



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:25 pm GMT

PDB ID : 2ASS  
Title : Crystal structure of the Skp1-Skp2-Cks1 complex  
Authors : Hao, B.; Zhang, N.; Schulman, B.A.; Wu, G.; Pagano, M.; Pavletich, N.P.  
Deposited on : 2005-08-24  
Resolution : 3.00 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 : trunk28620  
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) : recalc28949

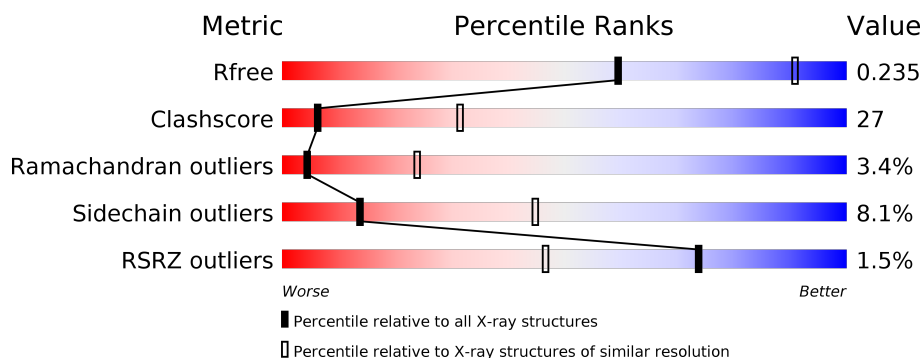
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	159	<div> <div>4%</div> <div> <div></div> <div>43%</div> <div>33%</div> <div>13%</div> <div>• 10%</div> </div> </div>
2	B	336	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>6%</div> <div>• •</div> </div> </div>
3	C	69	<div> <div></div> <div> <div>49%</div> <div>45%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	B	3	-	-	-	X
4	PO4	B	5	-	-	-	X
4	PO4	C	4	-	-	X	-
5	BEN	C	2	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4404 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 S-phase kinase-associated protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1133	718	184	225	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	ALA	PRO	ENGINEERED	UNP P63208

- Molecule 2 is a protein called S-phase kinase-associated protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	325	Total	C	N	O	S	0	0	0
			2572	1635	443	478	16			

- Molecule 3 is a protein called Cyclin-dependent kinases regulatory subunit 1.

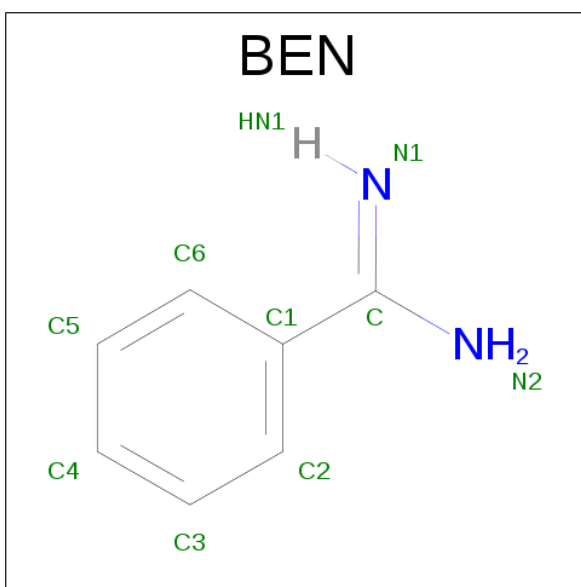
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	69	Total	C	N	O	S	0	0	0
			599	387	102	107	3			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			9	7	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	50	Total	O	0	0
			50	50		
6	C	10	Total	O	0	0
			10	10		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.33Å 149.33Å 99.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.00 19.94 – 2.98	Depositor EDS
% Data completeness (in resolution range)	95.7 (19.94-3.00) 94.3 (19.94-2.98)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.214 , 0.242 0.211 , 0.235	Depositor DCC
$R_{free}$ test set	1960 reflections (7.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BEN

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	0.52	1/1150 (0.1%)	0.76	4/1552 (0.3%)
2	B	0.85	3/2622 (0.1%)	0.90	8/3558 (0.2%)
3	C	0.41	0/619	0.76	0/837
All	All	0.73	4/4391 (0.1%)	0.85	12/5947 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2126	ARG	C-O	30.55	1.81	1.23
2	B	2127	TRP	N-CA	19.80	1.85	1.46
1	A	1059	HIS	C-O	-10.13	1.04	1.23
2	B	2125	LYS	C-O	-5.54	1.12	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2126	ARG	O-C-N	21.56	157.19	122.70
2	B	2126	ARG	CA-C-O	-11.81	95.31	120.10
2	B	2126	ARG	C-N-CA	10.16	147.10	121.70
2	B	2127	TRP	N-CA-CB	8.95	126.71	110.60
1	A	1059	HIS	N-CA-C	-8.73	87.43	111.00
1	A	1060	LYS	CA-C-N	-7.26	101.22	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2126	ARG	CB-CA-C	-7.19	96.02	110.40
2	B	2126	ARG	N-CA-C	-7.05	91.97	111.00
2	B	2127	TRP	N-CA-C	-6.43	93.63	111.00
1	A	1060	LYS	N-CA-CB	6.13	121.64	110.60
1	A	1147	GLU	N-CA-C	-5.84	95.22	111.00
2	B	2126	ARG	CA-C-N	-5.66	104.75	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1059	HIS	Mainchain

## 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	1133	0	1125	86	0
2	B	2572	0	2607	122	0
3	C	599	0	574	36	0
4	B	10	0	0	0	0
4	C	5	0	0	3	0
5	B	9	0	7	0	0
5	C	9	0	7	0	0
6	A	7	0	0	0	0
6	B	50	0	0	10	0
6	C	10	0	0	0	0
All	All	4404	0	4320	233	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 27.

All (233) 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)
2:B:2127:TRP:N	2:B:2127:TRP:CA	1.85	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2126:ARG:C	2:B:2126:ARG:O	1.81	1.16
1:A:1037:ASP:HA	1:A:1038:PRO:HA	1.34	1.09
1:A:1059:HIS:O	1:A:1060:LYS:HG2	1.58	1.01
2:B:2143:THR:HG22	2:B:2166:PRO:HD2	1.42	0.99
2:B:2102:ASP:OD1	2:B:2126:ARG:NH2	1.97	0.97
1:A:1059:HIS:O	1:A:1060:LYS:CG	2.13	0.94
2:B:2208:LEU:H	2:B:2229:ASN:HD22	1.20	0.89
2:B:2100:LEU:HD11	2:B:2104:LEU:HD23	1.57	0.86
1:A:1091:GLU:HA	1:A:1094:LYS:HG3	1.59	0.85
2:B:2100:LEU:HD12	2:B:2101:PRO:HD2	1.59	0.83
2:B:2141:ASP:OD1	2:B:2143:THR:HG23	1.79	0.82
1:A:1037:ASP:CA	1:A:1038:PRO:HA	2.09	0.82
2:B:2366:GLN:HE22	2:B:2391:SER:H	1.28	0.80
2:B:2415:ARG:NH1	2:B:2415:ARG:HB3	1.97	0.79
1:A:1082:THR:HG22	1:A:1083:ASP:H	1.48	0.78
1:A:1057:THR:O	1:A:1060:LYS:HE2	1.85	0.77
2:B:2185:HIS:HD2	2:B:2210:ASN:HD22	1.32	0.77
2:B:2113:CYS:SG	2:B:2116:GLU:HG2	2.26	0.75
3:C:3025:PRO:HD2	3:C:3028:ILE:HD11	1.69	0.74
1:A:1045:ASN:HD21	1:A:1048:ILE:H	1.32	0.74
1:A:1045:ASN:ND2	1:A:1048:ILE:H	1.85	0.73
1:A:1145:PHE:HB3	1:A:1150:GLU:HG2	1.70	0.73
1:A:1037:ASP:HA	1:A:1038:PRO:CA	2.16	0.71
1:A:1146:THR:HG22	1:A:1147:GLU:H	1.55	0.71
2:B:2287:GLN:HG2	2:B:2314:HIS:HB2	1.72	0.71
3:C:3040:GLU:HG3	3:C:3043:TRP:CZ2	2.26	0.71
1:A:1091:GLU:HB3	1:A:1094:LYS:HD2	1.73	0.70
1:A:1097:GLN:CG	2:B:2097:TRP:HE1	2.04	0.70
2:B:2349:ILE:HB	2:B:2352:THR:HG23	1.74	0.70
2:B:2401:ILE:HG13	2:B:2402:GLY:N	2.06	0.69
2:B:2143:THR:CG2	2:B:2166:PRO:HD2	2.22	0.69
2:B:2325:ASN:HA	2:B:2328:PHE:CE1	2.26	0.69
3:C:3013:ASP:HB2	3:C:3017:PHE:O	1.92	0.69
1:A:1019:GLU:HA	1:A:1022:LYS:HB3	1.74	0.69
2:B:2118:LEU:O	2:B:2121:SER:HB3	1.93	0.68
2:B:2126:ARG:CA	2:B:2126:ARG:O	2.41	0.68
2:B:2127:TRP:N	2:B:2127:TRP:C	2.47	0.68
2:B:2149:PRO:HA	2:B:2152:THR:HG23	1.75	0.68
1:A:1049:LEU:O	1:A:1053:ILE:HG13	1.94	0.67
2:B:2194:GLU:OE1	2:B:2194:GLU:HA	1.94	0.67
2:B:2366:GLN:NE2	2:B:2391:SER:H	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2143:THR:HG22	2:B:2164:ARG:HG2	1.78	0.66
2:B:2185:HIS:CD2	2:B:2210:ASN:HD22	2.14	0.66
1:A:1132:PRO:O	1:A:1136:ARG:HD3	1.95	0.65
3:C:3007:TYR:HB3	3:C:3023:MET:HB2	1.79	0.65
1:A:1086:PRO:O	1:A:1090:GLN:HG2	1.96	0.65
1:A:1019:GLU:O	1:A:1022:LYS:HB3	1.97	0.64
1:A:1136:ARG:NH2	1:A:1143:ASN:HD21	1.94	0.64
2:B:2203:SER:HA	6:B:67:HOH:O	1.96	0.64
1:A:1122:THR:O	1:A:1126:MET:HG3	1.97	0.64
2:B:2121:SER:O	2:B:2128:TYR:HB2	1.99	0.63
2:B:2102:ASP:OD1	2:B:2126:ARG:CZ	2.46	0.63
2:B:2208:LEU:H	2:B:2229:ASN:ND2	1.95	0.63
2:B:2415:ARG:HH11	2:B:2415:ARG:HB3	1.62	0.63
2:B:2194:GLU:HB2	6:B:28:HOH:O	1.98	0.63
2:B:2289:ASN:HB2	2:B:2396:ILE:HD12	1.80	0.63
1:A:1087:VAL:O	1:A:1090:GLN:HB2	1.98	0.62
2:B:2098:ASP:O	2:B:2099:SER:HB3	1.99	0.62
1:A:1037:ASP:C	1:A:1038:PRO:N	2.53	0.62
2:B:2225:THR:HB	6:B:67:HOH:O	1.99	0.61
2:B:2124:CYS:SG	2:B:2127:TRP:HB2	2.41	0.61
2:B:2098:ASP:OD1	2:B:2099:SER:N	2.34	0.61
2:B:2228:LYS:HE3	6:B:67:HOH:O	2.01	0.61
1:A:1131:THR:O	1:A:1135:ILE:HG12	2.00	0.61
1:A:1136:ARG:NH2	1:A:1143:ASN:ND2	2.49	0.60
2:B:2262:ASN:HD22	2:B:2262:ASN:C	2.02	0.60
2:B:2303:SER:HA	2:B:2330:GLU:OE2	2.01	0.60
1:A:1029:THR:O	1:A:1032:GLU:HG2	2.02	0.60
1:A:1146:THR:HB	1:A:1148:GLU:H	1.67	0.60
2:B:2152:THR:HG21	2:B:2170:MET:SD	2.42	0.60
2:B:2402:GLY:HA2	2:B:2406:ASN:HB2	1.83	0.60
1:A:1133:GLU:HA	1:A:1136:ARG:NH1	2.17	0.60
2:B:2344:ARG:NH2	3:C:3045:ASN:OD1	2.34	0.60
1:A:1059:HIS:O	1:A:1060:LYS:HG3	2.01	0.60
2:B:2277:ALA:O	2:B:2281:VAL:HG22	2.03	0.59
3:C:3020:ARG:NH1	4:C:4:PO4:O3	2.34	0.59
1:A:1045:ASN:C	1:A:1045:ASN:HD22	2.05	0.59
2:B:2143:THR:CG2	2:B:2164:ARG:HG2	2.32	0.59
3:C:3036:HIS:HD2	3:C:3037:LEU:O	1.86	0.59
2:B:2127:TRP:N	2:B:2128:TYR:N	2.51	0.58
2:B:2146:ASN:C	2:B:2146:ASN:HD22	2.07	0.58
1:A:1019:GLU:CG	1:A:1022:LYS:HD3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:ASP:O	1:A:1085:ILE:HB	2.03	0.58
3:C:3026:LYS:HE2	3:C:3065:HIS:CD2	2.39	0.58
1:A:1043:ASN:HB2	1:A:1109:TYR:CE2	2.39	0.58
2:B:2183:VAL:HG13	6:B:55:HOH:O	2.02	0.58
1:A:1093:LEU:C	1:A:1095:VAL:H	2.07	0.57
2:B:2325:ASN:HA	2:B:2328:PHE:CD1	2.40	0.57
1:A:1148:GLU:O	1:A:1152:GLN:HB2	2.05	0.57
2:B:2351:GLU:O	2:B:2354:LEU:HB2	2.05	0.56
2:B:2293:TYR:O	2:B:2295:LYS:N	2.38	0.56
3:C:3023:MET:HG2	3:C:3066:ILE:HD13	1.87	0.56
3:C:3025:PRO:HD2	3:C:3028:ILE:CD1	2.36	0.56
2:B:2409:ILE:O	2:B:2409:ILE:HG13	2.06	0.56
3:C:3005:GLN:OE1	3:C:3005:GLN:HA	2.06	0.56
3:C:3057:TYR:CE2	3:C:3058:MET:HG2	2.40	0.56
1:A:1088:TRP:O	1:A:1091:GLU:OE1	2.23	0.55
2:B:2163:PHE:HD2	2:B:2186:MET:CE	2.20	0.55
1:A:1025:VAL:HB	1:A:1111:ASP:OD2	2.07	0.55
1:A:1087:VAL:HA	1:A:1090:GLN:HG3	1.89	0.55
3:C:3005:GLN:HB3	3:C:3025:PRO:HG2	1.89	0.55
1:A:1097:GLN:HG2	2:B:2097:TRP:HE1	1.72	0.54
3:C:3023:MET:HG2	3:C:3066:ILE:CD1	2.36	0.54
1:A:1005:LYS:HB2	1:A:1038:PRO:HB3	1.89	0.54
2:B:2402:GLY:HA2	2:B:2406:ASN:CB	2.37	0.54
1:A:1123:VAL:HG11	2:B:2108:ILE:HD13	1.90	0.54
1:A:1005:LYS:O	1:A:1038:PRO:HB2	2.07	0.53
1:A:1136:ARG:CZ	1:A:1143:ASN:ND2	2.71	0.53
2:B:2116:GLU:O	2:B:2119:LYS:HB3	2.09	0.53
1:A:1082:THR:HG22	1:A:1083:ASP:N	2.20	0.53
2:B:2100:LEU:CD1	2:B:2104:LEU:HD23	2.36	0.53
1:A:1037:ASP:O	1:A:1038:PRO:N	2.43	0.52
1:A:1012:GLU:HG2	1:A:1014:PHE:CE1	2.44	0.52
1:A:1019:GLU:HG2	1:A:1022:LYS:HD3	1.90	0.52
2:B:2302:LEU:O	2:B:2306:VAL:HG23	2.09	0.52
3:C:3011:LYS:HE2	4:C:4:PO4:O3	2.10	0.52
2:B:2126:ARG:C	2:B:2129:ARG:H	2.13	0.52
3:C:3040:GLU:HA	3:C:3043:TRP:CE2	2.45	0.52
1:A:1019:GLU:HA	1:A:1022:LYS:CB	2.40	0.51
2:B:2265:TRP:CH2	3:C:3040:GLU:HB3	2.45	0.51
1:A:1149:GLU:HA	1:A:1152:GLN:HB3	1.92	0.51
3:C:3013:ASP:OD1	3:C:3014:ASP:O	2.29	0.51
1:A:1057:THR:O	1:A:1060:LYS:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:THR:O	1:A:1123:VAL:HG23	2.11	0.51
1:A:1133:GLU:HA	1:A:1136:ARG:HH11	1.76	0.51
2:B:2355:GLU:O	2:B:2358:GLU:HB2	2.11	0.51
3:C:3027:ASP:O	3:C:3030:LYS:HE2	2.10	0.51
1:A:1104:ILE:HG12	2:B:2104:LEU:HD21	1.93	0.50
2:B:2265:TRP:CZ2	3:C:3040:GLU:HB3	2.46	0.50
2:B:2348:ILE:HG21	2:B:2353:LEU:HD21	1.93	0.50
2:B:2371:VAL:HG11	2:B:2376:LEU:HA	1.92	0.50
2:B:2377:GLN:O	2:B:2381:GLU:HG2	2.11	0.50
2:B:2113:CYS:SG	2:B:2115:PRO:HG2	2.52	0.50
2:B:2144:GLY:HA2	2:B:2167:ARG:O	2.11	0.50
2:B:2221:PRO:O	2:B:2225:THR:HG23	2.11	0.50
2:B:2098:ASP:O	2:B:2099:SER:CB	2.60	0.50
2:B:2394:THR:HG22	3:C:3042:GLU:OE2	2.12	0.49
2:B:2349:ILE:O	2:B:2350:PRO:C	2.51	0.49
1:A:1142:LYS:CG	1:A:1143:ASN:H	2.25	0.49
2:B:2154:ARG:HD2	6:B:15:HOH:O	2.11	0.49
1:A:1149:GLU:O	1:A:1150:GLU:C	2.51	0.49
2:B:2149:PRO:HA	2:B:2152:THR:CG2	2.40	0.49
2:B:2358:GLU:O	2:B:2360:PRO:HD3	2.13	0.49
2:B:2300:SER:O	2:B:2303:SER:HB2	2.13	0.48
1:A:1146:THR:CG2	1:A:1147:GLU:H	2.19	0.48
1:A:1107:ALA:HB2	1:A:1115:LEU:HD13	1.95	0.48
2:B:2211:LEU:CD2	2:B:2226:LEU:HD21	2.44	0.48
1:A:1019:GLU:CA	1:A:1022:LYS:HB3	2.44	0.48
1:A:1037:ASP:CA	1:A:1038:PRO:CA	2.85	0.48
2:B:2126:ARG:C	2:B:2129:ARG:HB3	2.14	0.47
3:C:3012:TYR:CD1	3:C:3013:ASP:N	2.81	0.47
2:B:2164:ARG:HD2	2:B:2409:ILE:HG23	1.96	0.47
3:C:3006:ILE:HG22	3:C:3008:TYR:CE1	2.50	0.47
2:B:2100:LEU:CD1	2:B:2101:PRO:HD2	2.36	0.47
2:B:2146:ASN:HA	2:B:2169:PHE:HB2	1.97	0.47
2:B:2163:PHE:HD2	2:B:2186:MET:HE2	1.79	0.47
2:B:2143:THR:HG21	2:B:2164:ARG:CZ	2.45	0.47
1:A:1045:ASN:C	1:A:1045:ASN:ND2	2.67	0.46
2:B:2137:TRP:O	2:B:2160:VAL:HA	2.16	0.46
2:B:2366:GLN:HE21	2:B:2368:PHE:HE1	1.61	0.46
3:C:3027:ASP:O	3:C:3030:LYS:HG2	2.16	0.46
2:B:2112:LEU:HB3	2:B:2116:GLU:HB2	1.98	0.46
3:C:3040:GLU:HA	3:C:3043:TRP:NE1	2.31	0.46
2:B:2307:ARG:NH1	6:B:53:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:ASN:HD21	1:A:1048:ILE:HG12	1.81	0.46
1:A:1043:ASN:HB2	1:A:1109:TYR:CD2	2.51	0.45
1:A:1146:THR:O	1:A:1150:GLU:CG	2.63	0.45
2:B:2415:ARG:CZ	2:B:2415:ARG:HB3	2.45	0.45
2:B:2381:GLU:HA	2:B:2381:GLU:OE1	2.16	0.45
2:B:2390:CYS:HB2	6:B:56:HOH:O	2.16	0.45
1:A:1013:ILE:HD13	1:A:1038:PRO:HG3	1.97	0.45
2:B:2202:LEU:HA	2:B:2202:LEU:HD23	1.79	0.45
2:B:2171:ASP:CG	2:B:2171:ASP:O	2.55	0.44
2:B:2128:TYR:CD1	2:B:2128:TYR:C	2.91	0.44
3:C:3036:HIS:CD2	3:C:3037:LEU:O	2.70	0.44
1:A:1146:THR:HG22	1:A:1147:GLU:N	2.27	0.44
3:C:3025:PRO:O	3:C:3027:ASP:N	2.48	0.44
3:C:3051:SER:OG	4:C:4:PO4:O4	2.34	0.44
2:B:2395:THR:HG22	2:B:2401:ILE:CG2	2.47	0.44
3:C:3046:LEU:HD23	3:C:3046:LEU:HA	1.86	0.44
2:B:2291:SER:HB2	2:B:2318:SER:O	2.18	0.44
1:A:1045:ASN:HD22	1:A:1047:ALA:N	2.16	0.43
2:B:2401:ILE:CG1	2:B:2402:GLY:N	2.78	0.43
1:A:1049:LEU:HD22	1:A:1053:ILE:HD11	1.99	0.43
2:B:2231:ASN:HB2	6:B:61:HOH:O	2.18	0.43
2:B:2246:PHE:O	2:B:2250:THR:HG22	2.18	0.43
2:B:2219:SER:OG	2:B:2221:PRO:HD2	2.17	0.43
2:B:2403:ASN:O	2:B:2404:LYS:HB2	2.17	0.43
1:A:1038:PRO:O	1:A:1040:PRO:HD3	2.19	0.43
2:B:2132:SER:O	2:B:2133:ASP:O	2.37	0.43
1:A:1093:LEU:C	1:A:1095:VAL:N	2.71	0.42
3:C:3073:LEU:HD12	3:C:3073:LEU:HA	1.88	0.42
2:B:2262:ASN:ND2	2:B:2262:ASN:C	2.71	0.42
2:B:2324:LYS:O	2:B:2326:ASP:N	2.52	0.42
2:B:2156:LEU:HD21	2:B:2163:PHE:CD2	2.54	0.42
2:B:2328:PHE:N	2:B:2328:PHE:CD1	2.87	0.42
1:A:1142:LYS:HG2	1:A:1143:ASN:H	1.83	0.42
2:B:2134:GLU:O	2:B:2134:GLU:HG2	2.17	0.42
2:B:2234:ARG:HG2	2:B:2260:GLU:HB2	2.02	0.42
1:A:1058:HIS:C	1:A:1059:HIS:O	2.51	0.42
1:A:1159:TRP:CG	2:B:2151:VAL:HG11	2.54	0.42
2:B:2376:LEU:HD13	2:B:2380:LYS:HE2	2.00	0.42
3:C:3020:ARG:CG	3:C:3021:HIS:N	2.81	0.42
2:B:2277:ALA:O	2:B:2281:VAL:CG2	2.66	0.42
3:C:3005:GLN:HB3	3:C:3025:PRO:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:SER:OG	1:A:1045:ASN:HA	2.19	0.42
2:B:2271:GLU:HB2	2:B:2275:GLN:NE2	2.35	0.42
2:B:2190:ASN:CG	3:C:3037:LEU:HD13	2.40	0.42
3:C:3061:GLU:N	3:C:3062:PRO:CD	2.82	0.41
1:A:1027:ILE:O	1:A:1031:LEU:HG	2.21	0.41
2:B:2208:LEU:HB2	2:B:2229:ASN:ND2	2.35	0.41
2:B:2127:TRP:N	2:B:2128:TYR:H	2.19	0.41
2:B:2327:CYS:HA	2:B:2329:GLN:HE21	1.85	0.41
1:A:1037:ASP:CB	1:A:1038:PRO:HA	2.51	0.41
2:B:2354:LEU:HD12	2:B:2354:LEU:HA	1.94	0.41
1:A:1057:THR:O	1:A:1059:HIS:O	2.39	0.41
1:A:1035:GLY:O	1:A:1036:MET:HB2	2.20	0.41
2:B:2287:GLN:HG2	2:B:2314:HIS:CD2	2.56	0.41
1:A:1004:ILE:CG2	1:A:1005:LYS:N	2.84	0.41
1:A:1091:GLU:O	1:A:1094:LYS:HB2	2.21	0.41
2:B:2309:CYS:HB3	6:B:68:HOH:O	2.19	0.41
2:B:2198:LEU:HA	2:B:2198:LEU:HD12	1.91	0.41
1:A:1007:GLN:HB2	1:A:1038:PRO:HG2	2.03	0.40
1:A:1084:ASP:O	1:A:1085:ILE:CB	2.69	0.40
1:A:1093:LEU:O	1:A:1095:VAL:N	2.54	0.40
2:B:2302:LEU:HD22	2:B:2306:VAL:HG23	2.02	0.40
3:C:3040:GLU:HG3	3:C:3043:TRP:CH2	2.55	0.40
1:A:1128:LYS:HA	2:B:2116:GLU:OE1	2.21	0.40
1:A:1146:THR:HB	1:A:1148:GLU:N	2.35	0.40
1:A:1033:ASP:O	1:A:1034:LEU:C	2.60	0.40
1:A:1158:GLN:C	1:A:1160:CYS:H	2.24	0.40
3:C:3067:LEU:HB2	3:C:3069:PHE:HE1	1.85	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	137/159 (86%)	113 (82%)	14 (10%)	10 (7%)	1	6
2	B	323/336 (96%)	288 (89%)	28 (9%)	7 (2%)	8	36
3	C	67/69 (97%)	61 (91%)	5 (8%)	1 (2%)	12	48
All	All	527/564 (93%)	462 (88%)	47 (9%)	18 (3%)	4	24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1036	MET
2	B	2126	ARG
2	B	2133	ASP
2	B	2294	ARG
2	B	2325	ASN
2	B	2402	GLY
1	A	1060	LYS
1	A	1143	ASN
1	A	1146	THR
1	A	1159	TRP
1	A	1086	PRO
1	A	1094	LYS
1	A	1138	THR
1	A	1142	LYS
2	B	2134	GLU
1	A	1034	LEU
2	B	2404	LYS
3	C	3051	SER

### 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	128/145 (88%)	114 (89%)	14 (11%)	7	29
2	B	301/311 (97%)	279 (93%)	22 (7%)	16	50
3	C	66/66 (100%)	62 (94%)	4 (6%)	22	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	495/522 (95%)	455 (92%)	40 (8%)	14	45

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	ILE
1	A	1010	ASP
1	A	1019	GLU
1	A	1045	ASN
1	A	1049	LEU
1	A	1057	THR
1	A	1083	ASP
1	A	1090	GLN
1	A	1091	GLU
1	A	1115	LEU
1	A	1136	ARG
1	A	1139	PHE
1	A	1149	GLU
1	A	1154	ARG
2	B	2127	TRP
2	B	2128	TYR
2	B	2146	ASN
2	B	2152	THR
2	B	2171	ASP
2	B	2194	GLU
2	B	2220	ASP
2	B	2250	THR
2	B	2257	ARG
2	B	2262	ASN
2	B	2268	ASP
2	B	2271	GLU
2	B	2281	VAL
2	B	2290	LEU
2	B	2302	LEU
2	B	2324	LYS
2	B	2325	ASN
2	B	2329	GLN
2	B	2354	LEU
2	B	2376	LEU
2	B	2403	ASN
2	B	2417	THR
3	C	3046	LEU

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Mol	Chain	Res	Type
3	C	3058	MET
3	C	3068	LEU
3	C	3073	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1045	ASN
1	A	1054	GLN
1	A	1090	GLN
1	A	1125	ASN
1	A	1140	ASN
1	A	1143	ASN
2	B	2146	ASN
2	B	2185	HIS
2	B	2209	GLN
2	B	2229	ASN
2	B	2249	GLN
2	B	2262	ASN
2	B	2275	GLN
2	B	2329	GLN
2	B	2339	HIS
2	B	2366	GLN
2	B	2385	HIS
2	B	2419	GLN
3	C	3036	HIS

### 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

5 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	$\# Z  > 2$
5	BEN	B	1	-	9,9,9	1.62	2 (22%)	9,11,11	2.19	4 (44%)
4	PO4	B	3	-	4,4,4	1.41	0	6,6,6	0.41	0
4	PO4	B	5	-	4,4,4	1.38	0	6,6,6	0.40	0
5	BEN	C	2	-	9,9,9	1.59	2 (22%)	9,11,11	2.20	4 (44%)
4	PO4	C	4	-	4,4,4	1.56	0	6,6,6	0.37	0

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
5	BEN	B	1	-	-	0/4/4/4	0/1/1/1
4	PO4	B	3	-	-	0/0/0/0	0/0/0/0
4	PO4	B	5	-	-	0/0/0/0	0/0/0/0
5	BEN	C	2	-	-	0/4/4/4	0/1/1/1
4	PO4	C	4	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	BEN	C1-C	-2.80	1.42	1.47
5	C	2	BEN	C1-C	-2.22	1.43	1.47
5	B	1	BEN	C2-C1	2.08	1.42	1.39
5	C	2	BEN	C2-C1	2.19	1.42	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	BEN	C6-C1-C2	-3.10	114.28	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	BEN	C6-C1-C2	-3.01	114.41	118.58
5	B	1	BEN	C1-C-N2	2.00	121.19	118.12
5	C	2	BEN	C1-C-N2	2.20	121.50	118.12
5	B	1	BEN	C5-C6-C1	2.96	123.83	120.35
5	C	2	BEN	C5-C6-C1	3.25	124.17	120.35
5	C	2	BEN	C6-C1-C	3.39	124.80	120.66
5	B	1	BEN	C6-C1-C	3.64	125.11	120.66

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
4	C	4	PO4	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 [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	143/159 (89%)	0.03	6 (4%) 37 15	50, 86, 121, 139	0
2	B	325/336 (96%)	-0.67	2 (0%) 89 71	26, 47, 81, 122	0
3	C	69/69 (100%)	-0.57	0 100 100	33, 51, 72, 85	0
All	All	537/564 (95%)	-0.47	8 (1%) 74 47	26, 55, 113, 139	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1064	PRO	8.7
1	A	1063	PRO	6.6
1	A	1082	THR	4.1
1	A	1002	ALA	3.3
2	B	2095	VAL	2.8
1	A	1083	ASP	2.3
2	B	2419	GLN	2.3
1	A	1081	ARG	2.1

### 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
4	PO4	B	5	5/5	0.90	0.28	3.94	110,110,110,111	0
5	BEN	C	2	9/9	0.91	0.26	3.92	73,76,78,79	0
4	PO4	B	3	5/5	0.99	0.25	2.06	74,74,75,76	0
5	BEN	B	1	9/9	0.98	0.12	-0.58	41,42,42,42	0
4	PO4	C	4	5/5	0.97	0.13	-1.13	87,87,88,89	0

## 6.5 Other polymers

There are no such residues in this entry.