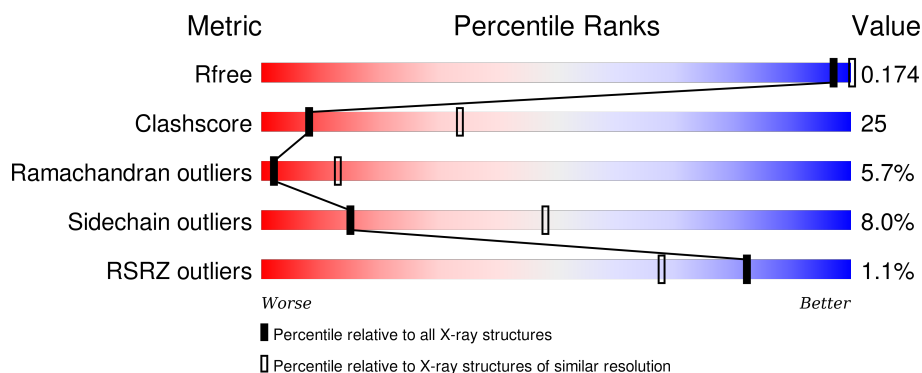
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.13 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	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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	420	<div> <div></div> <div>46% 31% 5% 17%</div> </div>
1	B	420	<div> <div></div> <div>45% 33% 5% 17%</div> </div>

## 2 Entry composition [i](#)

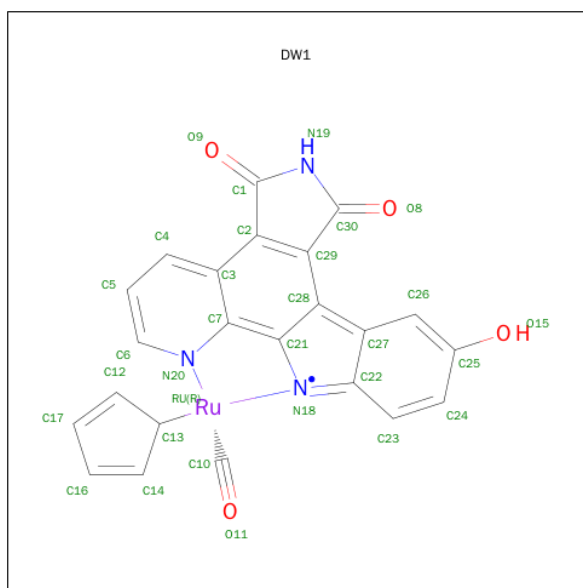
There are 3 unique types of molecules in this entry. The entry contains 5579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	6	1	0
			2710	1749	455	495	11			
1	B	349	Total	C	N	O	S	0	2	0
			2716	1754	455	496	11			

- Molecule 2 is RUTHENIUM PYRIDOCARBAZOLE (three-letter code: DW1) (formula:  $C_{23}H_{13}N_3O_4Ru$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Ru	0	0
			31	23	3	4	1		
2	B	1	Total	C	N	O	Ru	0	0
			31	23	3	4	1		

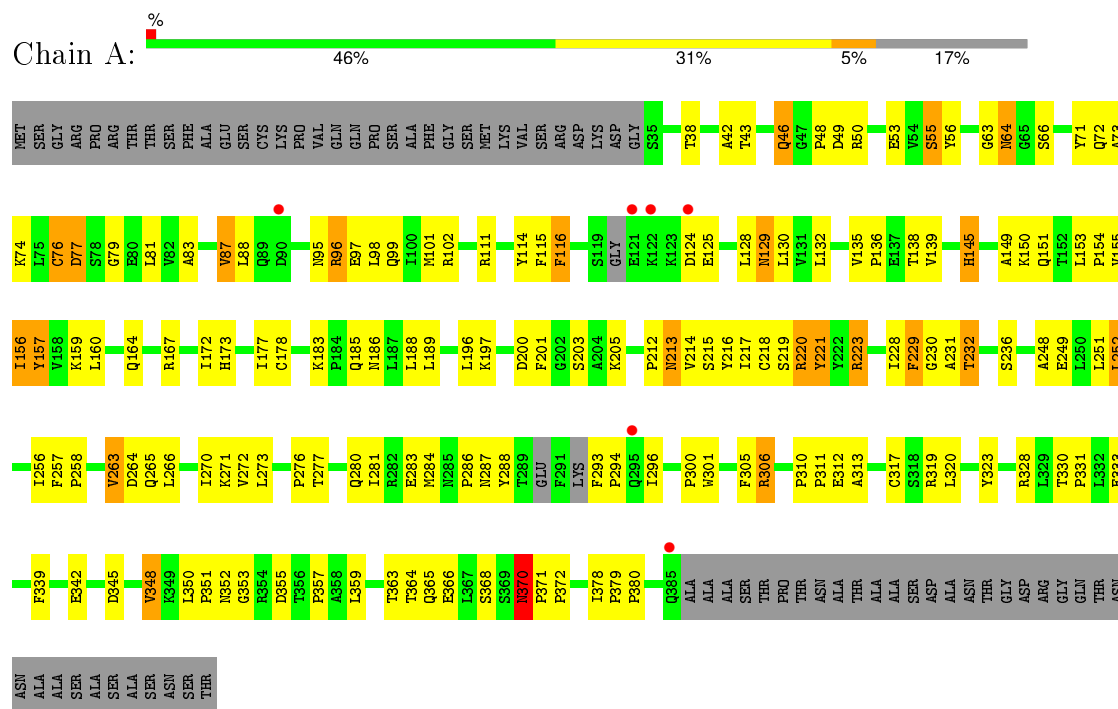
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	46	Total 46	O 46	0	0

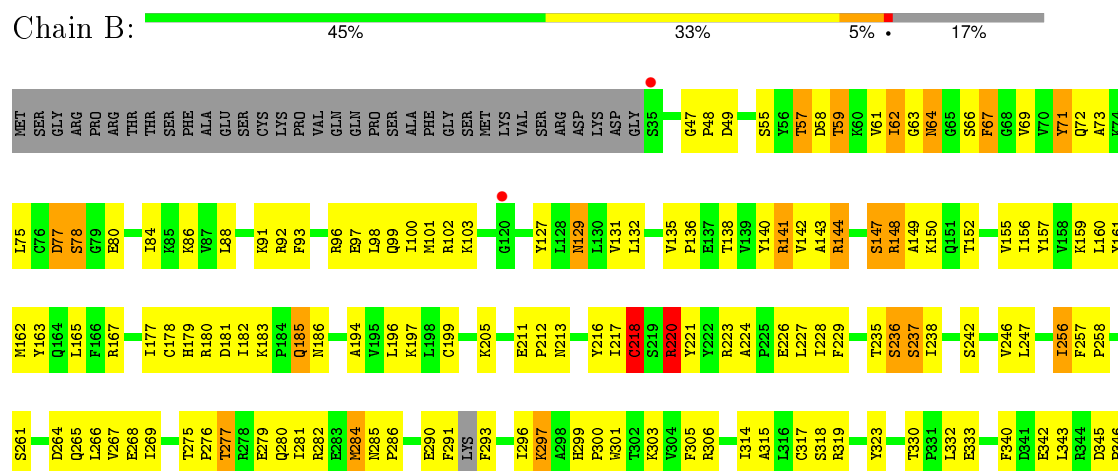
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Glycogen synthase kinase-3 beta



#### • Molecule 1: Glycogen synthase kinase-3 beta



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.04Å 86.11Å 177.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.22 – 3.13 38.22 – 3.13	Depositor EDS
% Data completeness (in resolution range)	92.6 (38.22-3.13) 92.6 (38.22-3.13)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.91 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.169 , 0.228 0.168 , 0.174	Depositor DCC
$R_{free}$ test set	1100 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.9	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21320 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: DW1

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	0.66	1/2784 (0.0%)	0.79	0/3800
1	B	0.64	0/2797	0.76	0/3823
All	All	0.65	1/5581 (0.0%)	0.77	0/7623

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	CYS	CB-SG	-5.50	1.72	1.81

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	2710	0	2646	125	0
1	B	2716	0	2653	144	0
2	A	31	0	11	0	0
2	B	31	0	12	1	0
3	A	45	0	0	3	0
3	B	46	0	0	4	0
All	All	5579	0	5322	266	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 25.

All (266) 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:B:220:ARG:HH11	1:B:220:ARG:HG2	0.97	1.08
1:B:220:ARG:HH11	1:B:220:ARG:CG	1.76	0.98
1:A:156:ILE:HG23	1:A:157:TYR:H	1.31	0.94
1:B:220:ARG:NH1	1:B:220:ARG:HG2	1.77	0.94
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.29	0.93
1:B:86:LYS:HE2	1:B:127:TYR:CD2	2.05	0.91
1:A:96:ARG:HG3	1:A:96:ARG:HH21	1.36	0.89
1:B:141:ARG:HG3	1:B:141:ARG:HH21	1.36	0.89
1:A:167:ARG:HD3	3:A:427:HOH:O	1.73	0.86
1:A:196:LEU:HD23	1:A:197:LYS:N	1.94	0.82
1:B:141:ARG:HG3	1:B:141:ARG:NH2	1.92	0.81
1:A:156:ILE:HG23	1:A:157:TYR:N	1.97	0.80
1:B:217:ILE:O	1:B:218:CYS:HB2	1.81	0.80
1:B:167:ARG:HD3	3:B:428:HOH:O	1.81	0.79
1:B:183:LYS:HE2	1:B:186:ASN:ND2	2.00	0.77
1:B:96:ARG:O	1:B:100:ILE:HG13	1.85	0.76
1:B:162:MET:HG3	1:B:247:LEU:HD13	1.68	0.74
1:A:342:GLU:O	1:A:348:VAL:HG21	1.90	0.72
1:A:156:ILE:CG2	1:A:157:TYR:H	2.04	0.70
1:A:215:SER:HB3	1:A:231:ALA:O	1.92	0.69
1:B:305:PHE:CD2	1:B:314:ILE:HG12	2.27	0.68
1:A:370:ASN:HD22	1:A:372:PRO:HD2	1.58	0.68
1:A:196:LEU:HD23	1:A:196:LEU:C	2.14	0.67
1:A:63:GLY:O	1:A:64:ASN:HB3	1.94	0.67
1:A:115:PHE:O	1:A:116:PHE:HB3	1.95	0.67
1:A:149:ALA:O	1:A:151:GLN:N	2.28	0.67
1:A:159:LYS:HE2	1:A:339:PHE:O	1.95	0.66
1:A:74:LYS:HE2	1:A:79:GLY:O	1.95	0.66
1:A:370:ASN:ND2	1:A:372:PRO:HD2	2.11	0.65
1:A:71:TYR:O	1:A:83:ALA:HA	1.95	0.65
1:B:358:ALA:HB1	1:B:361:ASN:ND2	2.12	0.65
1:B:315:ALA:O	1:B:319:ARG:HG2	1.97	0.64
1:B:96:ARG:CZ	1:B:205:LYS:HG3	2.27	0.64
1:B:370:ASN:OD1	1:B:372:PRO:HD2	1.98	0.64
1:B:220:ARG:HG3	1:B:221[B]:TYR:H	1.62	0.63
1:A:98:LEU:O	1:A:102:ARG:HG3	1.98	0.63
1:B:277:THR:O	1:B:281:ILE:HD12	1.97	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HD23	1:B:343:LEU:HD22	1.79	0.62
1:B:276:PRO:HB2	1:B:281:ILE:CD1	2.29	0.62
1:A:185:GLN:HB2	3:A:435:HOH:O	1.98	0.62
1:B:220:ARG:HG3	1:B:221[A]:TYR:H	1.63	0.61
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.08	0.61
1:A:320:LEU:O	1:A:328:ARG:HD3	2.02	0.59
1:A:312:GLU:H	1:A:312:GLU:CD	2.05	0.59
1:B:71:TYR:CD2	1:B:71:TYR:N	2.65	0.59
1:B:345:ASP:O	1:B:348:VAL:HG12	2.02	0.59
1:A:281:ILE:HA	1:A:284:MET:HE3	1.84	0.59
1:B:220:ARG:HG3	1:B:221[A]:TYR:N	2.18	0.59
1:B:141:ARG:CG	1:B:141:ARG:HH21	2.11	0.59
1:B:98:LEU:O	1:B:102:ARG:HG3	2.03	0.58
1:B:180:ARG:HG2	1:B:238:ILE:HD11	1.86	0.58
1:B:88:LEU:HD12	1:B:127:TYR:CE1	2.37	0.58
1:B:265:GLN:O	1:B:269:ILE:HG13	2.03	0.58
1:B:220:ARG:HG3	1:B:221[B]:TYR:N	2.18	0.57
1:A:160:LEU:O	1:A:164:GLN:HG3	2.04	0.57
1:A:363:THR:OG1	1:A:366:GLU:HG3	2.05	0.57
1:B:132:LEU:HD13	2:B:421:DW1:O9	2.03	0.57
1:A:357:PRO:O	1:A:359:LEU:HG	2.05	0.57
1:A:249:GLU:HB2	3:A:442:HOH:O	2.03	0.57
1:B:142:VAL:HG12	1:B:143:ALA:N	2.19	0.57
1:B:177:ILE:HG22	1:B:178:CYS:N	2.19	0.57
1:A:220:ARG:HG3	1:A:265:GLN:HE22	1.69	0.57
1:B:97:GLU:O	1:B:101:MET:HG2	2.05	0.57
1:A:72:GLN:NE2	1:A:81:LEU:HD22	2.20	0.57
1:B:61:VAL:HG12	1:B:61:VAL:O	2.04	0.56
1:A:205:LYS:NZ	1:A:213:ASN:HB3	2.20	0.56
1:B:100:ILE:HG23	1:B:177:ILE:HD12	1.87	0.56
1:B:129:ASN:HD22	1:B:129:ASN:N	2.04	0.56
1:B:345:ASP:OD1	1:B:346:PRO:HD2	2.06	0.56
1:B:357:PRO:O	1:B:359:LEU:HG	2.07	0.55
1:A:214:VAL:HB	1:A:216:TYR:CE2	2.41	0.55
1:A:330:THR:HG23	1:A:333:GLU:OE1	2.06	0.55
1:A:270:ILE:O	1:A:272:VAL:N	2.39	0.55
1:B:242:SER:O	1:B:246:VAL:HG23	2.06	0.55
1:B:268:GLU:HA	1:B:268:GLU:OE1	2.06	0.55
1:B:63:GLY:O	1:B:64:ASN:HB3	2.05	0.55
1:A:248:ALA:O	1:A:252:LEU:HB2	2.07	0.55
1:B:235:THR:O	1:B:237:SER:N	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:THR:H	1:A:280:GLN:HB2	1.71	0.54
1:A:96:ARG:HG3	1:A:96:ARG:NH2	2.13	0.54
1:B:185:GLN:HB2	3:B:461:HOH:O	2.06	0.54
1:A:95:ASN:ND2	1:A:128:LEU:HD23	2.22	0.54
1:B:220:ARG:NH1	1:B:220:ARG:CG	2.47	0.54
1:A:223:ARG:NH1	1:A:223:ARG:HG3	2.10	0.54
1:A:276:PRO:HB2	1:A:281:ILE:HG13	1.89	0.54
1:A:153:LEU:O	1:A:154:PRO:C	2.45	0.54
1:A:129:ASN:N	1:A:129:ASN:HD22	2.06	0.54
1:A:183:LYS:HE2	1:A:186:ASN:ND2	2.23	0.54
1:A:201:PHE:C	1:A:203:SER:H	2.10	0.54
1:A:130:LEU:HD23	1:A:130:LEU:N	2.22	0.54
1:A:149:ALA:C	1:A:151:GLN:H	2.12	0.53
1:B:284:MET:HE2	1:B:323:TYR:HB3	1.90	0.53
1:A:256:ILE:C	1:A:258:PRO:HD3	2.28	0.53
1:A:145:HIS:C	1:A:145:HIS:ND1	2.62	0.53
1:B:88:LEU:HA	1:B:127:TYR:HD1	1.73	0.53
1:A:46:GLN:HE22	1:A:111:ARG:HD2	1.74	0.53
1:B:228:ILE:HG21	1:B:266:LEU:HG	1.92	0.52
1:A:263:VAL:HG23	1:B:216:TYR:CD1	2.44	0.52
1:B:361:ASN:OD1	1:B:361:ASN:N	2.43	0.52
1:B:64:ASN:HA	1:B:67:PHE:CE1	2.45	0.52
1:B:135:VAL:HG13	1:B:136:PRO:HD2	1.91	0.52
1:A:270:ILE:C	1:A:272:VAL:H	2.14	0.51
1:B:301:TRP:CD1	1:B:318:SER:HB3	2.46	0.51
1:B:276:PRO:HB2	1:B:281:ILE:HG13	1.91	0.51
1:B:365:GLN:HA	1:B:365:GLN:HE21	1.75	0.51
1:B:220:ARG:CG	1:B:221[B]:TYR:H	2.24	0.51
1:B:103:LYS:NZ	3:B:427:HOH:O	2.43	0.51
1:A:351:PRO:C	1:A:353:GLY:H	2.13	0.51
1:B:160:LEU:HD11	1:B:350:LEU:HD21	1.92	0.51
1:B:194:ALA:CB	1:B:350:LEU:HD11	2.41	0.51
1:B:224:ALA:O	1:B:227:LEU:HB2	2.11	0.51
1:A:172:ILE:HG13	1:A:173:HIS:N	2.24	0.51
1:B:220:ARG:CG	1:B:221[A]:TYR:H	2.24	0.51
1:A:342:GLU:O	1:A:348:VAL:CG2	2.57	0.51
1:A:370:ASN:C	1:A:370:ASN:HD22	2.14	0.51
1:B:71:TYR:HD2	1:B:71:TYR:N	2.08	0.51
1:A:160:LEU:HD11	1:A:350:LEU:HD21	1.93	0.51
1:A:97:GLU:HG3	1:A:201:PHE:C	2.31	0.51
1:A:370:ASN:C	1:A:370:ASN:ND2	2.64	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:THR:O	1:B:367:LEU:N	2.41	0.50
1:B:71:TYR:H	1:B:71:TYR:HD2	1.60	0.50
1:A:263:VAL:HG23	1:B:216:TYR:CE1	2.46	0.50
1:B:62:ILE:HD11	1:B:72:GLN:HB2	1.93	0.50
1:B:226:GLU:HB3	1:B:284:MET:HB3	1.94	0.50
1:A:38:THR:O	1:A:55:SER:HA	2.12	0.50
1:B:129:ASN:N	1:B:129:ASN:ND2	2.59	0.50
1:A:72:GLN:CD	1:A:81:LEU:HD22	2.32	0.50
1:A:365:GLN:O	1:A:368:SER:HB3	2.12	0.50
1:B:352:ASN:HD21	1:B:354:ARG:HD3	1.77	0.50
1:A:280:GLN:O	1:A:283:GLU:HB2	2.12	0.49
1:A:220:ARG:O	1:A:221[A]:TYR:CB	2.60	0.49
1:A:160:LEU:HD11	1:A:350:LEU:CD2	2.42	0.49
1:B:279:GLU:O	1:B:280:GLN:C	2.51	0.49
1:B:275:THR:HG23	1:B:276:PRO:HD2	1.94	0.49
1:B:267:VAL:HG12	1:B:268:GLU:N	2.28	0.48
1:B:220:ARG:O	1:B:223:ARG:HG3	2.13	0.48
1:B:84:ILE:HG12	1:B:131:VAL:HG22	1.95	0.48
1:B:179:HIS:O	1:B:180:ARG:HB2	2.14	0.48
1:A:138:THR:O	1:A:139:VAL:C	2.50	0.48
1:B:358:ALA:HB1	1:B:361:ASN:HD21	1.78	0.48
1:A:263:VAL:HG12	1:A:264:ASP:N	2.28	0.48
1:A:177:ILE:CG2	1:A:178:CYS:N	2.77	0.48
1:B:194:ALA:HB2	1:B:350:LEU:HD11	1.96	0.48
1:A:101:MET:HE3	1:A:132:LEU:HD21	1.96	0.48
1:A:72:GLN:HG2	1:A:73:ALA:H	1.80	0.47
1:B:147:SER:O	1:B:148:ARG:C	2.53	0.47
1:B:157:TYR:CZ	1:B:351:PRO:HG2	2.50	0.47
1:A:177:ILE:HG22	1:A:178:CYS:N	2.29	0.47
1:A:305:PHE:O	1:A:306:ARG:O	2.32	0.47
1:B:220:ARG:CG	1:B:221[B]:TYR:N	2.78	0.47
1:B:220:ARG:CG	1:B:221[A]:TYR:N	2.78	0.47
1:A:348:VAL:HG12	1:A:348:VAL:O	2.14	0.47
1:A:196:LEU:CD2	1:A:196:LEU:C	2.83	0.47
1:B:332:LEU:HD12	1:B:332:LEU:HA	1.73	0.47
1:A:128:LEU:HD12	1:A:129:ASN:N	2.30	0.47
1:A:201:PHE:C	1:A:203:SER:N	2.68	0.47
1:A:43:THR:O	1:A:114:TYR:HA	2.15	0.47
1:B:276:PRO:HB2	1:B:281:ILE:HD11	1.97	0.46
1:A:286:PRO:C	1:A:288:TYR:H	2.19	0.46
1:A:251:LEU:HD11	1:A:313:ALA:HB1	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:C	1:A:230:GLY:H	2.17	0.46
1:A:257:PHE:N	1:A:258:PRO:HD3	2.30	0.46
1:A:220:ARG:HG3	1:A:265:GLN:NE2	2.29	0.46
1:B:266:LEU:HA	1:B:266:LEU:HD23	1.60	0.46
1:B:155:VAL:O	1:B:156:ILE:C	2.54	0.46
1:A:124:ASP:O	1:A:125:GLU:HG3	2.16	0.46
1:A:76:CYS:O	1:A:77:ASP:C	2.54	0.46
1:B:229:PHE:CE1	1:B:266:LEU:HD11	2.51	0.46
1:B:86:LYS:HE2	1:B:127:TYR:HD2	1.74	0.45
1:B:72:GLN:HG2	1:B:73:ALA:N	2.31	0.45
1:B:183:LYS:HE2	1:B:186:ASN:HD21	1.79	0.45
1:A:319:ARG:HA	1:A:319:ARG:HH11	1.81	0.45
1:B:59:THR:HA	1:B:72:GLN:O	2.17	0.45
1:B:96:ARG:O	1:B:96:ARG:HG3	2.16	0.45
1:B:299:HIS:CE1	1:B:303:LYS:CB	2.99	0.45
1:B:364:THR:HG22	1:B:365:GLN:N	2.31	0.45
1:B:296:ILE:HG22	1:B:297:LYS:O	2.16	0.45
1:B:363:THR:O	1:B:364:THR:C	2.54	0.45
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.62	0.45
1:A:95:ASN:O	1:A:99:GLN:HG3	2.17	0.45
1:B:78:SER:C	1:B:80:GLU:H	2.18	0.45
1:A:48:PRO:O	1:A:50:ARG:N	2.50	0.45
1:B:330:THR:OG1	1:B:333:GLU:HB2	2.17	0.45
1:B:91:LYS:C	1:B:93:PHE:H	2.20	0.44
1:B:86:LYS:CE	1:B:127:TYR:CD2	2.91	0.44
1:A:345:ASP:O	1:A:348:VAL:HB	2.16	0.44
1:B:305:PHE:O	1:B:306:ARG:C	2.56	0.44
1:B:357:PRO:O	1:B:359:LEU:N	2.50	0.44
1:A:129:ASN:N	1:A:129:ASN:ND2	2.64	0.44
1:B:332:LEU:HD21	1:B:367:LEU:HA	1.98	0.44
1:B:345:ASP:HA	1:B:346:PRO:HD3	1.74	0.44
1:A:135:VAL:HB	1:A:188:LEU:HB3	2.00	0.44
1:A:155:VAL:O	1:A:156:ILE:C	2.55	0.44
1:A:56:TYR:CD2	1:A:56:TYR:C	2.90	0.44
1:B:276:PRO:HB2	1:B:281:ILE:CG1	2.48	0.44
1:B:365:GLN:HA	1:B:365:GLN:NE2	2.33	0.44
1:A:371:PRO:N	1:A:372:PRO:CD	2.80	0.44
1:B:284:MET:HB2	1:B:285:ASN:H	1.53	0.44
1:A:342:GLU:O	1:A:342:GLU:HG2	2.17	0.44
1:B:264:ASP:O	1:B:268:GLU:HG2	2.18	0.44
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.70	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ALA:HB2	1:B:350:LEU:CD1	2.48	0.43
1:B:182:ILE:HB	1:B:242:SER:HB2	1.99	0.43
1:B:177:ILE:CG2	1:B:178:CYS:N	2.80	0.43
1:B:258:PRO:HD2	1:B:268:GLU:HG3	2.00	0.43
1:B:235:THR:O	1:B:236:SER:C	2.57	0.43
1:A:220:ARG:O	1:A:221[A]:TYR:HB2	2.18	0.43
1:A:330:THR:O	1:A:331:PRO:C	2.55	0.43
1:B:256:ILE:HD13	1:B:257:PHE:CE1	2.54	0.43
1:A:293:PHE:HA	1:A:294:PRO:HD3	1.73	0.43
1:B:162:MET:O	1:B:165:LEU:HB3	2.19	0.43
1:A:286:PRO:O	1:A:288:TYR:N	2.44	0.43
1:A:371:PRO:N	1:A:372:PRO:HD2	2.34	0.43
1:B:75:LEU:HD12	1:B:80:GLU:HB3	2.00	0.43
1:B:382:ALA:O	1:B:383:ARG:HB2	2.19	0.42
1:A:217:ILE:O	1:A:218:CYS:CB	2.66	0.42
1:A:213:ASN:O	1:A:232:THR:HG22	2.19	0.42
1:A:172:ILE:HG13	1:A:173:HIS:HD2	1.83	0.42
1:A:305:PHE:O	1:A:306:ARG:C	2.57	0.42
1:B:371:PRO:N	1:B:372:PRO:CD	2.82	0.42
1:A:229:PHE:CZ	1:A:293:PHE:HZ	2.38	0.42
1:B:69:VAL:CG1	1:B:71:TYR:CE2	3.02	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.64	0.42
1:B:135:VAL:HG13	1:B:136:PRO:CD	2.49	0.42
1:A:219:SER:O	1:A:220:ARG:C	2.57	0.42
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.87	0.42
1:B:98:LEU:HA	1:B:98:LEU:HD12	1.75	0.42
1:A:205:LYS:NZ	1:A:213:ASN:OD1	2.40	0.42
1:B:161:TYR:O	1:B:196:LEU:HD13	2.19	0.42
1:A:266:LEU:O	1:A:270:ILE:HG13	2.19	0.42
1:B:211:GLU:HA	1:B:212:PRO:HD3	1.79	0.42
1:B:365:GLN:CA	1:B:365:GLN:HE21	2.33	0.42
1:A:55:SER:HB2	1:A:76:CYS:SG	2.60	0.42
1:B:261:SER:O	1:B:265:GLN:HG3	2.20	0.41
1:B:148:ARG:O	1:B:150:LYS:N	2.52	0.41
1:A:42:ALA:HB1	1:A:114:TYR:HB3	2.02	0.41
1:B:156:ILE:HD13	1:B:342:GLU:OE1	2.20	0.41
1:B:197:LYS:NZ	3:B:429:HOH:O	2.52	0.41
1:B:299:HIS:ND1	1:B:300:PRO:HD2	2.35	0.41
1:B:163:TYR:HB2	1:B:340:PHE:CD1	2.55	0.41
1:B:59:THR:HG23	1:B:73:ALA:HB2	2.02	0.41
1:B:62:ILE:CG1	1:B:72:GLN:HB2	2.50	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ARG:NH1	1:A:223:ARG:CG	2.76	0.41
1:B:291:PHE:O	1:B:293:PHE:N	2.53	0.41
1:B:57:THR:O	1:B:58:ASP:HB2	2.19	0.41
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.97	0.41
1:B:160:LEU:CD2	1:B:343:LEU:HD22	2.48	0.41
1:A:379:PRO:O	1:A:380:PRO:C	2.58	0.41
1:B:69:VAL:HG11	1:B:71:TYR:CE2	2.56	0.41
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.80	0.41
1:A:129:ASN:C	1:A:130:LEU:HD23	2.42	0.41
1:B:96:ARG:NH2	1:B:205:LYS:HG3	2.35	0.41
1:A:135:VAL:HA	1:A:136:PRO:HD3	1.74	0.41
1:A:273:LEU:HB3	1:A:323:TYR:CE2	2.56	0.41
1:A:216:TYR:HB3	1:B:228:ILE:O	2.21	0.40
1:A:280:GLN:O	1:A:284:MET:CE	2.70	0.40
1:B:91:LYS:C	1:B:93:PHE:N	2.75	0.40
1:B:140:TYR:CE2	1:B:144:ARG:NH1	2.89	0.40
1:B:140:TYR:HE2	1:B:144:ARG:NH1	2.19	0.40
1:A:87:VAL:HG23	1:A:88:LEU:O	2.21	0.40
1:A:196:LEU:HD23	1:A:197:LYS:CA	2.51	0.40
1:A:330:THR:HG23	1:A:333:GLU:CD	2.42	0.40
1:B:155:VAL:O	1:B:159:LYS:HG3	2.21	0.40
1:B:282:ARG:HA	1:B:286:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

## 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	342/420 (81%)	283 (83%)	37 (11%)	22 (6%)	2	10
1	B	347/420 (83%)	290 (84%)	39 (11%)	18 (5%)	2	15
All	All	689/840 (82%)	573 (83%)	76 (11%)	40 (6%)	2	12

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	150	LYS
1	A	220	ARG
1	A	221[A]	TYR
1	A	221[B]	TYR
1	A	271	LYS
1	A	301	TRP
1	B	77	ASP
1	B	236	SER
1	B	290	GLU
1	A	49	ASP
1	A	287	ASN
1	A	352	ASN
1	B	62	ILE
1	B	149	ALA
1	B	181	ASP
1	B	358	ALA
1	A	64	ASN
1	A	76	CYS
1	A	116	PHE
1	A	156	ILE
1	B	48	PRO
1	B	64	ASN
1	B	67	PHE
1	B	92	ARG
1	B	365	GLN
1	A	348	VAL
1	B	47	GLY
1	B	218	CYS
1	B	220	ARG
1	B	277	THR
1	A	157	TYR
1	A	229	PHE
1	A	306	ARG
1	A	370	ASN
1	A	200	ASP
1	B	148	ARG
1	B	383	ARG
1	A	300	PRO
1	A	212	PRO



### 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	289/364 (79%)	270 (93%)	19 (7%)	21	56
1	B	291/364 (80%)	264 (91%)	27 (9%)	11	40
All	All	580/728 (80%)	534 (92%)	46 (8%)	15	48

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

Mol	Chain	Res	Type
1	A	46	GLN
1	A	53	GLU
1	A	55	SER
1	A	66	SER
1	A	87	VAL
1	A	96	ARG
1	A	129	ASN
1	A	145	HIS
1	A	213	ASN
1	A	223	ARG
1	A	232	THR
1	A	236	SER
1	A	252	LEU
1	A	263	VAL
1	A	296	ILE
1	A	355	ASP
1	A	364	THR
1	A	370	ASN
1	A	378	ILE
1	B	49	ASP
1	B	55	SER
1	B	57	THR
1	B	59	THR
1	B	66	SER
1	B	71	TYR
1	B	77	ASP
1	B	78	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	129	ASN
1	B	138	THR
1	B	141	ARG
1	B	144	ARG
1	B	147	SER
1	B	152	THR
1	B	185	GLN
1	B	199	CYS
1	B	213	ASN
1	B	218	CYS
1	B	220	ARG
1	B	237	SER
1	B	256	ILE
1	B	284	MET
1	B	297	LYS
1	B	317	CYS
1	B	347	ASN
1	B	365	GLN
1	B	369	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	186	ASN
1	A	370	ASN
1	B	129	ASN
1	B	186	ASN
1	B	365	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	DW1	A	421	-	30,37,37	1.42	3 (10%)	25,60,60	2.22	7 (28%)
2	DW1	B	421	-	30,37,37	1.40	4 (13%)	25,60,60	1.81	6 (24%)

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	DW1	A	421	-	-	0/0/28/28	0/7/7/7
2	DW1	B	421	-	-	0/0/28/28	0/7/7/7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	421	DW1	C28-C21	-4.17	1.37	1.42
2	B	421	DW1	C28-C21	-3.56	1.38	1.42
2	B	421	DW1	C7-C21	-2.60	1.37	1.43
2	A	421	DW1	C7-C21	-2.58	1.37	1.43
2	A	421	DW1	C23-C22	-2.22	1.36	1.41
2	B	421	DW1	C1-C2	-2.13	1.38	1.42
2	B	421	DW1	C26-C25	2.11	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	421	DW1	C25-C26-C27	-5.01	117.56	120.60
2	B	421	DW1	C25-C26-C27	-3.73	118.33	120.60
2	B	421	DW1	C2-C3-C7	-3.12	114.66	119.23
2	B	421	DW1	C2-C29-C28	-2.79	119.58	121.22
2	A	421	DW1	C2-C3-C7	-2.74	115.22	119.23
2	A	421	DW1	C2-C29-C28	-2.70	119.63	121.22
2	A	421	DW1	C23-C24-C25	2.69	123.49	120.18
2	A	421	DW1	C4-C3-C2	2.82	127.19	123.14
2	B	421	DW1	C4-C3-C2	2.87	127.27	123.14
2	B	421	DW1	C6-N20-C7	3.16	120.00	117.39
2	B	421	DW1	C7-C21-N18	4.12	121.63	116.59
2	A	421	DW1	C6-N20-C7	4.35	120.98	117.39
2	A	421	DW1	C7-C21-N18	5.83	123.72	116.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	421	DW1	1	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	A	348/420 (82%)	-0.41	6 (1%)	73 53	23, 44, 84, 112	1 (0%)
1	B	349/420 (83%)	-0.46	2 (0%)	90 81	20, 43, 85, 111	0
All	All	697/840 (82%)	-0.44	8 (1%)	82 68	20, 43, 86, 112	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	GLY	4.3
1	B	35	SER	3.1
1	A	122	LYS	3.0
1	A	295	GLN	2.8
1	A	90	ASP	2.6
1	A	385	GLN	2.6
1	A	124	ASP	2.5
1	A	121	GLU	2.2

### 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( $\text{\AA}^2$ )	Q<0.9
2	DW1	A	421	31/31	0.99	0.15	-0.30	32,39,44,46	0
2	DW1	B	421	31/31	0.99	0.14	-0.78	37,43,49,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.