



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:17 AM GMT

PDB ID : 1NXK  
Title : Crystal structure of staurosporine bound to MAP KAP kinase 2  
Authors : Underwood, K.W.; Parris, K.D.; Federico, E.; Mosyak, L.; Czerwinski, R.M.;  
Shane, T.; Taylor, M.; Svenson, K.; Liu, Y.; Hsiao, C.L.; Wolfrom, S.;  
Malakian, K.; Telliez, J.B.; Lin, L.L.; Kriz, R.W.; Seehra, J.; Somers, W.S.;  
Stahl, M.L.  
Deposited on : 2003-02-10  
Resolution : 2.70 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>

---

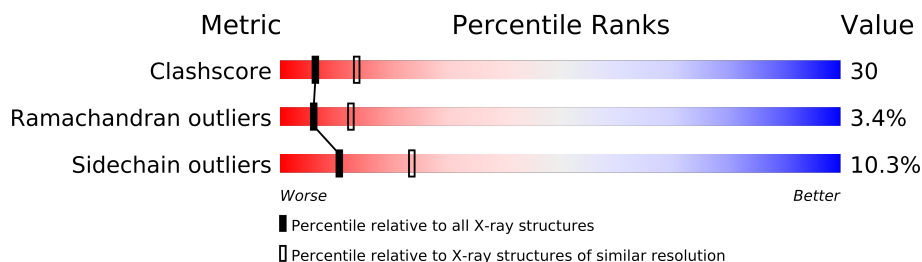
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	400	
1	B	400	
1	C	400	
1	D	400	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9405 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	Se	0	0	0
			2289	1471	388	413	6	11			
1	B	283	Total	C	N	O	S	Se	0	0	0
			2234	1425	382	410	6	11			
1	C	306	Total	C	N	O	S	Se	0	0	0
			2438	1557	421	442	6	12			
1	D	288	Total	C	N	O	S	Se	0	0	0
			2252	1452	373	410	6	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	314	MSE	MET	MODIFIED RESIDUE	UNP P49137

*Continued on next page...*

*Continued from previous page...*

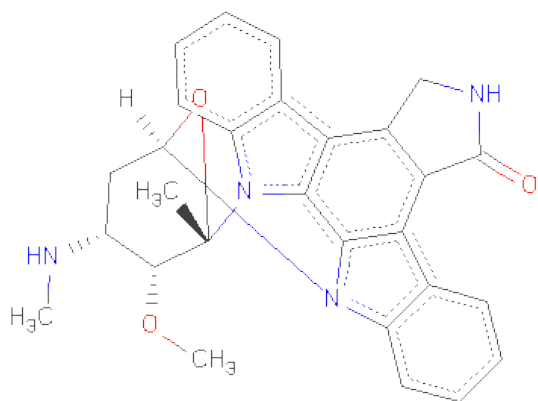
Chain	Residue	Modelled	Actual	Comment	Reference
B	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	356	MSE	MET	MODIFIED RESIDUE	UNP P49137

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is STAUROSPORINE (three-letter code: STU) (formula:  $C_{28}H_{26}N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	28	4	3		
3	B	1	Total	C	N	O	0	0
			35	28	4	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			35	28	4	3		
3	D	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	16	Total	O	0	0
			16	16		
4	C	9	Total	O	0	0
			9	9		
4	D	7	Total	O	0	0
			7	7		







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.20Å 160.20Å 133.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.70)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.239 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STU, SO4

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	0.76	3/2331 (0.1%)	0.95	3/3140 (0.1%)
1	B	0.79	2/2271 (0.1%)	0.99	3/3057 (0.1%)
1	C	0.75	1/2481 (0.0%)	0.91	2/3337 (0.1%)
1	D	0.66	0/2295	0.86	0/3100
All	All	0.74	6/9378 (0.1%)	0.93	8/12634 (0.1%)

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	3
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	NE1-CE2	8.77	1.49	1.37
1	C	324	TRP	NE1-CE2	8.66	1.48	1.37
1	A	109	TRP	NE1-CE2	8.65	1.48	1.37
1	A	291	TRP	NE1-CE2	8.64	1.48	1.37
1	B	247	TRP	NE1-CE2	8.64	1.48	1.37
1	A	244	CYS	CB-SG	-5.78	1.72	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	PHE	O-C-N	-7.70	110.39	122.70
1	B	303	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	282	GLY	N-CA-C	-5.54	99.25	113.10
1	B	110	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	183	ALA	N-CA-C	-5.30	96.70	111.00
1	C	64	LYS	N-CA-C	-5.16	97.06	111.00
1	A	242	LYS	O-C-N	5.05	130.79	122.70
1	A	64	LYS	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	103	ARG	Sidechain
1	A	119	ARG	Sidechain
1	B	158	PHE	Mainchain
1	B	176	TYR	Sidechain
1	C	340	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	176	TYR	Sidechain

## 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	2289	0	2258	148	0
1	B	2234	0	2197	137	0
1	C	2438	0	2414	152	0
1	D	2252	0	2194	157	0
2	B	10	0	0	0	0
3	A	35	0	26	3	0
3	B	35	0	26	2	0
3	C	35	0	26	1	0
3	D	35	0	26	7	0
4	A	10	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	0	0	0
4	C	9	0	0	0	0
4	D	7	0	0	0	0
All	All	9405	0	9167	561	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 30.

All (561) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:ASN:HD22	1:A:269:LEU:HG	1.30	0.96
1:A:158:PHE:CE1	1:A:162:GLU:HB3	2.00	0.95
1:C:328:SER:O	1:C:331:VAL:HG12	1.66	0.94
1:A:260:TYR:HE2	1:A:290:GLU:HG2	1.30	0.94
1:D:167:MSE:HG3	1:D:253:MSE:HG3	1.47	0.94
1:C:266:ASN:ND2	1:C:269:LEU:HG	1.81	0.94
1:D:314:MSE:HE3	1:D:319:PHE:HD1	1.32	0.94
1:C:332:PRO:HB2	1:C:334:THR:HG22	1.47	0.94
1:A:74:ILE:O	1:A:75:ASN:HB2	1.66	0.93
1:A:257:LEU:HA	1:A:336:LEU:HD13	1.51	0.92
1:D:300:MSE:HE3	1:D:303:ARG:HB2	1.49	0.92
1:B:278:ARG:HG2	1:B:283:GLN:HG3	1.49	0.92
1:D:266:ASN:HD22	1:D:269:LEU:HG	1.34	0.91
1:C:174:ILE:HG22	1:C:316:ILE:HG12	1.52	0.91
1:B:161:ARG:HG2	1:B:331:VAL:HG13	1.52	0.91
1:C:115:PRO:O	1:C:204:LYS:HE2	1.72	0.90
1:A:44:PRO:HG2	1:C:128:TYR:OH	1.71	0.90
1:A:198:ARG:HG2	1:A:199:PRO:CD	2.02	0.88
1:C:167:MSE:HG3	1:C:253:MSE:HE2	1.55	0.87
1:A:214:THR:O	1:A:215:THR:HG23	1.74	0.87
1:D:115:PRO:O	1:D:204:LYS:HE2	1.74	0.86
1:A:198:ARG:HG2	1:A:199:PRO:HD2	1.58	0.86
1:B:146:LEU:HD13	1:B:203:LEU:HD21	1.56	0.86
1:B:285:GLU:O	1:B:287:PRO:HD3	1.76	0.85
1:A:285:GLU:HG2	1:A:287:PRO:HD3	1.60	0.84
1:A:272:SER:HB2	1:A:283:GLN:HE22	1.40	0.84
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.13	0.83
1:A:179:SER:HB3	1:D:281:MSE:HE2	1.58	0.83
1:C:149:ARG:HB3	1:C:149:ARG:HH11	1.44	0.82
1:B:60:ILE:HG21	1:C:45:GLN:HG2	1.62	0.82
1:B:198:ARG:HB2	1:B:199:PRO:HD2	1.61	0.81
1:D:314:MSE:HE3	1:D:319:PHE:CD1	2.16	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:277:THR:O	1:D:281:MSE:HG2	1.82	0.80
1:A:233:GLU:HG2	1:D:310:PRO:HG3	1.63	0.80
1:A:45:GLN:HG2	1:C:60:ILE:HG21	1.63	0.79
1:D:314:MSE:CE	1:D:319:PHE:HD1	1.95	0.79
1:A:198:ARG:HD2	1:A:200:ASN:H	1.48	0.79
1:A:44:PRO:HG3	1:D:267:HIS:HB3	1.64	0.79
1:D:225:TYR:O	1:D:226:THR:HB	1.83	0.78
1:A:198:ARG:HG2	1:A:199:PRO:N	1.99	0.77
1:C:65:VAL:HA	1:C:81:ILE:HG22	1.65	0.77
1:B:98:CYS:HB2	1:B:99:PRO:HD2	1.66	0.77
1:D:301:LEU:HD13	1:D:322:HIS:CD2	2.20	0.77
1:B:74:ILE:HG22	1:B:75:ASN:ND2	2.00	0.76
1:B:151:GLN:NE2	1:B:343:LYS:HA	2.00	0.76
1:C:275:MSE:HA	1:C:278:ARG:HG3	1.68	0.76
1:B:46:PHE:C	1:B:48:VAL:H	1.88	0.75
1:D:83:ASN:O	1:D:87:GLN:HA	1.87	0.75
1:B:67:SER:HB2	1:C:42:GLN:HB3	1.67	0.75
1:B:86:THR:O	1:B:87:GLN:HB3	1.85	0.75
1:D:300:MSE:SE	1:D:303:ARG:HH11	2.19	0.75
1:A:272:SER:OG	1:A:277:THR:HG22	1.87	0.75
1:A:192:LEU:HB3	1:A:203:LEU:HD11	1.69	0.74
1:B:344:GLU:O	1:B:345:ASP:CB	2.33	0.74
1:D:78:VAL:HG21	3:D:401:STU:C17	2.16	0.74
1:A:227:PRO:HB3	1:A:229:TYR:CE2	2.23	0.74
1:B:86:THR:O	1:B:87:GLN:CB	2.35	0.73
1:A:295:SER:OG	1:A:298:VAL:HG23	1.88	0.73
1:B:305:LEU:HD21	1:B:314:MSE:CE	2.18	0.73
1:A:227:PRO:O	1:A:230:VAL:HG12	1.89	0.72
1:A:42:GLN:HG3	1:A:42:GLN:O	1.89	0.72
1:B:198:ARG:HB2	1:B:199:PRO:CD	2.19	0.72
1:D:74:ILE:HB	1:D:209:GLY:HA3	1.72	0.71
1:B:227:PRO:O	1:B:230:VAL:HG12	1.89	0.71
1:C:43:PHE:CB	1:C:44:PRO:CD	2.68	0.71
1:D:147:PHE:HE2	1:D:256:LEU:HD23	1.54	0.71
1:D:277:THR:O	1:D:281:MSE:CG	2.37	0.71
1:C:149:ARG:HB3	1:C:153:ARG:HH12	1.54	0.71
1:D:267:HIS:HA	1:D:273:PRO:HB3	1.72	0.71
1:B:253:MSE:HE1	1:B:319:PHE:HE1	1.54	0.71
1:D:260:TYR:OH	1:D:287:PRO:HG2	1.92	0.70
1:B:305:LEU:HD21	1:B:314:MSE:HE3	1.74	0.70
1:D:138:MSE:SE	3:D:401:STU:H13	2.42	0.70
1:B:151:GLN:HE21	1:B:343:LYS:HA	1.57	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:GLU:HG2	1:D:310:PRO:CG	2.22	0.69
1:C:301:LEU:HD13	1:C:322:HIS:CD2	2.28	0.69
1:D:269:LEU:HD12	1:D:278:ARG:NH1	2.07	0.69
1:C:127:LEU:HA	1:C:131:ARG:O	1.92	0.69
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.73	0.69
1:C:167:MSE:HE2	1:C:253:MSE:HE3	1.73	0.68
1:D:184:HIS:CD2	1:D:205:LEU:HD21	2.28	0.68
1:C:128:TYR:O	1:C:131:ARG:HB2	1.92	0.68
1:C:344:GLU:O	1:C:345:ASP:HB2	1.92	0.68
1:B:344:GLU:O	1:B:345:ASP:HB3	1.93	0.68
1:C:184:HIS:CD2	1:C:186:ASP:H	2.12	0.68
1:C:184:HIS:HD2	1:C:186:ASP:H	1.40	0.68
1:B:328:SER:O	1:B:331:VAL:HG12	1.94	0.68
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.28	0.67
1:D:307:LYS:HD2	1:D:312:GLN:HB3	1.76	0.67
1:D:266:ASN:ND2	1:D:269:LEU:HG	2.09	0.67
1:B:289:PRO:HA	1:B:292:SER:OG	1.94	0.67
1:A:337:HIS:O	1:A:341:VAL:HG23	1.94	0.67
1:C:357:THR:O	1:C:357:THR:HG22	1.94	0.67
1:C:150:ILE:O	1:C:153:ARG:HB2	1.94	0.67
1:A:272:SER:HB2	1:A:283:GLN:NE2	2.09	0.67
1:A:43:PHE:CD1	1:A:44:PRO:HD2	2.29	0.67
1:A:198:ARG:HD2	1:A:200:ASN:N	2.09	0.67
1:C:324:TRP:HE3	1:C:325:ILE:HD12	1.59	0.66
1:C:190:GLU:H	1:C:190:GLU:CD	1.98	0.66
1:D:188:LYS:HB2	1:D:190:GLU:OE1	1.96	0.66
1:A:260:TYR:OH	1:A:287:PRO:HG2	1.96	0.66
1:B:295:SER:HB2	1:B:298:VAL:HG23	1.78	0.66
1:C:149:ARG:HB3	1:C:153:ARG:NH1	2.09	0.66
1:B:162:GLU:O	1:B:166:ILE:HG13	1.96	0.66
1:D:150:ILE:CG2	1:D:342:LEU:HD23	2.25	0.66
1:A:266:ASN:ND2	1:A:269:LEU:HG	2.07	0.66
1:C:160:GLU:HB3	1:C:334:THR:HG23	1.77	0.66
1:B:253:MSE:HE1	1:B:319:PHE:CE1	2.31	0.65
1:C:264:TYR:CE1	1:C:348:ARG:NE	2.64	0.65
1:B:74:ILE:HD13	1:B:210:PHE:CD2	2.31	0.65
1:A:309:GLU:O	1:A:310:PRO:C	2.33	0.65
1:C:43:PHE:CB	1:C:44:PRO:HD2	2.27	0.65
1:B:337:HIS:HA	1:B:340:ARG:HE	1.62	0.65
1:D:300:MSE:CE	1:D:303:ARG:HB2	2.25	0.65
1:D:264:TYR:O	1:D:278:ARG:NH2	2.30	0.65
1:A:186:ASP:HB2	1:A:210:PHE:HD2	1.62	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:150:ILE:HG22	1:D:342:LEU:HD23	1.78	0.65
1:D:149:ARG:HH21	1:D:197:LYS:HA	1.61	0.65
1:D:150:ILE:HG21	1:D:338:THR:HG22	1.79	0.64
1:D:184:HIS:O	1:D:185:ARG:HB2	1.96	0.64
1:B:107:LEU:HD21	1:B:213:GLU:HG3	1.78	0.64
1:A:344:GLU:O	1:A:345:ASP:HB2	1.96	0.64
1:D:254:TYR:CG	1:D:262:PRO:HG3	2.33	0.64
1:B:289:PRO:O	1:B:292:SER:OG	2.17	0.63
1:D:86:THR:OG1	1:D:88:GLU:HG2	1.98	0.63
1:C:289:PRO:HG2	1:C:290:GLU:H	1.63	0.63
1:A:95:LEU:O	1:A:133:CYS:HB2	1.99	0.63
1:C:146:LEU:HD11	1:C:166:ILE:HD13	1.80	0.63
1:D:186:ASP:HB2	1:D:210:PHE:HD2	1.64	0.63
1:C:160:GLU:CB	1:C:334:THR:HG23	2.28	0.62
1:D:300:MSE:SE	1:D:303:ARG:HD2	2.48	0.62
1:D:74:ILE:HG22	1:D:75:ASN:ND2	2.14	0.62
1:D:225:TYR:O	1:D:226:THR:CB	2.45	0.62
1:B:331:VAL:HG23	1:B:332:PRO:HD2	1.81	0.62
1:B:69:VAL:HG22	1:B:79:LEU:CD2	2.29	0.62
1:D:264:TYR:O	1:D:275:MSE:HB2	2.00	0.62
1:D:141:LEU:HD13	1:D:193:LEU:HB2	1.81	0.62
1:C:345:ASP:O	1:C:346:LYS:O	2.16	0.62
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.82	0.62
1:A:260:TYR:CE2	1:A:290:GLU:HG2	2.22	0.62
1:A:47:HIS:NE2	1:D:269:LEU:O	2.33	0.61
1:A:258:CYS:HB2	1:A:290:GLU:HB3	1.83	0.61
1:D:93:LYS:HE2	1:D:95:LEU:HD21	1.83	0.61
1:C:174:ILE:CG2	1:C:316:ILE:HG12	2.29	0.60
1:C:153:ARG:O	1:C:156:GLN:NE2	2.34	0.60
1:D:337:HIS:HB3	1:D:341:VAL:HG23	1.83	0.60
1:C:322:HIS:ND1	1:C:323:PRO:HD2	2.16	0.60
1:C:264:TYR:CZ	1:C:348:ARG:NE	2.68	0.60
1:B:146:LEU:HD13	1:B:203:LEU:CD2	2.27	0.60
1:A:305:LEU:CD2	1:A:314:MSE:HE3	2.31	0.60
1:A:272:SER:CB	1:A:277:THR:HG22	2.32	0.60
1:D:90:PHE:CE2	1:D:121:VAL:HG21	2.37	0.60
1:D:305:LEU:HD21	1:D:314:MSE:HE2	1.83	0.60
1:A:264:TYR:CD1	1:A:264:TYR:N	2.70	0.60
1:C:94:MSE:HE3	1:C:135:LEU:HD21	1.83	0.60
1:B:305:LEU:CD2	1:B:314:MSE:CE	2.79	0.60
1:A:150:ILE:HG22	1:A:342:LEU:HD23	1.84	0.60
1:A:298:VAL:HG22	1:A:324:TRP:NE1	2.16	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:SER:HA	1:A:324:TRP:CZ3	2.37	0.59
1:C:44:PRO:O	1:C:47:HIS:HB2	2.01	0.59
1:A:305:LEU:HG	1:A:314:MSE:CE	2.32	0.59
1:B:167:MSE:HE2	1:B:253:MSE:HE3	1.85	0.59
1:C:149:ARG:CB	1:C:149:ARG:HH11	2.12	0.59
1:B:178:HIS:CE1	1:B:242:LYS:HB3	2.37	0.59
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.84	0.59
1:B:299:LYS:O	1:B:303:ARG:HG3	2.02	0.59
1:C:337:HIS:HA	1:C:340:ARG:CZ	2.32	0.59
1:B:186:ASP:HB2	1:B:210:PHE:HD2	1.67	0.59
1:B:167:MSE:HG3	1:B:253:MSE:HE2	1.83	0.59
1:B:56:LYS:HD3	1:B:125:GLU:HB3	1.85	0.58
1:D:289:PRO:HA	1:D:292:SER:OG	2.03	0.58
1:A:111:ALA:HB1	1:A:177:LEU:HD21	1.85	0.58
3:B:403:STU:H16	3:B:403:STU:H261	1.85	0.58
1:C:158:PHE:O	1:C:336:LEU:HB2	2.03	0.58
1:C:140:CYS:O	1:C:141:LEU:HD23	2.04	0.58
1:A:233:GLU:OE2	1:D:313:ARG:NH1	2.37	0.58
1:C:260:TYR:HB2	1:C:261:PRO:HD2	1.86	0.58
1:A:179:SER:HA	1:D:281:MSE:SE	2.54	0.58
1:C:41:GLN:O	1:C:42:GLN:HB2	2.04	0.58
1:D:141:LEU:CD1	1:D:193:LEU:HB2	2.34	0.58
1:A:198:ARG:HD2	1:A:200:ASN:CA	2.34	0.57
1:C:266:ASN:HD22	1:C:269:LEU:HG	1.66	0.57
1:C:332:PRO:HB2	1:C:334:THR:CG2	2.31	0.57
1:B:234:VAL:HG12	1:B:234:VAL:O	2.03	0.57
1:A:149:ARG:HD3	1:A:194:TYR:CD2	2.40	0.57
1:B:67:SER:CB	1:C:42:GLN:HB3	2.35	0.57
1:D:74:ILE:HD12	1:D:209:GLY:HA3	1.86	0.57
1:D:190:GLU:H	1:D:190:GLU:CD	2.08	0.57
1:D:300:MSE:HE3	1:D:303:ARG:CB	2.29	0.56
1:B:93:LYS:HE2	1:B:95:LEU:HD21	1.87	0.56
1:B:289:PRO:O	1:B:290:GLU:C	2.42	0.56
1:A:227:PRO:CB	1:A:229:TYR:CE2	2.87	0.56
1:C:357:THR:HG23	1:D:72:LEU:CD1	2.36	0.56
1:C:260:TYR:CE1	1:C:348:ARG:NH1	2.74	0.56
1:B:232:PRO:O	1:B:235:LEU:HB2	2.06	0.56
1:C:151:GLN:C	1:C:153:ARG:H	2.09	0.56
1:B:98:CYS:HB2	1:B:99:PRO:CD	2.35	0.56
1:D:88:GLU:HG3	1:D:90:PHE:CE1	2.40	0.56
1:D:168:LYS:O	1:D:172:GLU:HG3	2.06	0.56
1:D:66:THR:HG21	1:D:82:PHE:HE1	1.69	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:274:GLY:C	1:B:278:ARG:HH21	2.08	0.56
1:B:147:PHE:HE2	1:B:256:LEU:HD23	1.71	0.56
1:B:109:TRP:O	1:B:112:SER:HB3	2.06	0.56
1:A:45:GLN:HG2	1:C:60:ILE:CG2	2.35	0.56
1:B:69:VAL:HG22	1:B:79:LEU:HD23	1.86	0.56
1:B:264:TYR:HA	1:B:275:MSE:SE	2.56	0.56
1:D:264:TYR:N	1:D:264:TYR:CD1	2.74	0.55
1:B:258:CYS:HB2	1:B:290:GLU:HB3	1.87	0.55
1:A:272:SER:OG	1:A:277:THR:CG2	2.54	0.55
1:A:115:PRO:O	1:A:202:ILE:HD11	2.06	0.55
1:B:284:TYR:O	1:B:285:GLU:HB3	2.05	0.55
1:B:46:PHE:C	1:B:48:VAL:N	2.60	0.55
1:D:290:GLU:CD	1:D:290:GLU:H	2.09	0.55
1:C:349:TRP:O	1:C:353:LYS:HG3	2.07	0.55
1:B:130:GLY:O	1:C:110:ARG:HD2	2.07	0.55
1:D:118:VAL:O	1:D:118:VAL:HG13	2.05	0.55
1:C:153:ARG:NE	1:C:153:ARG:HA	2.22	0.55
1:D:189:PRO:HG2	1:D:190:GLU:OE2	2.07	0.55
1:C:117:ILE:HD13	1:C:208:PHE:HZ	1.72	0.55
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.72	0.54
1:C:86:THR:OG1	1:C:88:GLU:HG3	2.07	0.54
1:B:115:PRO:O	1:B:202:ILE:HD11	2.07	0.54
1:A:198:ARG:CD	1:A:200:ASN:H	2.19	0.54
1:A:288:ASN:HB3	1:A:289:PRO:HA	1.90	0.54
1:B:278:ARG:CG	1:B:283:GLN:HG3	2.32	0.54
1:B:65:VAL:HA	1:B:81:ILE:HG22	1.90	0.54
1:C:253:MSE:HE1	1:C:319:PHE:HE1	1.73	0.54
1:A:271:ILE:O	1:A:272:SER:C	2.46	0.54
1:A:230:VAL:HG21	1:A:235:LEU:CD2	2.38	0.54
1:C:184:HIS:CE1	1:C:207:ASP:O	2.61	0.54
1:B:90:PHE:CD2	1:B:121:VAL:HG21	2.43	0.54
3:C:401:STU:H16	3:C:401:STU:H261	1.90	0.54
1:B:46:PHE:O	1:B:48:VAL:N	2.39	0.53
1:B:324:TRP:CE3	1:B:325:ILE:HD12	2.43	0.53
1:A:124:TYR:HB2	1:A:135:LEU:HB2	1.91	0.53
1:D:337:HIS:O	1:D:338:THR:C	2.46	0.53
1:C:108:HIS:CG	1:C:120:ILE:HD11	2.43	0.53
1:A:233:GLU:CG	1:D:310:PRO:HG3	2.36	0.53
1:B:83:ASN:O	1:B:87:GLN:N	2.41	0.53
1:B:305:LEU:CD2	1:B:314:MSE:HE2	2.38	0.53
1:D:305:LEU:CG	1:D:314:MSE:HE2	2.39	0.53
1:A:305:LEU:HD21	1:A:314:MSE:HE3	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:ASN:CB	1:A:289:PRO:HA	2.39	0.53
1:B:285:GLU:C	1:B:287:PRO:HD3	2.28	0.53
1:C:97:ASP:O	1:C:98:CYS:HB3	2.09	0.53
1:D:158:PHE:O	1:D:336:LEU:HB2	2.08	0.53
1:B:115:PRO:O	1:B:204:LYS:HE2	2.09	0.53
1:A:147:PHE:CE1	1:A:255:ILE:HG21	2.43	0.53
1:C:266:ASN:ND2	1:C:269:LEU:CG	2.63	0.52
1:C:149:ARG:HG3	1:C:194:TYR:CD2	2.44	0.52
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.45	0.52
1:C:264:TYR:CE1	1:C:348:ARG:CZ	2.92	0.52
1:C:142:ASP:OD1	1:C:196:SER:HA	2.08	0.52
1:D:118:VAL:HG23	1:D:139:GLU:HG2	1.92	0.52
1:D:267:HIS:HA	1:D:273:PRO:CB	2.40	0.52
1:B:287:PRO:O	1:B:291:TRP:HD1	1.92	0.52
1:B:322:HIS:ND1	1:B:323:PRO:N	2.57	0.52
1:D:78:VAL:HA	1:D:92:LEU:O	2.10	0.52
1:A:230:VAL:HG21	1:A:235:LEU:HD21	1.92	0.52
1:C:195:THR:OG1	1:C:201:ALA:HB1	2.09	0.52
3:A:401:STU:H261	3:A:401:STU:H16	1.91	0.52
1:D:277:THR:O	1:D:281:MSE:CB	2.58	0.52
1:B:82:PHE:CE2	1:B:89:LYS:HB3	2.45	0.52
1:D:305:LEU:CD2	1:D:314:MSE:HE2	2.40	0.52
1:A:44:PRO:HG3	1:D:267:HIS:CB	2.36	0.52
1:C:149:ARG:HH11	1:C:153:ARG:HH12	1.58	0.52
1:A:70:LEU:O	3:A:401:STU:H25	2.09	0.52
1:D:66:THR:HG21	1:D:82:PHE:CE1	2.45	0.52
1:D:184:HIS:HB3	1:D:187:VAL:HG23	1.91	0.51
1:A:179:SER:CB	1:D:281:MSE:HE2	2.34	0.51
1:C:242:LYS:O	1:C:245:ASP:HB2	2.10	0.51
1:A:167:MSE:HE2	1:A:253:MSE:HE3	1.91	0.51
1:D:70:LEU:HD22	3:D:401:STU:C3	2.40	0.51
1:B:298:VAL:HG22	1:B:324:TRP:CD1	2.46	0.51
1:B:307:LYS:HD3	1:B:312:GLN:HG2	1.92	0.51
1:A:52:LEU:HD21	1:A:123:VAL:HG21	1.93	0.51
1:A:188:LYS:HB2	1:A:189:PRO:HD2	1.93	0.51
1:D:240:TYR:CE2	1:D:311:THR:HG22	2.46	0.51
1:B:150:ILE:O	1:B:153:ARG:HB3	2.11	0.51
1:C:181:ASN:HB3	1:C:214:THR:OG1	2.10	0.51
1:D:254:TYR:CD1	1:D:262:PRO:HG3	2.46	0.51
1:C:196:SER:H	1:C:201:ALA:HB1	1.76	0.51
1:A:138:MSE:SE	3:A:401:STU:H13	2.61	0.51
1:A:286:PHE:HB3	1:A:291:TRP:CG	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:278:ARG:HG2	1:B:283:GLN:CG	2.32	0.51
1:D:138:MSE:SE	3:D:401:STU:C13	3.07	0.51
1:D:88:GLU:HG3	1:D:90:PHE:HE1	1.76	0.50
1:A:50:SER:HB2	1:C:56:LYS:O	2.10	0.50
1:A:338:THR:O	1:A:342:LEU:HB2	2.11	0.50
1:D:328:SER:O	1:D:331:VAL:HG12	2.11	0.50
1:B:128:TYR:HD1	1:C:48:VAL:CG2	2.25	0.50
1:B:214:THR:HG22	1:B:241:ASP:HB2	1.94	0.50
1:A:327:GLN:C	1:A:329:THR:H	2.14	0.50
1:B:67:SER:HB3	1:C:42:GLN:HG2	1.92	0.50
1:D:158:PHE:HZ	1:D:166:ILE:CD1	2.25	0.50
1:A:49:LYS:HD2	1:A:113:GLN:OE1	2.10	0.50
1:D:92:LEU:HD11	1:D:135:LEU:HB3	1.93	0.50
1:B:328:SER:O	1:B:330:LYS:N	2.44	0.50
1:B:80:GLN:NE2	1:B:89:LYS:HD2	2.27	0.50
1:A:258:CYS:SG	1:A:260:TYR:CE2	2.98	0.49
1:D:300:MSE:CE	1:D:303:ARG:HD2	2.42	0.49
1:B:324:TRP:HE3	1:B:325:ILE:HD12	1.77	0.49
1:D:300:MSE:CE	1:D:303:ARG:CB	2.87	0.49
1:B:328:SER:C	1:B:330:LYS:N	2.64	0.49
1:C:146:LEU:O	1:C:150:ILE:HD13	2.13	0.49
1:C:324:TRP:CE3	1:C:325:ILE:HD12	2.44	0.49
1:A:332:PRO:CB	1:A:334:THR:HG22	2.42	0.49
1:C:272:SER:N	1:C:273:PRO:HD3	2.28	0.49
1:D:266:ASN:O	1:D:273:PRO:HA	2.13	0.49
1:A:97:ASP:H	1:A:133:CYS:HA	1.77	0.49
1:D:49:LYS:HG2	1:D:50:SER:N	2.27	0.49
1:C:337:HIS:O	1:C:341:VAL:HG23	2.12	0.49
1:A:278:ARG:HE	1:A:283:GLN:HE21	1.59	0.49
1:A:264:TYR:N	1:A:264:TYR:HD1	2.09	0.49
1:D:69:VAL:HG22	1:D:79:LEU:HD23	1.94	0.49
1:D:86:THR:O	1:D:87:GLN:HB3	2.12	0.49
1:A:327:GLN:O	1:A:329:THR:N	2.46	0.49
1:C:329:THR:HG23	1:C:330:LYS:N	2.28	0.49
1:C:90:PHE:CE2	1:C:121:VAL:HG21	2.48	0.49
1:D:335:PRO:O	1:D:336:LEU:HD12	2.12	0.49
1:D:257:LEU:CD1	1:D:298:VAL:HG11	2.43	0.49
1:A:288:ASN:ND2	1:A:292:SER:OG	2.45	0.49
1:B:341:VAL:O	1:B:344:GLU:HB2	2.12	0.49
1:C:357:THR:HG23	1:D:72:LEU:HD11	1.94	0.49
1:C:66:THR:HG21	1:C:82:PHE:HE2	1.78	0.49
1:D:158:PHE:HZ	1:D:166:ILE:HD12	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:LYS:HG3	1:A:325:ILE:HG23	1.95	0.49
1:D:257:LEU:HD11	1:D:298:VAL:HG11	1.95	0.48
1:D:324:TRP:HE3	1:D:325:ILE:HD12	1.78	0.48
1:D:301:LEU:HD11	1:D:314:MSE:HE1	1.95	0.48
1:B:198:ARG:CB	1:B:199:PRO:CD	2.88	0.48
1:A:245:ASP:O	1:A:248:SER:HB2	2.13	0.48
1:D:305:LEU:HG	1:D:314:MSE:HE2	1.94	0.48
1:C:93:LYS:HE2	1:C:95:LEU:HD21	1.94	0.48
1:D:214:THR:HG21	1:D:242:LYS:CE	2.43	0.48
1:A:274:GLY:O	1:A:278:ARG:HG3	2.14	0.48
1:C:149:ARG:NH1	1:C:153:ARG:HH12	2.11	0.48
1:B:69:VAL:HG22	1:B:79:LEU:HD21	1.94	0.48
1:C:331:VAL:HG23	1:C:332:PRO:HD2	1.95	0.48
1:D:74:ILE:CB	1:D:209:GLY:HA3	2.42	0.48
1:B:149:ARG:NH2	1:B:196:SER:O	2.44	0.48
1:D:114:CYS:HB2	1:D:176:TYR:CD2	2.48	0.48
1:D:74:ILE:CD1	1:D:209:GLY:HA3	2.42	0.48
1:A:337:HIS:CD2	1:A:337:HIS:N	2.82	0.48
1:B:57:ASN:HA	1:C:50:SER:HB2	1.96	0.48
1:B:89:LYS:O	1:B:140:CYS:HB2	2.14	0.48
1:D:85:ARG:O	1:D:86:THR:C	2.51	0.48
1:A:247:TRP:HB2	1:A:313:ARG:NH1	2.29	0.48
1:B:69:VAL:HA	1:B:79:LEU:HD23	1.95	0.48
1:D:127:LEU:HD12	1:D:132:LYS:HA	1.95	0.48
1:A:253:MSE:HE1	1:A:325:ILE:HD11	1.96	0.48
1:C:230:VAL:HG22	1:C:234:VAL:HB	1.96	0.48
1:A:69:VAL:HA	1:A:79:LEU:HD23	1.96	0.48
1:C:180:ILE:HD11	1:C:182:ILE:HD12	1.95	0.48
1:C:52:LEU:HD21	1:C:123:VAL:HG21	1.95	0.48
1:D:202:ILE:HG13	1:D:203:LEU:N	2.27	0.47
1:A:214:THR:O	1:A:215:THR:CG2	2.55	0.47
1:D:150:ILE:HG21	1:D:338:THR:CG2	2.44	0.47
1:C:264:TYR:OH	1:C:348:ARG:NH2	2.46	0.47
1:A:127:LEU:HD11	1:B:110:ARG:HD3	1.95	0.47
1:C:267:HIS:HA	1:C:273:PRO:HB3	1.96	0.47
1:A:44:PRO:CG	1:C:128:TYR:OH	2.53	0.47
1:D:225:TYR:CG	1:D:226:THR:N	2.81	0.47
1:C:233:GLU:H	1:C:233:GLU:HG3	1.22	0.47
1:A:338:THR:HG22	1:A:342:LEU:HD22	1.97	0.47
1:A:50:SER:HB3	1:C:58:ALA:N	2.28	0.47
1:C:41:GLN:O	1:C:42:GLN:NE2	2.48	0.47
1:B:300:MSE:SE	1:B:303:ARG:HH11	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:138:MSE:SE	3:B:403:STU:H13	2.65	0.47
1:C:90:PHE:HE2	1:C:121:VAL:HG21	1.80	0.47
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.50	0.47
1:C:274:GLY:O	1:C:278:ARG:HG2	2.14	0.47
1:A:281:MSE:HB2	1:A:283:GLN:HG3	1.97	0.47
1:D:70:LEU:C	3:D:401:STU:H25	2.35	0.47
1:D:187:VAL:O	1:D:187:VAL:HG12	2.15	0.47
1:C:160:GLU:HA	1:C:336:LEU:HD21	1.97	0.47
1:B:328:SER:C	1:B:330:LYS:H	2.17	0.47
1:B:74:ILE:CD1	1:B:210:PHE:CD2	2.98	0.47
1:A:111:ALA:HB1	1:A:117:ILE:HD13	1.96	0.47
1:C:190:GLU:N	1:C:190:GLU:CD	2.66	0.46
1:B:289:PRO:CA	1:B:292:SER:OG	2.63	0.46
1:B:94:MSE:HE3	1:B:135:LEU:HD21	1.97	0.46
1:B:74:ILE:HB	1:B:209:GLY:HA3	1.96	0.46
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.97	0.46
1:A:150:ILE:CG2	1:A:342:LEU:HD23	2.45	0.46
1:B:143:GLY:HA3	1:B:196:SER:O	2.15	0.46
1:B:168:LYS:O	1:B:172:GLU:HG3	2.15	0.46
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.70	0.46
1:A:80:GLN:CD	1:A:89:LYS:HD2	2.36	0.46
1:D:233:GLU:H	1:D:233:GLU:HG3	1.24	0.46
1:D:52:LEU:HD21	1:D:123:VAL:HG21	1.97	0.46
1:C:332:PRO:C	1:C:334:THR:H	2.19	0.46
1:C:98:CYS:HB2	1:C:99:PRO:CD	2.45	0.46
1:D:324:TRP:HE3	1:D:325:ILE:CD1	2.29	0.46
1:B:60:ILE:HG21	1:C:45:GLN:CG	2.40	0.46
1:B:52:LEU:HB2	1:B:109:TRP:CD2	2.50	0.46
1:A:56:LYS:O	1:B:50:SER:HB2	2.15	0.46
1:A:43:PHE:CG	1:A:44:PRO:HD2	2.51	0.46
1:C:127:LEU:HD12	1:C:132:LYS:HA	1.96	0.46
1:D:83:ASN:OD1	1:D:85:ARG:N	2.49	0.46
1:D:43:PHE:CD2	1:D:45:GLN:N	2.84	0.46
1:B:331:VAL:HG23	1:B:332:PRO:CD	2.46	0.46
1:D:143:GLY:HA3	1:D:194:TYR:CB	2.46	0.46
1:B:289:PRO:HD2	1:B:290:GLU:OE2	2.16	0.45
1:A:167:MSE:SE	1:A:256:LEU:HD12	2.67	0.45
1:C:266:ASN:HD22	1:C:269:LEU:CG	2.29	0.45
1:B:149:ARG:HH21	1:B:197:LYS:HA	1.81	0.45
1:D:128:TYR:C	1:D:128:TYR:CD2	2.89	0.45
1:D:72:LEU:HA	1:D:77:LYS:HA	1.97	0.45
1:D:183:ALA:O	1:D:211:ALA:HA	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:153:ARG:HA	1:C:153:ARG:HE	1.80	0.45
1:A:150:ILE:HG22	1:A:151:GLN:N	2.32	0.45
1:A:253:MSE:CE	1:A:325:ILE:HD11	2.47	0.45
1:D:306:LEU:HA	1:D:306:LEU:HD23	1.69	0.45
1:D:147:PHE:CE2	1:D:256:LEU:HD23	2.42	0.45
1:D:338:THR:O	1:D:339:SER:C	2.55	0.45
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.89	0.45
1:D:86:THR:O	1:D:87:GLN:CB	2.64	0.45
1:A:158:PHE:CZ	1:A:166:ILE:HD12	2.51	0.45
1:B:289:PRO:O	1:B:292:SER:N	2.45	0.45
1:D:150:ILE:O	1:D:153:ARG:HB2	2.17	0.45
1:A:146:LEU:HG	1:A:147:PHE:CD2	2.52	0.45
1:C:118:VAL:HG13	1:C:118:VAL:O	2.17	0.45
1:D:96:GLN:HB2	1:D:96:GLN:HE21	1.61	0.45
1:A:67:SER:OG	1:A:67:SER:O	2.31	0.45
1:B:316:ILE:HA	1:B:316:ILE:HD12	1.78	0.45
1:D:299:LYS:O	1:D:303:ARG:HG3	2.16	0.45
1:B:124:TYR:HB2	1:B:135:LEU:HB2	1.98	0.45
1:A:81:ILE:HG21	1:A:92:LEU:HD22	1.98	0.45
1:C:296:GLU:O	1:C:300:MSE:HB2	2.16	0.45
1:D:278:ARG:HG3	1:D:278:ARG:NH1	2.32	0.44
1:C:42:GLN:HB2	1:C:42:GLN:HE21	1.29	0.44
1:A:305:LEU:HG	1:A:314:MSE:HE1	1.99	0.44
1:B:202:ILE:HD11	1:B:204:LYS:HE2	2.00	0.44
1:D:111:ALA:HB1	1:D:177:LEU:HD21	1.99	0.44
1:C:151:GLN:C	1:C:153:ARG:N	2.70	0.44
1:C:301:LEU:HD12	1:C:314:MSE:HE1	1.98	0.44
1:B:190:GLU:CD	1:B:190:GLU:H	2.21	0.44
1:A:257:LEU:O	1:A:336:LEU:HD22	2.18	0.44
1:C:342:LEU:HA	1:C:342:LEU:HD12	1.83	0.44
1:B:111:ALA:HB1	1:B:117:ILE:HD13	2.00	0.44
1:B:83:ASN:HB3	1:B:86:THR:OG1	2.18	0.44
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.81	0.44
1:A:49:LYS:O	1:C:126:ASN:HB3	2.17	0.44
1:A:90:PHE:HE2	1:A:121:VAL:HG21	1.81	0.44
1:C:73:GLY:N	1:C:76:GLY:O	2.49	0.44
1:C:160:GLU:HB2	1:C:334:THR:HG23	1.98	0.44
1:A:44:PRO:CG	1:D:267:HIS:HB3	2.42	0.44
1:D:277:THR:O	1:D:281:MSE:HB2	2.17	0.44
1:C:357:THR:CG2	1:D:72:LEU:HD13	2.47	0.44
1:C:86:THR:O	1:C:87:GLN:CB	2.65	0.44
1:D:43:PHE:CG	1:D:44:PRO:HD2	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:94:MSE:HG2	1:C:135:LEU:CD2	2.48	0.44
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.31	0.44
1:C:301:LEU:CD1	1:C:314:MSE:HE1	2.48	0.44
1:B:255:ILE:O	1:B:256:LEU:C	2.54	0.44
1:A:322:HIS:ND1	1:A:323:PRO:HD2	2.32	0.44
1:A:80:GLN:NE2	1:A:89:LYS:HD2	2.32	0.44
1:D:255:ILE:O	1:D:255:ILE:HG22	2.18	0.44
1:C:136:ILE:HG22	1:C:138:MSE:HG3	2.00	0.44
1:A:198:ARG:HD2	1:A:200:ASN:CB	2.48	0.44
1:B:289:PRO:O	1:B:291:TRP:N	2.50	0.44
1:D:185:ARG:HH11	1:D:212:LYS:HB2	1.83	0.44
1:C:249:LEU:HD12	1:C:249:LEU:HA	1.72	0.44
1:A:110:ARG:HH11	1:A:110:ARG:HD2	1.60	0.43
1:C:357:THR:HG23	1:D:72:LEU:HD13	1.99	0.43
1:C:161:ARG:O	1:C:165:GLU:HG3	2.17	0.43
1:D:87:GLN:HB2	1:D:87:GLN:HE21	1.43	0.43
1:B:275:MSE:O	1:B:279:ILE:HG13	2.18	0.43
1:B:97:ASP:OD2	1:B:102:ARG:NH2	2.50	0.43
1:B:284:TYR:N	1:B:284:TYR:CD1	2.86	0.43
1:A:260:TYR:HB2	1:A:261:PRO:HD2	1.99	0.43
1:D:301:LEU:CD1	1:D:314:MSE:HE1	2.48	0.43
1:A:295:SER:HG	1:A:298:VAL:HG23	1.81	0.43
1:D:69:VAL:HG22	1:D:79:LEU:CD2	2.49	0.43
1:B:80:GLN:CD	1:B:89:LYS:HD2	2.38	0.43
1:C:145:GLU:O	1:C:146:LEU:C	2.57	0.43
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.90	0.43
1:B:100:LYS:O	1:B:103:ARG:HB3	2.19	0.43
1:C:336:LEU:C	1:C:338:THR:H	2.20	0.43
1:A:289:PRO:O	1:A:290:GLU:C	2.56	0.43
1:C:57:ASN:HD22	1:C:57:ASN:H	1.67	0.43
1:B:56:LYS:O	1:C:50:SER:HB2	2.18	0.43
1:A:98:CYS:O	1:A:101:ALA:HB3	2.19	0.43
1:C:159:THR:HA	1:C:334:THR:O	2.18	0.42
3:D:401:STU:H16	3:D:401:STU:H261	2.00	0.42
1:B:56:LYS:HE3	1:B:125:GLU:CD	2.40	0.42
1:B:63:TYR:HA	1:B:82:PHE:O	2.18	0.42
1:C:227:PRO:O	1:C:230:VAL:HG12	2.19	0.42
1:B:290:GLU:CD	1:B:290:GLU:H	2.22	0.42
1:B:87:GLN:HB2	1:B:87:GLN:HE21	1.30	0.42
1:C:108:HIS:HB3	1:C:120:ILE:HD11	2.01	0.42
1:C:241:ASP:C	1:C:243:SER:N	2.70	0.42
1:A:257:LEU:HD12	1:A:291:TRP:CH2	2.54	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:ARG:CG	1:A:199:PRO:HD2	2.40	0.42
1:D:65:VAL:HA	1:D:81:ILE:HG22	2.01	0.42
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.60	0.42
1:D:74:ILE:HD12	1:D:209:GLY:CA	2.49	0.42
1:D:118:VAL:CG1	1:D:118:VAL:O	2.67	0.42
1:A:77:LYS:H	1:A:77:LYS:HG3	1.62	0.42
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.62	0.42
1:C:334:THR:HA	1:C:335:PRO:HD3	1.63	0.42
1:D:43:PHE:HA	1:D:44:PRO:HD3	1.91	0.42
1:C:94:MSE:HA	1:C:135:LEU:HD23	2.01	0.42
1:C:253:MSE:HE1	1:C:319:PHE:CE1	2.54	0.42
1:B:151:GLN:O	1:B:152:ASP:C	2.58	0.42
1:C:238:GLU:O	1:C:239:LYS:O	2.37	0.42
1:A:50:SER:HB3	1:C:58:ALA:H	1.84	0.42
1:C:192:LEU:HB3	1:C:203:LEU:HD11	2.02	0.42
1:C:147:PHE:O	1:C:151:GLN:HG2	2.20	0.41
1:C:180:ILE:CD1	1:C:182:ILE:HD12	2.50	0.41
1:B:175:GLN:HA	1:B:316:ILE:HG21	2.02	0.41
1:A:98:CYS:H	1:A:101:ALA:HB3	1.84	0.41
1:D:237:PRO:HB2	1:D:238:GLU:H	1.62	0.41
1:C:304:ASN:HD22	1:C:304:ASN:HA	1.68	0.41
1:C:307:LYS:HD3	1:C:312:GLN:HB3	2.02	0.41
1:B:95:LEU:O	1:B:133:CYS:HB2	2.21	0.41
1:C:82:PHE:HA	1:C:88:GLU:O	2.20	0.41
1:C:63:TYR:CD1	1:C:81:ILE:HD12	2.55	0.41
1:D:97:ASP:H	1:D:133:CYS:HA	1.85	0.41
1:B:322:HIS:ND1	1:B:323:PRO:HD2	2.35	0.41
1:A:228:TYR:OH	1:D:190:GLU:OE2	2.33	0.41
1:C:289:PRO:O	1:C:291:TRP:N	2.52	0.41
1:A:331:VAL:HA	1:A:332:PRO:HD3	1.88	0.41
1:D:95:LEU:O	1:D:133:CYS:HB2	2.20	0.41
1:C:240:TYR:O	1:C:243:SER:HB2	2.20	0.41
1:C:254:TYR:C	1:C:254:TYR:CD1	2.92	0.41
1:A:110:ARG:HG2	1:C:127:LEU:HD21	2.03	0.41
1:B:74:ILE:O	1:B:75:ASN:HB2	2.21	0.41
1:D:258:CYS:SG	1:D:260:TYR:CE2	3.13	0.41
1:A:253:MSE:O	1:A:254:TYR:C	2.59	0.41
1:A:240:TYR:HE2	1:D:309:GLU:OE2	2.03	0.41
1:D:289:PRO:O	1:D:290:GLU:C	2.59	0.41
1:B:128:TYR:C	1:B:128:TYR:CD2	2.94	0.41
1:A:310:PRO:O	1:A:313:ARG:HB2	2.21	0.41
1:C:94:MSE:HE2	1:C:94:MSE:HB3	1.98	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:ALA:CB	1:A:177:LEU:HD21	2.51	0.41
1:A:56:LYS:NZ	1:A:125:GLU:OE2	2.53	0.41
1:B:183:ALA:O	1:B:211:ALA:HA	2.21	0.41
1:C:159:THR:C	1:C:336:LEU:HD22	2.41	0.41
1:B:337:HIS:N	1:B:337:HIS:CD2	2.89	0.41
1:C:168:LYS:HD2	1:C:325:ILE:O	2.21	0.41
1:D:190:GLU:N	1:D:190:GLU:CD	2.74	0.41
1:C:168:LYS:O	1:C:172:GLU:HG3	2.20	0.41
1:D:271:ILE:HA	1:D:271:ILE:HD13	1.77	0.41
1:D:70:LEU:HB3	3:D:401:STU:C20	2.51	0.41
1:A:152:ASP:O	1:A:153:ARG:HG3	2.21	0.41
1:B:289:PRO:HG2	1:B:337:HIS:CE1	2.56	0.40
1:A:305:LEU:O	1:A:313:ARG:HD3	2.20	0.40
1:A:334:THR:HA	1:A:335:PRO:HD3	1.79	0.40
1:D:264:TYR:N	1:D:264:TYR:HD1	2.15	0.40
1:A:227:PRO:C	1:A:229:TYR:H	2.25	0.40
1:A:138:MSE:HB2	1:A:138:MSE:HE3	2.00	0.40
1:A:167:MSE:HG3	1:A:253:MSE:HG3	2.04	0.40
1:D:43:PHE:HD2	1:D:45:GLN:N	2.18	0.40
1:C:139:GLU:OE1	1:C:204:LYS:NZ	2.54	0.40
1:A:272:SER:HA	1:A:277:THR:HG21	2.03	0.40
1:C:264:TYR:OH	1:C:348:ARG:NE	2.55	0.40
1:A:332:PRO:C	1:A:334:THR:H	2.25	0.40
1:D:185:ARG:NH1	1:D:212:LYS:HD2	2.37	0.40
1:B:149:ARG:NH2	1:B:197:LYS:HA	2.37	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	284/400 (71%)	250 (88%)	25 (9%)	9 (3%)	6	14
1	B	277/400 (69%)	241 (87%)	26 (9%)	10 (4%)	5	11
1	C	302/400 (76%)	261 (86%)	30 (10%)	11 (4%)	5	11

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	282/400 (70%)	241 (86%)	32 (11%)	9 (3%)	6	14
All	All	1145/1600 (72%)	993 (87%)	113 (10%)	39 (3%)	6	12

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
1	B	66	THR
1	B	239	LYS
1	C	42	GLN
1	C	237	PRO
1	C	239	LYS
1	C	289	PRO
1	C	290	GLU
1	C	346	LYS
1	A	237	PRO
1	A	239	LYS
1	A	328	SER
1	B	146	LEU
1	B	207	ASP
1	B	238	GLU
1	D	152	ASP
1	D	195	THR
1	D	237	PRO
1	D	292	SER
1	D	338	THR
1	B	237	PRO
1	B	329	THR
1	C	345	ASP
1	D	151	GLN
1	D	238	GLU
1	B	47	HIS
1	B	290	GLU
1	C	207	ASP
1	C	228	TYR
1	C	267	HIS
1	D	207	ASP
1	A	238	GLU
1	A	310	PRO
1	C	112	SER
1	D	226	THR
1	A	273	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	287	PRO
1	A	309	GLU
1	B	332	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	246/345 (71%)	224 (91%)	22 (9%)	14	31
1	B	241/345 (70%)	213 (88%)	28 (12%)	8	18
1	C	263/345 (76%)	231 (88%)	32 (12%)	7	17
1	D	241/345 (70%)	221 (92%)	20 (8%)	16	35
All	All	991/1380 (72%)	889 (90%)	102 (10%)	10	23

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	45	GLN
1	A	77	LYS
1	A	80	GLN
1	A	106	GLU
1	A	127	LEU
1	A	134	LEU
1	A	142	ASP
1	A	149	ARG
1	A	198	ARG
1	A	202	ILE
1	A	215	THR
1	A	233	GLU
1	A	249	LEU
1	A	271	ILE
1	A	285	GLU
1	A	297	GLU
1	A	304	ASN
1	A	325	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	331	VAL
1	A	334	THR
1	A	342	LEU
1	B	45	GLN
1	B	47	HIS
1	B	66	THR
1	B	87	GLN
1	B	100	LYS
1	B	102	ARG
1	B	119	ARG
1	B	134	LEU
1	B	149	ARG
1	B	156	GLN
1	B	161	ARG
1	B	162	GLU
1	B	198	ARG
1	B	202	ILE
1	B	212	LYS
1	B	233	GLU
1	B	243	SER
1	B	249	LEU
1	B	256	LEU
1	B	265	SER
1	B	292	SER
1	B	295	SER
1	B	297	GLU
1	B	304	ASN
1	B	331	VAL
1	B	334	THR
1	B	336	LEU
1	B	342	LEU
1	C	42	GLN
1	C	45	GLN
1	C	47	HIS
1	C	87	GLN
1	C	106	GLU
1	C	127	LEU
1	C	131	ARG
1	C	133	CYS
1	C	145	GLU
1	C	149	ARG
1	C	153	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	162	GLU
1	C	198	ARG
1	C	202	ILE
1	C	233	GLU
1	C	235	LEU
1	C	243	SER
1	C	249	LEU
1	C	287	PRO
1	C	290	GLU
1	C	297	GLU
1	C	308	THR
1	C	311	THR
1	C	316	ILE
1	C	325	ILE
1	C	326	MSE
1	C	333	GLN
1	C	334	THR
1	C	336	LEU
1	C	337	HIS
1	C	342	LEU
1	C	354	GLU
1	D	45	GLN
1	D	66	THR
1	D	87	GLN
1	D	96	GLN
1	D	127	LEU
1	D	134	LEU
1	D	142	ASP
1	D	175	GLN
1	D	195	THR
1	D	202	ILE
1	D	233	GLU
1	D	256	LEU
1	D	264	TYR
1	D	271	ILE
1	D	295	SER
1	D	297	GLU
1	D	308	THR
1	D	327	GLN
1	D	334	THR
1	D	336	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	45	GLN
1	A	68	GLN
1	A	80	GLN
1	A	181	ASN
1	A	266	ASN
1	A	283	GLN
1	A	288	ASN
1	A	337	HIS
1	B	45	GLN
1	B	68	GLN
1	B	75	ASN
1	B	87	GLN
1	B	151	GLN
1	B	156	GLN
1	B	283	GLN
1	B	337	HIS
1	C	42	GLN
1	C	57	ASN
1	C	87	GLN
1	C	151	GLN
1	C	156	GLN
1	C	184	HIS
1	C	266	ASN
1	C	283	GLN
1	C	304	ASN
1	C	327	GLN
1	C	333	GLN
1	D	45	GLN
1	D	68	GLN
1	D	75	ASN
1	D	87	GLN
1	D	96	GLN
1	D	175	GLN
1	D	266	ASN
1	D	304	ASN
1	D	333	GLN

### 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 ⓘ

6 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$
3	STU	A	401	-	40,42,42	2.21	12 (30%)	62,68,68	2.06	18 (29%)
2	SO4	B	401	-	4,4,4	1.54	1 (25%)	6,6,6	0.64	0
2	SO4	B	402	-	4,4,4	1.58	1 (25%)	6,6,6	0.64	0
3	STU	B	403	-	40,42,42	2.22	14 (35%)	62,68,68	1.61	10 (16%)
3	STU	C	401	-	40,42,42	2.12	15 (37%)	62,68,68	2.04	16 (25%)
3	STU	D	401	-	40,42,42	2.25	16 (40%)	62,68,68	1.75	14 (22%)

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
3	STU	A	401	-	-	0/4/42/42	0/0/8/8
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	STU	B	403	-	-	0/4/42/42	0/0/8/8
3	STU	C	401	-	-	0/4/42/42	0/0/8/8
3	STU	D	401	-	-	0/4/42/42	0/0/8/8

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	STU	C21-C22	5.10	1.60	1.53
3	B	403	STU	C23-N4	5.03	1.58	1.47
3	D	401	STU	C23-N4	5.02	1.58	1.47
3	A	401	STU	C23-N4	5.01	1.58	1.47
3	D	401	STU	C18-N2	4.63	1.45	1.39
3	B	403	STU	C7-C6	4.40	1.50	1.43
3	A	401	STU	C18-N2	4.37	1.44	1.39
3	B	403	STU	C21-C22	4.28	1.59	1.53
3	C	401	STU	C21-C22	4.27	1.59	1.53
3	B	403	STU	C19-N3	4.24	1.44	1.39
3	D	401	STU	C7-C6	4.21	1.50	1.43
3	C	401	STU	C23-N4	4.06	1.56	1.47
3	C	401	STU	C7-C6	3.96	1.49	1.43
3	D	401	STU	C11-C18	3.91	1.47	1.42
3	A	401	STU	C24-C25	3.89	1.57	1.51
3	D	401	STU	C22-C23	3.80	1.59	1.52
3	B	403	STU	C6-C19	3.75	1.47	1.42
3	D	401	STU	C17-N2	3.62	1.43	1.39
3	C	401	STU	C19-N3	3.60	1.43	1.39
3	C	401	STU	C18-N2	3.56	1.43	1.39
3	B	403	STU	C5-C20	3.55	1.47	1.41
3	A	401	STU	C11-C18	3.48	1.47	1.42
3	D	401	STU	C24-C25	3.32	1.56	1.51
3	A	401	STU	C12-C17	3.26	1.46	1.41
3	C	401	STU	C24-C25	3.23	1.56	1.51
3	B	403	STU	C9-C10	3.20	1.55	1.50
3	B	403	STU	C24-C25	3.18	1.56	1.51
3	C	401	STU	C5-C20	3.06	1.46	1.41
3	C	401	STU	C3-C2	3.02	1.46	1.37
3	D	401	STU	C12-C17	2.94	1.46	1.41
3	A	401	STU	C7-C10	-2.92	1.31	1.40
3	B	403	STU	C7-C10	-2.91	1.31	1.40
3	C	401	STU	C11-C18	2.82	1.46	1.42
3	A	401	STU	C14-C15	2.78	1.45	1.37
3	C	401	STU	C7-C10	-2.76	1.32	1.40
3	D	401	STU	C6-C19	2.72	1.46	1.42
3	C	401	STU	C22-C23	2.69	1.57	1.52
3	D	401	STU	C21-C22	2.65	1.57	1.53
3	B	403	STU	C18-N2	2.65	1.42	1.39
3	D	401	STU	C7-C10	-2.65	1.32	1.40
3	A	401	STU	C7-C6	2.62	1.47	1.43
3	D	401	STU	C9-C10	2.59	1.54	1.50
3	B	403	STU	C19-C18	-2.58	1.35	1.41

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	STU	C20-N3	-2.53	1.35	1.39
3	B	403	STU	C10-C11	2.52	1.46	1.42
3	C	401	STU	C24-C23	2.50	1.57	1.53
2	B	402	SO4	O4-S	2.50	1.55	1.47
2	B	401	SO4	O4-S	2.41	1.55	1.47
3	A	401	STU	C22-C23	2.35	1.57	1.52
3	D	401	STU	C14-C15	2.28	1.44	1.37
3	A	401	STU	C5-C20	2.20	1.44	1.41
3	C	401	STU	C14-C15	2.18	1.44	1.37
3	D	401	STU	C19-C18	-2.14	1.36	1.41
3	D	401	STU	C3-C2	2.10	1.44	1.37
3	A	401	STU	C3-C2	2.09	1.43	1.37
3	B	403	STU	C14-C15	2.08	1.43	1.37
3	B	403	STU	C3-C2	2.07	1.43	1.37
3	D	401	STU	C5-C20	2.06	1.44	1.41
3	C	401	STU	C9-C10	2.01	1.53	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	STU	C28-N4-C23	-7.50	109.64	113.82
3	A	401	STU	C28-N4-C23	-7.32	109.74	113.82
3	B	403	STU	C24-C25-N3	-5.20	106.50	112.48
3	C	401	STU	C24-C25-N3	-4.94	106.79	112.48
3	C	401	STU	C7-C6-C19	-4.88	114.50	121.81
3	A	401	STU	C7-C6-C19	-4.87	114.51	121.81
3	D	401	STU	C7-C6-C19	-4.56	114.98	121.81
3	A	401	STU	C6-C7-C8	-4.46	125.45	128.93
3	B	403	STU	C7-C6-C19	-4.46	115.13	121.81
3	A	401	STU	C24-C25-N3	-4.40	107.41	112.48
3	C	401	STU	C10-C9-N1	-3.57	98.48	101.45
3	D	401	STU	C9-N1-C8	3.52	117.45	113.15
3	D	401	STU	C28-N4-C23	-3.50	111.87	113.82
3	C	401	STU	C9-N1-C8	3.48	117.40	113.15
3	D	401	STU	C10-C9-N1	-3.46	98.57	101.45
3	A	401	STU	C10-C9-N1	-3.38	98.63	101.45
3	D	401	STU	C24-C25-N3	-3.29	108.69	112.48
3	C	401	STU	C6-C7-C8	-3.28	126.37	128.93
3	A	401	STU	C9-N1-C8	3.24	117.11	113.15
3	A	401	STU	C21-O4-C25	3.24	128.00	116.37
3	D	401	STU	C7-C8-N1	-3.21	102.90	106.39
3	D	401	STU	C24-C23-N4	-3.18	104.48	112.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	STU	C10-C7-C6	3.09	123.43	120.39
3	A	401	STU	C7-C8-N1	-3.09	103.04	106.39
3	C	401	STU	C22-C21-N2	-3.05	108.30	112.78
3	B	403	STU	C9-N1-C8	2.94	116.74	113.15
3	C	401	STU	C21-O4-C25	2.94	126.93	116.37
3	A	401	STU	C22-C21-N2	-2.90	108.53	112.78
3	C	401	STU	C7-C8-N1	-2.88	103.26	106.39
3	D	401	STU	C21-O4-C25	2.81	126.49	116.37
3	B	403	STU	C21-O4-C25	2.70	126.07	116.37
3	C	401	STU	O4-C25-C24	-2.70	107.69	112.00
3	C	401	STU	C10-C7-C6	2.68	123.02	120.39
3	B	403	STU	O4-C25-C24	-2.67	107.74	112.00
3	B	403	STU	C11-C12-C17	2.61	109.22	106.37
3	C	401	STU	C11-C12-C17	2.54	109.15	106.37
3	B	403	STU	C22-C21-N2	-2.52	109.09	112.78
3	A	401	STU	O4-C25-C24	-2.49	108.02	112.00
3	B	403	STU	C7-C8-N1	-2.41	103.78	106.39
3	B	403	STU	C10-C9-N1	-2.35	99.50	101.45
3	D	401	STU	C11-C12-C17	2.32	108.90	106.37
3	C	401	STU	C24-C23-N4	-2.32	106.62	112.33
3	A	401	STU	C11-C12-C17	2.31	108.89	106.37
3	D	401	STU	C6-C7-C8	-2.29	127.14	128.93
3	D	401	STU	C22-C23-N4	2.24	114.53	110.54
3	A	401	STU	C18-N2-C17	2.21	110.53	106.19
3	A	401	STU	C12-C17-N2	-2.21	106.45	109.40
3	A	401	STU	C26-C21-N2	2.17	112.26	111.09
3	A	401	STU	C24-C23-N4	-2.16	107.00	112.33
3	D	401	STU	O4-C25-C24	-2.14	108.58	112.00
3	A	401	STU	C10-C7-C8	2.11	111.12	108.89
3	C	401	STU	C12-C17-N2	-2.07	106.64	109.40
3	D	401	STU	C15-C14-C13	-2.07	117.45	120.47
3	C	401	STU	C18-N2-C17	2.06	110.24	106.19
3	D	401	STU	C16-C17-N2	2.06	134.47	130.55
3	C	401	STU	C21-C22-C23	-2.05	104.13	111.00
3	A	401	STU	C5-C6-C19	2.01	109.60	106.05
3	B	403	STU	C12-C17-N2	-2.00	106.72	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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.