



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:35 PM GMT

PDB ID : 1FS1  
Title : INSIGHTS INTO SCF UBIQUITIN LIGASES FROM THE STRUCTURE  
OF THE SKP1-SKP2 COMPLEX  
Authors : Schulman, B.A.; Carrano, A.C.; Jeffrey, P.D.; Bowen, Z.; Kinnucan, E.R.E.;  
Finnin, M.S.; Elledge, S.J.; Harper, J.W.; Pagano, M.; Pavletich, N.P.  
Deposited on : 2000-09-08  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

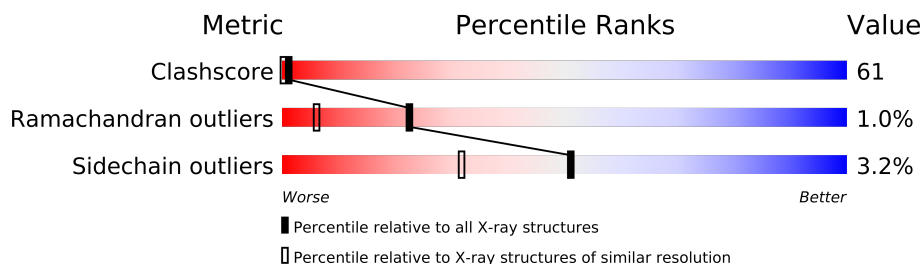
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 Å.

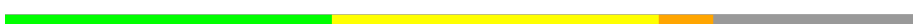
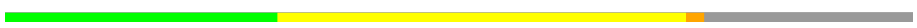
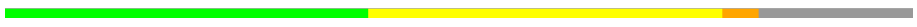
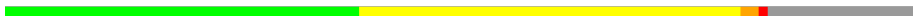
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	53	
1	C	53	
2	B	141	
2	D	141	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3067 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYCLIN A/CDK2-ASSOCIATED P19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	41	Total	C	N	O	S	0	0	0
			333	219	52	59	3			
1	C	41	Total	C	N	O	S	0	0	0
			330	218	52	57	3			

- Molecule 2 is a protein called CYCLIN A/CDK2-ASSOCIATED P45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			909	584	146	174	5			
2	D	118	Total	C	N	O	S	0	0	0
			925	594	149	177	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	GLY	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208
D	?	-	GLY	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	196	Total 196	O 196	0	0
3	C	69	Total 69	O 69	0	0
3	D	236	Total 236	O 236	0	0



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.54Å 41.60Å 87.23Å 90.00° 93.42° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.61	1/342 (0.3%)	0.83	0/465
1	C	0.60	0/339	0.81	0/461
2	B	0.67	0/923	0.90	2/1248 (0.2%)
2	D	0.71	0/939	0.92	2/1271 (0.2%)
All	All	0.67	1/2543 (0.0%)	0.88	4/3445 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	CYS	CB-SG	-6.10	1.71	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	PRO	N-CA-CB	6.49	111.09	103.30
2	D	2	PRO	N-CA-CB	6.45	111.04	103.30
2	B	35	GLY	N-CA-C	-6.02	98.05	113.10
2	D	96	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	333	0	333	56	0
1	C	330	0	331	67	0
2	B	909	0	928	95	0
2	D	925	0	944	105	0
3	A	69	0	0	43	0
3	B	196	0	0	56	0
3	C	69	0	0	42	0
3	D	236	0	0	61	0
All	All	3067	0	2536	307	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 61.

All (307) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:13:ILE:HG13	3:D:346:HOH:O	1.41	1.17
2:D:30:MET:HE3	3:D:345:HOH:O	1.45	1.16
2:D:26:THR:HG21	3:D:329:HOH:O	1.49	1.12
2:B:20:ILE:HG22	3:B:312:HOH:O	1.49	1.10
2:D:137:LYS:HD2	3:D:351:HOH:O	1.53	1.09
1:C:137:LYS:H	1:C:137:LYS:HD2	1.16	1.05
2:D:18:VAL:HG23	3:D:338:HOH:O	1.57	1.03
1:A:110:ASP:HB2	3:A:194:HOH:O	1.60	1.02
2:D:44:PRO:HB3	3:D:336:HOH:O	1.59	1.00
2:B:32:GLU:HG3	3:B:325:HOH:O	1.60	0.99
1:C:112:LEU:HG	3:C:200:HOH:O	1.62	0.99
2:B:43:ASP:HB3	2:B:44:PRO:HD3	1.44	0.99
1:C:109:TRP:HE1	2:D:139:PHE:HB3	1.29	0.98
2:D:31:LEU:HB2	3:D:325:HOH:O	1.64	0.97
2:D:26:THR:HB	3:D:347:HOH:O	1.66	0.96
1:C:123:CYS:SG	3:D:340:HOH:O	2.24	0.95
2:B:130:LYS:HE3	3:B:341:HOH:O	1.65	0.95
1:A:131:LYS:HE3	3:A:192:HOH:O	1.64	0.94
1:A:149:TRP:HD1	3:A:215:HOH:O	1.49	0.94
1:C:129:LEU:HD13	3:C:206:HOH:O	1.65	0.94
3:B:169:HOH:O	2:D:66:LYS:HD3	1.68	0.92
1:C:115:GLU:HG2	3:C:161:HOH:O	1.70	0.92
1:A:145:ASP:HB2	3:A:198:HOH:O	1.70	0.90
2:B:28:LYS:HG3	3:B:325:HOH:O	1.72	0.89
1:C:137:LYS:CD	1:C:137:LYS:H	1.85	0.89
1:C:112:LEU:CD2	3:C:200:HOH:O	2.21	0.89
1:A:137:LYS:HD3	3:A:210:HOH:O	1.72	0.89
2:B:138:THR:HA	3:B:292:HOH:O	1.73	0.89

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:GLU:CB	3:A:205:HOH:O	2.20	0.88
1:A:113:PRO:HG2	3:B:326:HOH:O	1.73	0.87
2:D:65:HIS:HD2	2:D:68:ASP:OD2	1.58	0.86
2:B:4:ILE:HG23	2:B:18:VAL:HG12	1.55	0.86
2:B:32:GLU:CG	3:B:325:HOH:O	2.21	0.86
1:A:137:LYS:CD	3:A:210:HOH:O	2.23	0.85
1:A:149:TRP:CD1	3:A:215:HOH:O	2.25	0.85
2:B:97:GLN:HB2	3:B:328:HOH:O	1.75	0.85
2:B:118:VAL:HB	3:B:197:HOH:O	1.75	0.85
1:C:109:TRP:HE1	2:D:139:PHE:CB	1.89	0.84
1:A:146:GLU:CA	3:A:205:HOH:O	2.24	0.84
2:D:93:LEU:HD12	3:D:282:HOH:O	1.76	0.84
3:B:322:HOH:O	2:D:88:TRP:CZ2	2.30	0.84
2:B:91:GLU:HG2	3:B:289:HOH:O	1.76	0.84
2:D:113:LYS:HE3	3:D:357:HOH:O	1.78	0.84
2:D:130:LYS:HE3	3:D:378:HOH:O	1.77	0.83
1:C:112:LEU:CG	3:C:200:HOH:O	2.23	0.83
2:D:33:ASP:HB3	3:D:209:HOH:O	1.77	0.83
2:D:89:ASP:HA	3:D:204:HOH:O	1.79	0.83
1:A:121:PHE:HB3	3:A:214:HOH:O	1.78	0.82
1:A:146:GLU:HA	3:A:205:HOH:O	1.80	0.82
1:A:116:LEU:HG	3:A:158:HOH:O	1.77	0.82
1:A:115:GLU:HG3	3:A:170:HOH:O	1.79	0.82
1:C:144:SER:CB	3:C:221:HOH:O	2.28	0.82
1:A:121:PHE:CB	3:A:214:HOH:O	2.26	0.82
3:B:322:HOH:O	2:D:88:TRP:CH2	2.32	0.81
1:A:121:PHE:CD1	3:A:214:HOH:O	2.33	0.81
1:C:144:SER:HB3	3:C:221:HOH:O	1.80	0.81
2:B:19:GLU:HG3	3:B:214:HOH:O	1.80	0.81
1:A:137:LYS:O	1:A:141:ARG:HG3	1.81	0.81
2:D:91:GLU:HB2	3:D:298:HOH:O	1.80	0.80
1:C:109:TRP:NE1	2:D:139:PHE:HB3	1.97	0.79
1:C:132:VAL:HG12	3:C:156:HOH:O	1.82	0.79
1:C:144:SER:HA	3:C:221:HOH:O	1.82	0.78
1:C:137:LYS:N	1:C:137:LYS:HD2	1.98	0.78
1:C:148:LEU:HD11	3:C:202:HOH:O	1.83	0.78
2:D:32:GLU:HG3	3:D:359:HOH:O	1.82	0.77
2:D:27:ILE:O	2:D:31:LEU:HG	1.84	0.77
1:C:148:LEU:HD21	3:C:202:HOH:O	1.83	0.77
2:B:93:LEU:HD21	3:B:279:HOH:O	1.85	0.76
1:C:126:LEU:HG	3:C:172:HOH:O	1.85	0.76
2:B:106:ALA:HB1	3:B:323:HOH:O	1.86	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:ASP:CB	3:A:194:HOH:O	2.27	0.75
1:A:131:LYS:HE2	3:A:183:HOH:O	1.83	0.75
2:D:26:THR:CB	3:D:347:HOH:O	2.30	0.75
2:B:121:LYS:HG3	3:B:187:HOH:O	1.86	0.75
1:A:131:LYS:CD	3:A:192:HOH:O	2.34	0.75
2:D:118:VAL:HG22	3:D:282:HOH:O	1.86	0.74
1:C:139:TRP:CH2	3:C:212:HOH:O	2.40	0.74
2:B:140:ASN:HA	3:B:280:HOH:O	1.87	0.74
1:A:113:PRO:HB2	3:A:158:HOH:O	1.88	0.73
2:B:20:ILE:HB	3:B:287:HOH:O	1.87	0.72
1:A:131:LYS:CE	3:A:192:HOH:O	2.29	0.72
2:D:5:LYS:HE2	3:D:178:HOH:O	1.88	0.72
1:A:141:ARG:HD2	3:A:159:HOH:O	1.89	0.71
2:B:113:LYS:NZ	3:B:209:HOH:O	2.23	0.71
2:B:122:THR:HG21	3:B:339:HOH:O	1.89	0.71
1:A:136:CYS:SG	3:A:157:HOH:O	2.49	0.71
2:D:43:ASP:O	2:D:44:PRO:C	2.28	0.71
1:A:137:LYS:NZ	3:A:206:HOH:O	2.25	0.70
2:D:132:PRO:HG2	3:D:327:HOH:O	1.89	0.70
2:B:22:LYS:HB3	2:B:22:LYS:NZ	2.07	0.69
1:C:121:PHE:HE2	3:C:212:HOH:O	1.76	0.69
1:C:129:LEU:HB3	3:C:206:HOH:O	1.91	0.68
1:A:146:GLU:HG3	3:A:205:HOH:O	1.93	0.68
2:B:43:ASP:HB3	2:B:44:PRO:CD	2.23	0.68
3:C:195:HOH:O	2:D:127:ILE:HD13	1.93	0.68
1:A:111:SER:HB3	2:B:101:PHE:CE1	2.28	0.68
3:A:204:HOH:O	2:B:101:PHE:CE2	2.47	0.68
1:C:112:LEU:HB2	3:C:184:HOH:O	1.93	0.67
1:C:129:LEU:HD21	3:C:211:HOH:O	1.92	0.67
2:B:110:LEU:HD11	3:B:323:HOH:O	1.93	0.67
2:D:30:MET:SD	3:D:319:HOH:O	2.52	0.67
1:C:132:VAL:HG13	1:C:139:TRP:CE3	2.28	0.67
2:D:131:THR:OG1	2:D:134:GLU:HG3	1.95	0.67
2:D:113:LYS:HG3	3:D:357:HOH:O	1.94	0.67
1:C:129:LEU:HD22	3:C:206:HOH:O	1.94	0.66
1:A:137:LYS:HE2	3:A:206:HOH:O	1.95	0.66
2:D:65:HIS:HE1	2:D:89:ASP:OD1	1.79	0.66
2:D:121:LYS:HG2	3:D:255:HOH:O	1.95	0.66
2:B:94:LYS:HE2	3:B:261:HOH:O	1.95	0.66
2:D:4:ILE:HG21	2:D:31:LEU:HD22	1.77	0.66
1:A:137:LYS:N	1:A:137:LYS:HD2	2.11	0.66
1:C:148:LEU:CD2	3:C:202:HOH:O	2.43	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:17:ASP:O	2:B:20:ILE:HG23	1.96	0.65
2:D:91:GLU:CG	3:D:151:HOH:O	2.43	0.65
2:B:13:ILE:HD11	3:B:163:HOH:O	1.96	0.65
3:C:157:HOH:O	2:D:128:LYS:HD3	1.96	0.65
2:B:122:THR:CG2	3:B:339:HOH:O	2.44	0.64
2:D:31:LEU:HB2	3:D:359:HOH:O	1.97	0.64
1:C:131:LYS:HD3	2:D:130:LYS:O	1.98	0.63
1:A:120:ILE:HD13	2:B:123:VAL:HG11	1.79	0.63
2:B:107:ALA:N	3:B:270:HOH:O	2.30	0.63
1:A:128:GLU:HG2	3:A:160:HOH:O	1.99	0.63
1:C:124:LEU:HD11	3:C:195:HOH:O	1.98	0.63
1:A:137:LYS:HD2	1:A:137:LYS:H	1.62	0.63
2:D:91:GLU:HG3	3:D:151:HOH:O	1.97	0.63
2:B:132:PRO:O	2:B:136:ARG:HG3	1.97	0.63
2:D:65:HIS:CD2	2:D:68:ASP:OD2	2.47	0.63
2:D:133:GLU:HG2	3:D:240:HOH:O	1.99	0.62
3:A:204:HOH:O	2:B:101:PHE:HE2	1.81	0.62
2:B:88:TRP:HB3	3:B:267:HOH:O	2.00	0.61
2:D:26:THR:HG22	3:D:337:HOH:O	1.99	0.61
1:A:142:LEU:HA	3:A:198:HOH:O	2.00	0.61
2:B:118:VAL:HG23	3:B:201:HOH:O	1.99	0.61
2:B:65:HIS:HD2	2:B:68:ASP:OD2	1.80	0.61
2:B:32:GLU:CD	3:B:325:HOH:O	2.38	0.61
1:C:137:LYS:NZ	3:C:154:HOH:O	2.33	0.61
2:D:90:GLN:O	2:D:94:LYS:HG3	2.01	0.61
2:D:8:SER:C	3:D:309:HOH:O	2.38	0.61
1:C:132:VAL:CG1	3:C:156:HOH:O	2.45	0.60
1:A:111:SER:HB3	2:B:101:PHE:CZ	2.36	0.60
1:C:148:LEU:CD1	3:C:202:HOH:O	2.42	0.60
1:C:117:LEU:CD1	3:C:213:HOH:O	2.49	0.60
1:C:123:CYS:HB3	3:D:255:HOH:O	2.00	0.60
1:C:117:LEU:HD11	3:C:213:HOH:O	2.01	0.60
1:A:113:PRO:HD2	3:A:158:HOH:O	2.01	0.60
2:B:97:GLN:HE22	2:B:139:PHE:HA	1.67	0.59
1:A:109:TRP:N	3:A:197:HOH:O	2.35	0.59
1:C:116:LEU:HD13	2:D:104:ILE:HG22	1.84	0.59
2:B:97:GLN:NE2	2:B:139:PHE:HA	2.17	0.59
2:D:36:MET:C	2:D:43:ASP:O	2.39	0.59
2:B:98:GLY:O	2:B:102:GLU:HG3	2.02	0.59
2:D:26:THR:C	3:D:347:HOH:O	2.41	0.59
2:B:16:VAL:HG21	2:B:20:ILE:HD13	1.84	0.58
2:D:113:LYS:CG	3:D:357:HOH:O	2.48	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:137:LYS:HB2	3:C:170:HOH:O	2.01	0.58
2:D:117:ASP:C	2:D:117:ASP:OD1	2.41	0.58
1:A:141:ARG:HG3	3:A:161:HOH:O	2.03	0.58
2:B:92:PHE:CE2	3:B:279:HOH:O	2.53	0.58
2:B:36:MET:HA	3:B:276:HOH:O	2.03	0.58
2:B:44:PRO:HB3	3:B:150:HOH:O	2.03	0.57
1:A:137:LYS:CE	3:A:206:HOH:O	2.49	0.57
2:B:57:LYS:NZ	2:B:60:GLN:HE22	2.03	0.57
2:B:110:LEU:CD1	3:B:323:HOH:O	2.52	0.57
2:B:138:THR:OG1	2:B:139:PHE:CD1	2.58	0.57
1:A:145:ASP:OD1	1:A:146:GLU:N	2.37	0.56
1:C:128:GLU:CD	2:D:128:LYS:HD2	2.26	0.56
1:C:113:PRO:HG3	3:D:258:HOH:O	2.05	0.56
1:A:146:GLU:HB2	3:A:205:HOH:O	1.96	0.56
1:C:139:TRP:CZ2	3:C:212:HOH:O	2.57	0.56
2:D:136:ARG:NH1	3:D:244:HOH:O	2.37	0.56
1:C:113:PRO:HG2	1:C:116:LEU:HG	1.87	0.56
2:B:92:PHE:HE2	3:B:279:HOH:O	1.86	0.56
1:A:121:PHE:HD1	3:A:214:HOH:O	1.79	0.56
2:D:22:LYS:NZ	3:D:230:HOH:O	2.39	0.56
2:B:65:HIS:HE1	2:B:89:ASP:OD1	1.89	0.55
2:B:124:ALA:HA	2:B:127:ILE:HD12	1.89	0.55
2:D:132:PRO:HB2	2:D:136:ARG:HH12	1.70	0.55
2:D:92:PHE:HB3	3:D:204:HOH:O	2.05	0.55
2:D:31:LEU:HD23	2:D:45:VAL:HG21	1.87	0.55
1:C:113:PRO:O	1:C:116:LEU:N	2.37	0.55
2:D:19:GLU:HG2	3:D:194:HOH:O	2.06	0.55
3:B:169:HOH:O	2:D:66:LYS:CD	2.40	0.54
2:B:34:LEU:HD13	3:B:243:HOH:O	2.07	0.53
2:B:138:THR:OG1	2:B:139:PHE:HD1	1.92	0.53
1:C:144:SER:CA	3:C:221:HOH:O	2.38	0.53
1:C:137:LYS:O	1:C:141:ARG:HG3	2.09	0.53
1:A:146:GLU:CG	3:A:205:HOH:O	2.43	0.53
2:B:4:ILE:HG23	2:B:18:VAL:CG1	2.33	0.53
2:D:13:ILE:CG1	3:D:346:HOH:O	2.20	0.52
2:B:134:GLU:N	2:B:134:GLU:OE1	2.42	0.52
2:B:50:VAL:HG11	3:B:323:HOH:O	2.09	0.52
2:D:48:PRO:HG2	3:D:181:HOH:O	2.09	0.52
2:D:30:MET:CE	3:D:319:HOH:O	2.57	0.52
2:D:137:LYS:HE2	3:D:184:HOH:O	2.08	0.52
2:B:139:PHE:HB3	3:B:281:HOH:O	2.08	0.52
2:B:35:GLY:O	2:B:36:MET:O	2.28	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:4:ILE:HG13	2:D:5:LYS:N	2.24	0.52
1:A:109:TRP:HB2	3:B:281:HOH:O	2.09	0.52
1:C:129:LEU:HG	3:C:185:HOH:O	2.10	0.52
1:A:109:TRP:O	1:A:110:ASP:OD1	2.28	0.52
1:C:129:LEU:CD1	3:C:206:HOH:O	2.40	0.51
2:B:34:LEU:CD1	3:B:243:HOH:O	2.58	0.51
2:D:4:ILE:HG21	2:D:31:LEU:CD2	2.41	0.51
2:D:108:ASN:ND2	3:D:258:HOH:O	2.43	0.51
1:C:109:TRP:NE1	2:D:139:PHE:CD2	2.79	0.51
1:C:137:LYS:HE3	3:C:182:HOH:O	2.09	0.51
2:D:56:LYS:HG2	2:D:60:GLN:HE21	1.77	0.50
1:A:109:TRP:HE1	2:B:97:GLN:HG2	1.75	0.50
1:C:124:LEU:HB3	1:C:128:GLU:HB3	1.93	0.50
1:C:116:LEU:HB3	3:C:167:HOH:O	2.10	0.50
2:B:97:GLN:CG	3:B:311:HOH:O	2.59	0.50
1:C:129:LEU:CG	3:C:206:HOH:O	2.58	0.50
2:B:130:LYS:CE	3:B:341:HOH:O	2.40	0.50
1:C:128:GLU:OE1	2:D:128:LYS:HE3	2.12	0.50
1:A:128:GLU:CG	3:A:160:HOH:O	2.57	0.50
2:B:7:GLN:HG3	3:B:163:HOH:O	2.11	0.49
2:D:133:GLU:CG	3:D:240:HOH:O	2.59	0.49
2:B:86:PRO:HB2	2:B:89:ASP:OD2	2.11	0.49
2:D:7:GLN:NE2	3:D:360:HOH:O	2.45	0.49
2:D:140:ASN:OD1	2:D:140:ASN:O	2.31	0.49
2:D:19:GLU:HG3	3:D:366:HOH:O	2.12	0.49
2:B:50:VAL:O	2:B:50:VAL:HG23	2.12	0.49
2:D:43:ASP:HB2	3:D:284:HOH:O	2.12	0.49
2:D:24:SER:HA	2:D:112:ILE:HG12	1.95	0.49
1:C:113:PRO:HD2	1:C:116:LEU:HD12	1.94	0.48
2:B:97:GLN:HG2	3:B:311:HOH:O	2.14	0.48
2:D:139:PHE:O	2:D:140:ASN:HB3	2.13	0.48
1:A:141:ARG:CG	3:A:161:HOH:O	2.62	0.48
1:C:125:CYS:SG	3:C:175:HOH:O	2.60	0.48
2:B:28:LYS:CG	3:B:325:HOH:O	2.47	0.47
2:D:117:ASP:HB2	3:D:185:HOH:O	2.14	0.47
2:D:29:THR:HG21	3:D:304:HOH:O	2.15	0.47
2:B:28:LYS:NZ	3:B:172:HOH:O	2.44	0.47
2:D:5:LYS:CE	3:D:178:HOH:O	2.56	0.47
1:A:129:LEU:O	1:A:132:VAL:HG22	2.14	0.47
2:D:137:LYS:CE	3:D:184:HOH:O	2.63	0.47
2:D:31:LEU:CB	3:D:325:HOH:O	2.40	0.47
2:B:65:HIS:CE1	2:B:89:ASP:OD1	2.66	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:118:LEU:CD1	3:C:196:HOH:O	2.63	0.47
2:B:2:PRO:N	2:D:67:ASP:OD1	2.48	0.47
2:B:16:VAL:HG21	2:B:20:ILE:CD1	2.45	0.47
2:D:137:LYS:NZ	3:D:184:HOH:O	2.47	0.46
2:D:49:ASN:HD22	2:D:109:TYR:HE1	1.57	0.46
1:C:145:ASP:O	1:C:146:GLU:C	2.51	0.46
2:D:7:GLN:HB2	3:D:336:HOH:O	2.14	0.46
2:D:65:HIS:CE1	2:D:89:ASP:OD1	2.64	0.46
2:B:101:PHE:CD2	3:B:272:HOH:O	2.56	0.46
1:A:148:LEU:CD1	3:A:214:HOH:O	2.63	0.46
2:B:126:MET:O	2:B:130:LYS:HD2	2.16	0.46
2:B:93:LEU:HD11	3:B:197:HOH:O	2.17	0.46
2:D:49:ASN:HB2	2:D:109:TYR:CZ	2.51	0.46
2:D:19:GLU:CG	3:D:194:HOH:O	2.61	0.45
2:B:44:PRO:HA	3:B:150:HOH:O	2.15	0.45
2:D:22:LYS:HG3	2:D:28:LYS:HD2	1.98	0.45
2:D:136:ARG:CZ	3:D:244:HOH:O	2.63	0.45
1:A:132:VAL:HG23	1:A:143:ALA:HB2	1.99	0.45
2:B:106:ALA:HB3	3:B:270:HOH:O	2.15	0.45
1:C:114:ASP:HB3	1:C:142:LEU:HD21	1.98	0.45
2:B:30:MET:HE2	2:B:30:MET:HB3	1.75	0.45
1:C:124:LEU:HB2	3:C:185:HOH:O	2.17	0.45
2:D:131:THR:O	2:D:135:ILE:HG13	2.17	0.45
1:A:137:LYS:CD	1:A:137:LYS:H	2.27	0.45
2:D:49:ASN:HB2	2:D:109:TYR:CE1	2.52	0.44
1:A:110:ASP:CG	3:A:194:HOH:O	2.52	0.44
2:B:44:PRO:CA	3:B:150:HOH:O	2.66	0.44
2:D:43:ASP:N	3:D:284:HOH:O	2.50	0.44
2:B:54:ILE:HD11	2:B:102:GLU:OE2	2.18	0.44
2:D:16:VAL:O	2:D:16:VAL:HG23	2.18	0.44
2:B:57:LYS:HZ2	2:B:60:GLN:HE22	1.65	0.43
2:B:44:PRO:CB	3:B:150:HOH:O	2.65	0.43
2:B:86:PRO:HG2	3:B:166:HOH:O	2.18	0.43
1:A:124:LEU:HB3	1:A:128:GLU:HB3	2.00	0.43
1:C:132:VAL:HG13	1:C:139:TRP:HE3	1.81	0.43
1:C:124:LEU:HD22	1:C:128:GLU:HG2	2.01	0.43
2:B:104:ILE:HD11	2:B:123:VAL:HG21	2.00	0.43
2:D:133:GLU:O	2:D:137:LYS:HG3	2.19	0.43
2:B:20:ILE:HA	3:B:312:HOH:O	2.18	0.43
1:A:109:TRP:HA	3:A:162:HOH:O	2.17	0.43
2:B:16:VAL:CG2	2:B:20:ILE:HD13	2.49	0.42
1:A:131:LYS:CE	3:A:183:HOH:O	2.55	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:47:LEU:C	3:D:309:HOH:O	2.57	0.42
2:B:125:ASN:HA	2:B:125:ASN:HD22	1.65	0.42
2:D:31:LEU:CD2	2:D:45:VAL:HG21	2.48	0.42
1:C:112:LEU:HD23	3:C:200:HOH:O	2.04	0.42
1:C:116:LEU:HG	3:D:258:HOH:O	2.19	0.42
2:B:137:LYS:HE3	2:B:137:LYS:HB2	1.86	0.42
2:D:94:LYS:HD2	3:D:356:HOH:O	2.19	0.42
2:D:93:LEU:HD11	2:D:118:VAL:HG13	2.02	0.42
2:B:22:LYS:HB3	2:B:22:LYS:HZ3	1.80	0.42
2:B:60:GLN:HG3	2:D:15:GLU:HG2	2.01	0.42
2:B:30:MET:CE	2:B:45:VAL:HG13	2.50	0.42
1:C:109:TRP:CD1	2:D:139:PHE:HB3	2.55	0.41
2:B:126:MET:HE1	3:B:241:HOH:O	2.20	0.41
2:D:28:LYS:HA	3:D:359:HOH:O	2.20	0.41
1:A:145:ASP:OD1	1:A:145:ASP:C	2.58	0.41
2:B:50:VAL:HG13	2:B:109:TYR:CD2	2.56	0.41
1:C:141:ARG:CZ	3:C:158:HOH:O	2.69	0.41
2:D:127:ILE:HG23	2:D:135:ILE:HD13	2.03	0.41
1:C:118:LEU:HD13	3:C:168:HOH:O	2.21	0.41
1:C:109:TRP:NE1	2:D:139:PHE:CG	2.82	0.41
3:A:204:HOH:O	2:B:101:PHE:CZ	2.72	0.41
2:B:35:GLY:O	2:B:36:MET:C	2.59	0.41
2:D:107:ALA:HB2	2:D:115:LEU:HG	2.03	0.41
2:D:13:ILE:HD11	3:D:317:HOH:O	2.21	0.40
2:B:136:ARG:NH1	3:B:236:HOH:O	2.53	0.40
1:C:109:TRP:N	3:C:163:HOH:O	2.53	0.40
2:B:127:ILE:HG23	2:B:135:ILE:HD13	2.04	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	A	39/53 (74%)	37 (95%)	2 (5%)	0	100 100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	39/53 (74%)	34 (87%)	5 (13%)	0	100	100
2	B	112/141 (79%)	104 (93%)	7 (6%)	1 (1%)	25	7
2	D	114/141 (81%)	110 (96%)	2 (2%)	2 (2%)	13	2
All	All	304/388 (78%)	285 (94%)	16 (5%)	3 (1%)	22	6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	44	PRO
2	D	43	ASP
2	B	36	MET

### 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	38/49 (78%)	36 (95%)	2 (5%)	32	13
1	C	37/49 (76%)	36 (97%)	1 (3%)	57	39
2	B	103/130 (79%)	100 (97%)	3 (3%)	55	37
2	D	105/130 (81%)	102 (97%)	3 (3%)	55	37
All	All	283/358 (79%)	274 (97%)	9 (3%)	51	32

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	137	LYS
2	B	22	LYS
2	B	101	PHE
2	B	133	GLU
1	C	137	LYS
2	D	44	PRO
2	D	113	LYS
2	D	117	ASP



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	GLN
2	B	65	HIS
2	B	97	GLN
2	B	125	ASN
2	D	60	GLN
2	D	65	HIS
2	D	125	ASN
2	D	140	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.