



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 AM GMT

PDB ID : 2DR0  
Title : Crystal structure of human carboxylesterase in complex with taurocholate  
Authors : Bencharit, S.; Redinbo, M.R.  
Deposited on : 2006-06-02  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

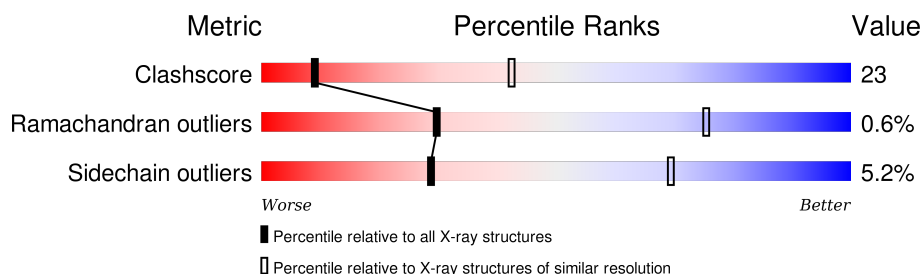
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	542	
1	B	542	
1	C	542	

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
6	TCH	A	101	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TCH	A	102	X	-	X	-
6	TCH	B	201	X	-	-	-
6	TCH	B	202	X	-	X	-
6	TCH	C	301	X	-	-	-
6	TCH	C	302	X	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12988 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.

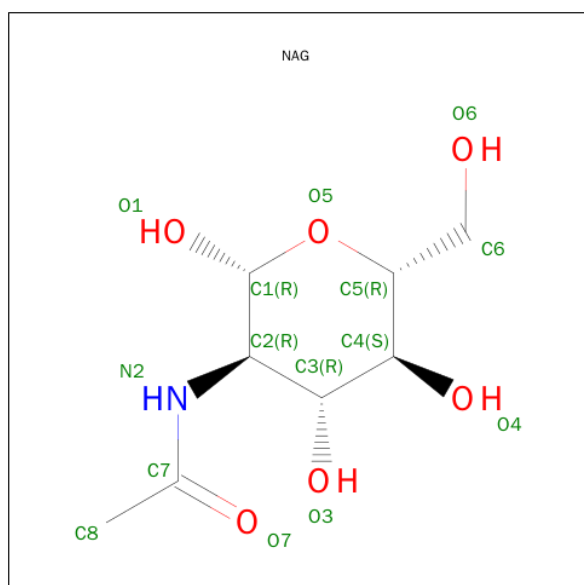
- Molecule 1 is a protein called Liver carboxylesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	C	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			

There are 3 discrepancies between the modelled and reference sequences:

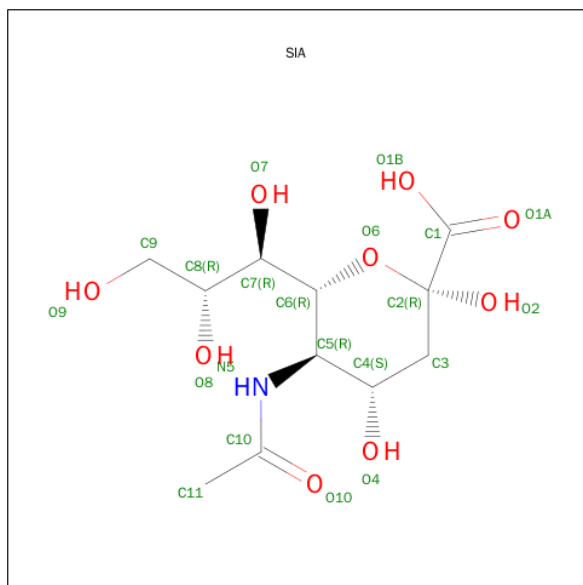
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P23141
B	?	-	GLN	DELETION	UNP P23141
C	?	-	GLN	DELETION	UNP P23141

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



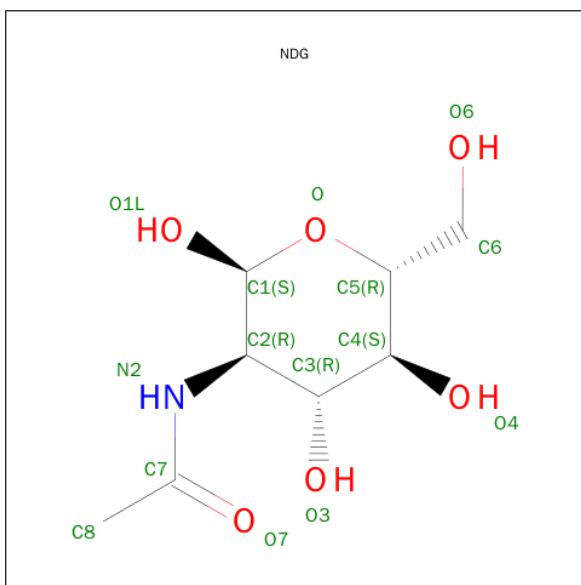
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	C	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



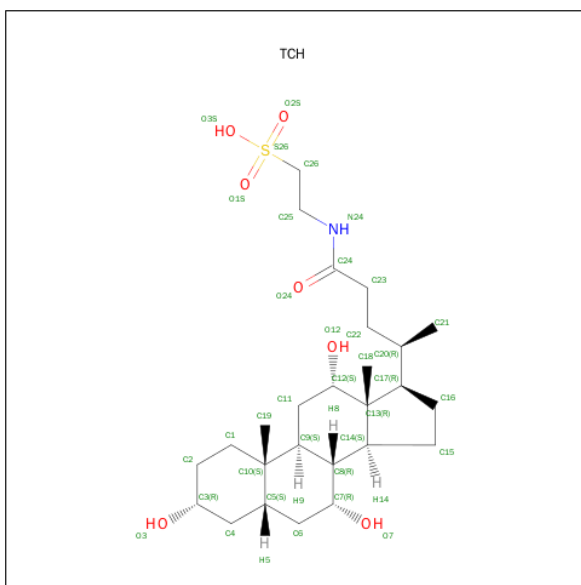
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

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

- Molecule 6 is TAUROCHOLIC ACID (three-letter code: TCH) (formula:  $C_{26}H_{45}NO_7S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
6	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
6	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
6	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
6	C	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
6	C	1	Total	C	N	O	S	0	0
			35	26	1	7	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	104	Total 104	O 104	0	0
7	B	72	Total 72	O 72	0	0
7	C	77	Total 77	O 77	0	0

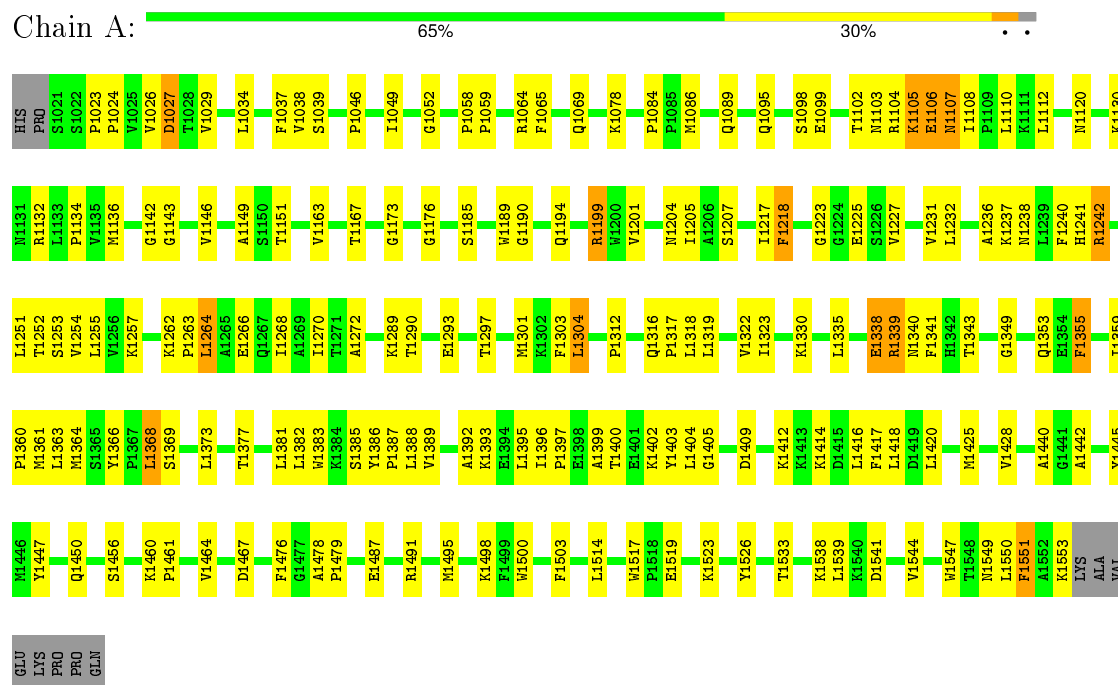


### 3 Residue-property plots

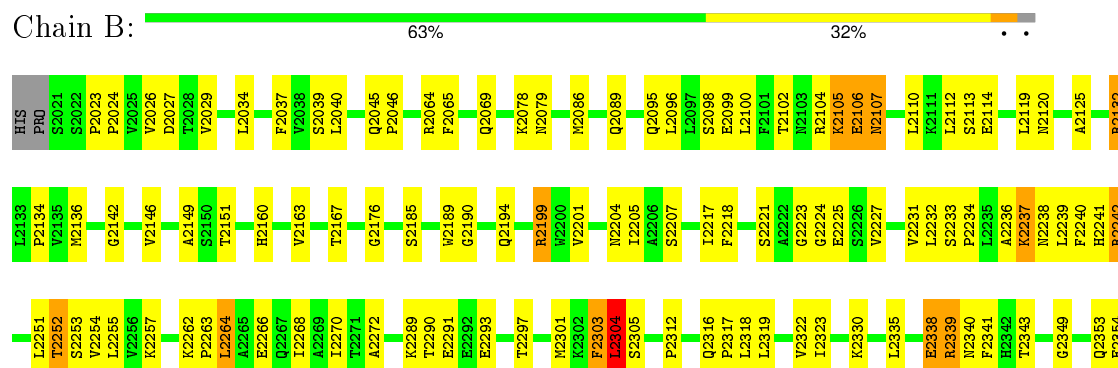
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

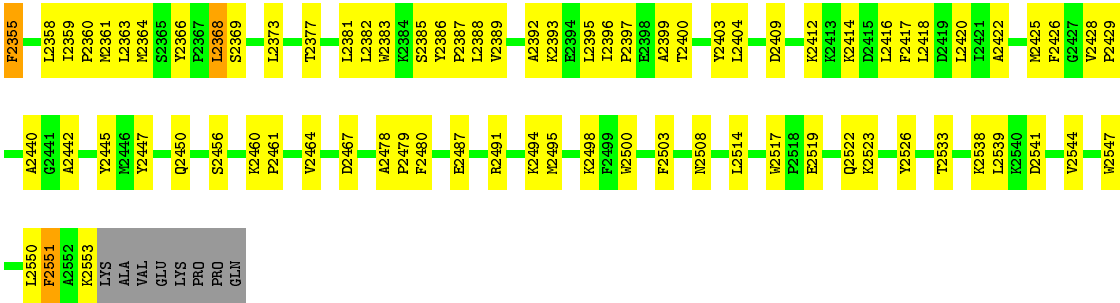
Note EDS was not executed.

- Molecule 1: Liver carboxylesterase 1



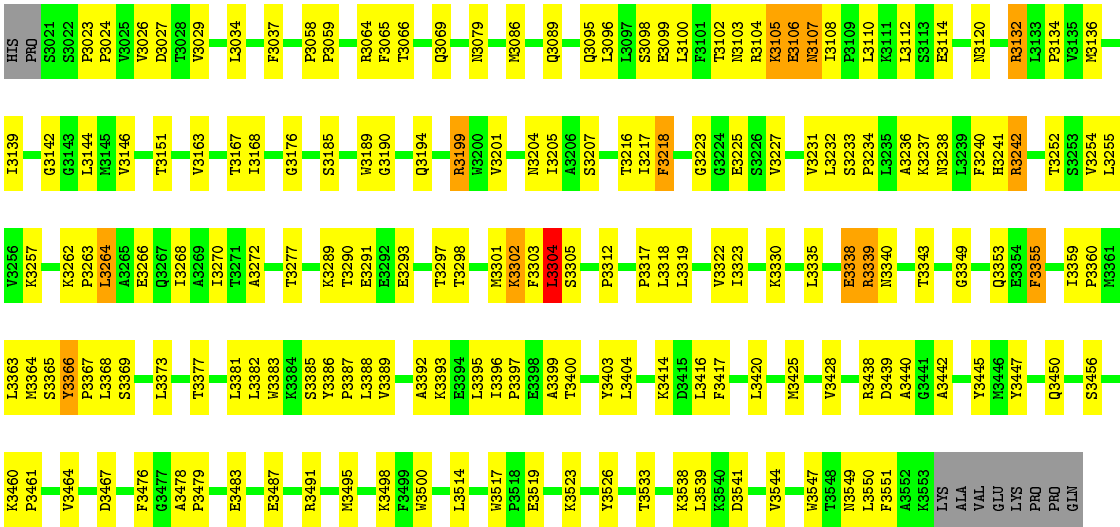
- Molecule 1: Liver carboxylesterase 1





● Molecule 1: Liver carboxylesterase 1

Chain C: 66% 30% . .



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.42Å 179.95Å 201.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.61 – 3.20	Depositor
% Data completeness (in resolution range)	98.6 (30.61-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.219 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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: TCH, SIA, NAG, NDG, 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	0.49	2/4236 (0.0%)	0.61	0/5754
1	B	0.44	0/4236	0.61	2/5754 (0.0%)
1	C	0.46	1/4236 (0.0%)	0.61	1/5754 (0.0%)
All	All	0.46	3/12708 (0.0%)	0.61	3/17262 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1549	ASN	CG-OD1	-9.65	1.02	1.24
1	A	1549	ASN	CG-ND2	-9.52	1.09	1.32
1	C	3549	ASN	CG-OD1	-5.01	1.12	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2303	PHE	N-CA-C	6.79	129.34	111.00
1	C	3304	LEU	CA-CB-CG	-6.53	100.29	115.30
1	B	2304	LEU	CA-CB-CG	-5.45	102.77	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4130	179	0
1	B	4130	0	4131	197	0
1	C	4130	0	4130	210	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	21	0	18	2	0
3	B	21	0	18	6	0
3	C	21	0	18	5	0
4	C	14	0	13	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	1	0
6	A	70	0	87	31	0
6	B	70	0	87	39	0
6	C	70	0	87	48	0
7	A	104	0	0	11	0
7	B	72	0	0	13	0
7	C	77	0	0	11	0
All	All	12988	0	12745	589	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 23.

All (589) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3252:THR:HG21	6:C:302:TCH:O3	1.33	1.22
1:A:1304:LEU:HD13	6:A:102:TCH:C18	1.69	1.22
1:C:3255:LEU:HG	6:C:302:TCH:H2	1.15	1.13
1:C:3301:MET:HB2	1:C:3303:PHE:CZ	1.87	1.08
1:C:3255:LEU:HG	6:C:302:TCH:C2	1.84	1.08
1:B:2359:ILE:HG12	6:B:202:TCH:H15	1.34	1.07
1:A:1304:LEU:HD22	6:A:102:TCH:C24	1.92	0.99
1:B:2199:ARG:HB3	1:B:2199:ARG:HH11	1.28	0.98
1:C:3304:LEU:CD1	6:C:302:TCH:C18	2.41	0.97
1:A:1199:ARG:HH11	1:A:1199:ARG:HB3	1.28	0.97
1:C:3199:ARG:HB3	1:C:3199:ARG:HH11	1.30	0.96
1:B:2491:ARG:HB2	1:B:2491:ARG:HH11	1.31	0.96
1:A:1369:SER:HA	6:A:101:TCH:H11	1.48	0.95
1:C:3304:LEU:HD13	6:C:302:TCH:C18	1.96	0.95
3:B:282:SIA:H113	1:C:3262:LYS:HZ3	1.32	0.95
1:C:3255:LEU:CG	6:C:302:TCH:H2	1.95	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:LEU:HD13	6:A:102:TCH:H18B	1.50	0.94
3:B:282:SIA:H113	1:C:3262:LYS:NZ	1.83	0.93
1:C:3304:LEU:HD13	6:C:302:TCH:H18B	1.51	0.93
1:B:2369:SER:HA	6:B:201:TCH:H11	1.51	0.93
1:C:3359:ILE:HG12	6:C:302:TCH:H15	1.52	0.90
1:C:3363:LEU:O	6:C:302:TCH:H25A	1.72	0.90
1:A:1304:LEU:CD1	6:A:102:TCH:C18	2.50	0.90
1:C:3491:ARG:HH11	1:C:3491:ARG:HB2	1.36	0.89
1:C:3254:VAL:HG11	6:C:302:TCH:H4A	1.55	0.88
1:C:3304:LEU:HD22	6:C:302:TCH:H37	1.54	0.88
1:B:2363:LEU:O	6:B:202:TCH:H25A	1.73	0.88
1:C:3252:THR:CG2	6:C:302:TCH:O3	2.22	0.87
1:C:3301:MET:O	1:C:3302:LYS:O	1.92	0.87
1:A:1491:ARG:HB2	1:A:1491:ARG:HH11	1.40	0.87
1:C:3369:SER:HA	6:C:301:TCH:H11	1.56	0.86
1:A:1487:GLU:HG3	1:A:1491:ARG:HH12	1.40	0.86
1:C:3359:ILE:HG23	6:C:302:TCH:H15A	1.57	0.85
1:C:3425:MET:CE	6:C:302:TCH:H6	2.08	0.84
1:C:3487:GLU:HG3	1:C:3491:ARG:HH12	1.43	0.83
1:B:2359:ILE:HG12	6:B:202:TCH:C15	2.08	0.83
1:C:3254:VAL:CG1	6:C:302:TCH:H2A	2.09	0.82
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.61	0.82
1:B:2363:LEU:HD13	6:B:202:TCH:H22	1.61	0.82
1:C:3301:MET:CB	1:C:3303:PHE:CZ	2.61	0.82
1:A:1143:GLY:HA3	6:A:102:TCH:H11A	1.62	0.81
1:C:3304:LEU:CD1	6:C:302:TCH:H18A	2.09	0.81
1:A:1304:LEU:HD13	6:A:102:TCH:H18	1.63	0.80
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.64	0.80
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.62	0.79
1:A:1359:ILE:HG23	6:A:102:TCH:H7	1.62	0.79
1:A:1290:THR:OG1	1:A:1293:GLU:HG3	1.83	0.79
1:B:2403:TYR:O	1:B:2416:LEU:HD13	1.83	0.79
1:A:1317:PRO:HG2	1:A:1318:LEU:HD23	1.62	0.79
1:B:2290:THR:OG1	1:B:2293:GLU:HG3	1.81	0.79
1:A:1241:HIS:O	1:A:1242:ARG:HG3	1.83	0.79
1:B:2491:ARG:HB2	1:B:2491:ARG:NH1	1.96	0.79
1:C:3086:MET:HE2	1:C:3110:LEU:HB2	1.65	0.79
1:B:2338:GLU:HG2	1:B:2340:ASN:H	1.48	0.79
1:C:3304:LEU:CD2	6:C:302:TCH:H37	2.12	0.78
1:B:2426:PHE:CE2	6:B:202:TCH:H4	2.18	0.78
1:A:1304:LEU:CD2	6:A:102:TCH:H25A	2.14	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2316:GLN:HG3	7:B:7076:HOH:O	1.83	0.78
1:C:3317:PRO:HG2	1:C:3318:LEU:HD23	1.66	0.78
1:B:2317:PRO:HG2	1:B:2318:LEU:HD23	1.65	0.78
1:A:1338:GLU:HG2	1:A:1340:ASN:H	1.49	0.78
1:A:1304:LEU:HD21	1:A:1363:LEU:O	1.85	0.77
1:A:1461:PRO:HG2	1:A:1464:VAL:HG23	1.66	0.77
1:B:2400:THR:HG23	1:B:2404:LEU:HD12	1.67	0.77
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.67	0.77
1:B:2461:PRO:HG2	1:B:2464:VAL:HG23	1.66	0.77
1:C:3338:GLU:HG2	1:C:3340:ASN:H	1.48	0.77
1:C:3254:VAL:HG13	1:C:3255:LEU:N	1.99	0.77
1:C:3297:THR:O	1:C:3301:MET:HG2	1.84	0.76
1:C:3403:TYR:O	1:C:3416:LEU:HD13	1.86	0.76
1:A:1403:TYR:O	1:A:1416:LEU:HD13	1.85	0.76
1:C:3304:LEU:HD11	6:C:302:TCH:C18	2.15	0.76
1:B:2363:LEU:O	6:B:202:TCH:C25	2.33	0.76
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.68	0.76
1:C:3491:ARG:HB2	1:C:3491:ARG:NH1	2.01	0.75
1:C:3241:HIS:O	1:C:3242:ARG:HG3	1.86	0.75
1:B:2487:GLU:HG3	1:B:2491:ARG:HH12	1.50	0.75
1:C:3461:PRO:HG2	1:C:3464:VAL:HG23	1.68	0.75
1:A:1400:THR:HG23	1:A:1404:LEU:HD12	1.67	0.75
1:C:3304:LEU:CD1	6:C:302:TCH:H18B	2.13	0.74
1:C:3290:THR:OG1	1:C:3293:GLU:HG3	1.87	0.74
1:A:1456:SER:HB3	1:A:1460:LYS:HD3	1.69	0.74
1:A:1105:LYS:HD2	1:A:1106:GLU:N	2.03	0.74
1:B:2241:HIS:O	1:B:2242:ARG:HG3	1.87	0.73
1:B:2023:PRO:HB2	1:B:2034:LEU:HD21	1.70	0.73
1:C:3023:PRO:HB2	1:C:3034:LEU:HD21	1.70	0.73
1:B:2086:MET:HE2	1:B:2110:LEU:HD12	1.71	0.73
1:C:3363:LEU:HD13	6:C:302:TCH:H22	1.71	0.72
1:A:1086:MET:HE2	1:A:1110:LEU:HD12	1.71	0.72
1:C:3363:LEU:O	6:C:302:TCH:C25	2.37	0.72
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.71	0.72
1:C:3400:THR:HG23	1:C:3404:LEU:HD12	1.71	0.72
1:B:2095:GLN:O	1:B:2099:GLU:HG3	1.90	0.71
1:A:1491:ARG:HB2	1:A:1491:ARG:NH1	2.04	0.71
1:C:3254:VAL:HG13	6:C:302:TCH:H2A	1.71	0.71
1:C:3024:PRO:HG3	1:C:3037:PHE:CE1	2.26	0.71
1:C:3254:VAL:HG11	6:C:302:TCH:H19A	1.73	0.71
1:A:1024:PRO:HG3	1:A:1037:PHE:CE1	2.26	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3414:LYS:NZ	6:C:301:TCH:H4A	2.06	0.71
1:C:3105:LYS:HD2	1:C:3106:GLU:N	2.06	0.70
1:C:3304:LEU:HD11	6:C:302:TCH:H18A	1.72	0.70
1:B:2304:LEU:HG	1:B:2305:SER:N	2.04	0.70
1:B:2254:VAL:HG13	1:B:2255:LEU:N	2.06	0.69
1:C:3425:MET:HE3	6:C:302:TCH:H6	1.73	0.69
1:B:2461:PRO:HG2	1:B:2464:VAL:CG2	2.23	0.69
1:B:2024:PRO:HG3	1:B:2037:PHE:CE1	2.28	0.69
1:C:3368:LEU:O	6:C:301:TCH:H19B	1.92	0.69
1:A:1364:MET:HE1	1:A:1388:LEU:HD11	1.75	0.69
1:A:1461:PRO:HG2	1:A:1464:VAL:CG2	2.22	0.68
1:B:2105:LYS:HD2	1:B:2106:GLU:N	2.07	0.68
1:B:2304:LEU:HD22	6:B:202:TCH:O24	1.94	0.68
1:A:1095:GLN:O	1:A:1099:GLU:HG3	1.94	0.68
1:A:1024:PRO:HG3	1:A:1037:PHE:CZ	2.30	0.67
1:C:3024:PRO:HG3	1:C:3037:PHE:CZ	2.30	0.67
1:C:3456:SER:HB3	1:C:3460:LYS:HD3	1.76	0.67
1:C:3359:ILE:HG23	6:C:302:TCH:C15	2.25	0.67
1:B:2426:PHE:CZ	6:B:202:TCH:H4	2.29	0.67
1:C:3086:MET:HE2	1:C:3110:LEU:HD12	1.76	0.67
1:B:2382:LEU:HD23	1:B:2396:ILE:HG23	1.77	0.67
1:C:3438:ARG:HG2	7:C:7206:HOH:O	1.95	0.67
1:C:3382:LEU:HD23	1:C:3396:ILE:HG23	1.74	0.66
1:A:1382:LEU:HD23	1:A:1396:ILE:HG23	1.76	0.66
1:B:2339:ARG:HG2	1:B:2440:ALA:HA	1.78	0.66
1:C:3461:PRO:HG2	1:C:3464:VAL:CG2	2.26	0.66
1:A:1255:LEU:HD11	6:A:102:TCH:H2	1.76	0.66
1:C:3095:GLN:O	1:C:3099:GLU:HG3	1.96	0.66
6:C:302:TCH:O2S	7:C:7197:HOH:O	2.12	0.66
1:A:1254:VAL:HG13	1:A:1255:LEU:N	2.11	0.66
1:B:2359:ILE:HG23	6:B:202:TCH:H15A	1.77	0.66
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.78	0.65
1:C:3254:VAL:HG21	6:C:302:TCH:C19	2.27	0.65
1:C:3252:THR:HG21	6:C:302:TCH:HO3	1.56	0.65
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	1.79	0.65
1:A:1339:ARG:HG2	1:A:1440:ALA:HA	1.79	0.65
1:A:1487:GLU:HG3	1:A:1491:ARG:NH1	2.11	0.65
1:B:2024:PRO:HG3	1:B:2037:PHE:CZ	2.32	0.65
1:B:2086:MET:HE2	1:B:2110:LEU:HB2	1.79	0.64
1:A:1304:LEU:CD2	6:A:102:TCH:C24	2.71	0.64
1:B:2368:LEU:O	6:B:201:TCH:H19B	1.97	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1428:VAL:HG13	1:A:1544:VAL:HG22	1.79	0.64
1:B:2078:LYS:HG3	3:B:282:SIA:O1B	1.97	0.64
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.79	0.64
1:B:2113:SER:HB2	1:C:3277:THR:HG21	1.79	0.64
1:B:2304:LEU:HD13	6:B:202:TCH:C24	2.27	0.64
1:C:3428:VAL:HG13	1:C:3544:VAL:HG22	1.79	0.63
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.80	0.63
1:C:3303:PHE:O	1:C:3304:LEU:C	2.37	0.63
1:C:3254:VAL:HG21	6:C:302:TCH:H19A	1.79	0.63
1:B:2426:PHE:CZ	6:B:202:TCH:H6	2.34	0.63
1:B:2425:MET:HE3	6:B:202:TCH:H6	1.82	0.62
1:B:2359:ILE:HA	6:B:202:TCH:H15A	1.81	0.62
1:C:3339:ARG:HG2	1:C:3440:ALA:HA	1.81	0.62
1:C:3254:VAL:HG11	6:C:302:TCH:H2A	1.82	0.62
1:C:3304:LEU:HD13	6:C:302:TCH:H18A	1.73	0.61
1:C:3487:GLU:HG3	1:C:3491:ARG:NH1	2.14	0.61
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.81	0.61
1:A:1223:GLY:O	1:A:1227:VAL:HG23	2.00	0.61
1:A:1414:LYS:NZ	6:A:101:TCH:H4A	2.15	0.61
1:C:3304:LEU:HD11	1:C:3364:MET:HG2	1.83	0.61
1:A:1400:THR:CG2	1:A:1404:LEU:HD12	2.31	0.61
1:B:2400:THR:CG2	1:B:2404:LEU:HD12	2.31	0.61
1:A:1368:LEU:O	6:A:101:TCH:H19B	2.00	0.60
1:B:2428:VAL:HG13	1:B:2544:VAL:HG22	1.83	0.60
1:C:3495:MET:HE3	1:C:3533:THR:HG21	1.84	0.60
1:C:3403:TYR:CG	1:C:3420:LEU:HD23	2.36	0.60
1:A:1086:MET:HE2	1:A:1110:LEU:HB2	1.84	0.60
1:A:1495:MET:HE3	1:A:1533:THR:HG21	1.83	0.60
1:B:2373:LEU:HD11	1:B:2377:THR:CG2	2.32	0.60
1:A:1086:MET:HG3	1:A:1112:LEU:HD23	1.82	0.60
1:A:1363:LEU:HD13	6:A:102:TCH:H16A	1.83	0.59
1:C:3255:LEU:CD1	6:C:302:TCH:H2	2.32	0.59
1:B:2089:GLN:HB2	1:B:2146:VAL:HG12	1.84	0.59
1:C:3223:GLY:O	1:C:3227:VAL:HG23	2.01	0.59
1:A:1262:LYS:NZ	3:C:382:SIA:H111	2.17	0.59
1:B:2262:LYS:HB3	1:B:2263:PRO:HD3	1.83	0.59
1:A:1373:LEU:HD11	1:A:1377:THR:CG2	2.32	0.59
1:C:3106:GLU:HG3	1:C:3106:GLU:O	2.03	0.59
1:A:1146:VAL:HG21	6:A:102:TCH:H21	1.85	0.59
1:C:3373:LEU:HD11	1:C:3377:THR:CG2	2.32	0.59
1:A:1262:LYS:HB3	1:A:1263:PRO:HD3	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2304:LEU:HD11	6:B:202:TCH:H25A	1.84	0.59
1:B:2495:MET:HE3	1:B:2533:THR:HG21	1.85	0.59
1:B:2079:ASN:O	3:B:282:SIA:O2	2.18	0.58
1:C:3303:PHE:O	1:C:3305:SER:N	2.36	0.58
1:B:2086:MET:HG3	1:B:2112:LEU:HD23	1.85	0.58
1:A:1084:PRO:HA	7:A:7039:HOH:O	2.02	0.58
1:B:2223:GLY:O	1:B:2227:VAL:HG23	2.03	0.58
1:C:3262:LYS:HB3	1:C:3263:PRO:HD3	1.85	0.58
1:B:2368:LEU:HD21	1:B:2373:LEU:HD22	1.85	0.58
1:C:3237:LYS:O	1:C:3238:ASN:HB2	2.04	0.58
1:C:3355:PHE:HE2	1:C:3425:MET:HE1	1.69	0.58
1:A:1304:LEU:HD23	6:A:102:TCH:H25A	1.85	0.58
1:C:3400:THR:CG2	1:C:3404:LEU:HD12	2.34	0.58
1:A:1026:VAL:CG1	1:A:1207:SER:HB3	2.34	0.58
1:A:1089:GLN:OE1	1:A:1146:VAL:HB	2.04	0.57
1:B:2403:TYR:CG	1:B:2420:LEU:HD23	2.39	0.57
1:A:1403:TYR:CG	1:A:1420:LEU:HD23	2.39	0.57
1:B:2498:LYS:HB3	1:B:2514:LEU:HD11	1.87	0.57
1:B:2426:PHE:HZ	6:B:202:TCH:H6	1.69	0.57
1:C:3414:LYS:HZ1	6:C:301:TCH:H4A	1.69	0.57
1:B:2487:GLU:HG3	1:B:2491:ARG:NH1	2.20	0.57
1:B:2099:GLU:HG2	1:B:2107:ASN:OD1	2.04	0.57
1:B:2236:ALA:HB1	1:B:2240:PHE:HE1	1.69	0.57
1:A:1297:THR:O	1:A:1301:MET:HG2	2.05	0.57
1:C:3254:VAL:CG1	6:C:302:TCH:H19A	2.35	0.56
1:B:2106:GLU:O	1:B:2106:GLU:HG3	2.05	0.56
1:A:1237:LYS:O	1:A:1238:ASN:HB2	2.04	0.56
1:B:2199:ARG:HH11	1:B:2199:ARG:CB	2.10	0.56
1:B:2237:LYS:O	1:B:2238:ASN:HB2	2.05	0.56
1:B:2480:PHE:HB3	7:B:7056:HOH:O	2.06	0.56
1:A:1106:GLU:HG3	1:A:1106:GLU:O	2.06	0.56
1:C:3298:THR:O	1:C:3303:PHE:HE1	1.89	0.56
1:B:2363:LEU:HD13	6:B:202:TCH:C22	2.32	0.56
1:B:2522:GLN:HB2	7:B:7021:HOH:O	2.04	0.56
1:C:3298:THR:O	1:C:3303:PHE:CE1	2.59	0.56
1:C:3368:LEU:HD21	1:C:3373:LEU:HD22	1.88	0.56
1:C:3254:VAL:CG1	1:C:3255:LEU:N	2.69	0.56
1:C:3086:MET:HG3	1:C:3112:LEU:HD23	1.87	0.56
1:A:1395:LEU:HB3	1:A:1550:LEU:HD11	1.88	0.55
1:C:3364:MET:HE1	1:C:3388:LEU:HD11	1.88	0.55
1:A:1105:LYS:HD2	1:A:1106:GLU:H	1.71	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3236:ALA:HB1	1:C:3240:PHE:HE1	1.72	0.55
1:A:1359:ILE:CG2	6:A:102:TCH:H7	2.34	0.55
1:C:3089:GLN:OE1	1:C:3146:VAL:HB	2.07	0.55
1:C:3254:VAL:CG2	6:C:302:TCH:H19A	2.37	0.55
1:A:1359:ILE:HG12	6:A:102:TCH:O7	2.07	0.55
1:C:3199:ARG:CB	1:C:3199:ARG:HH11	2.12	0.55
1:A:1304:LEU:CD1	6:A:102:TCH:H18	2.28	0.55
1:A:1236:ALA:HB1	1:A:1240:PHE:HE1	1.72	0.55
1:A:1368:LEU:HD21	1:A:1373:LEU:HD22	1.88	0.55
1:B:2217:ILE:HD12	1:B:2227:VAL:HG13	1.89	0.55
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.42	0.55
1:C:3363:LEU:HD22	6:C:302:TCH:HN24	1.72	0.54
1:B:2312:PRO:HG2	1:B:2383:TRP:CD1	2.42	0.54
1:C:3266:GLU:O	1:C:3270:ILE:HG13	2.07	0.54
1:A:1355:PHE:CD1	1:A:1360:PRO:HG3	2.42	0.54
1:B:2364:MET:HE1	1:B:2388:LEU:HD21	1.87	0.54
3:B:282:SIA:H113	1:C:3262:LYS:HZ1	1.71	0.54
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.23	0.54
1:B:2297:THR:O	1:B:2301:MET:HG2	2.07	0.54
1:B:2414:LYS:NZ	6:B:201:TCH:H4A	2.22	0.54
1:A:1029:VAL:HG23	1:A:1204:ASN:OD1	2.08	0.54
1:B:2363:LEU:HD12	6:B:202:TCH:H16A	1.88	0.54
1:C:3086:MET:CE	1:C:3110:LEU:HD12	2.36	0.54
1:A:1498:LYS:HB3	1:A:1514:LEU:HD11	1.89	0.54
1:A:1099:GLU:HG2	1:A:1107:ASN:OD1	2.07	0.54
1:C:3498:LYS:HB3	1:C:3514:LEU:HD11	1.89	0.54
1:C:3301:MET:O	1:C:3302:LYS:C	2.39	0.54
1:A:1304:LEU:CD1	6:A:102:TCH:H18A	2.36	0.54
1:A:1217:ILE:HD12	1:A:1227:VAL:HG13	1.90	0.54
1:C:3312:PRO:HG2	1:C:3383:TRP:CD1	2.43	0.54
1:B:2355:PHE:CD1	1:B:2360:PRO:HG3	2.43	0.53
1:B:2318:LEU:HD23	1:B:2318:LEU:N	2.23	0.53
1:B:2254:VAL:CG1	1:B:2255:LEU:N	2.71	0.53
1:B:2304:LEU:CD2	6:B:202:TCH:O24	2.56	0.53
1:A:1369:SER:HB2	6:A:101:TCH:H18B	1.90	0.53
1:C:3029:VAL:HG23	1:C:3204:ASN:OD1	2.08	0.53
1:B:2026:VAL:CG1	1:B:2207:SER:HB3	2.38	0.53
1:B:2447:TYR:HB3	1:B:2517:TRP:CZ2	2.43	0.53
1:C:3304:LEU:CD1	1:C:3364:MET:HG2	2.38	0.53
1:C:3099:GLU:HG2	1:C:3107:ASN:OD1	2.07	0.53
1:B:2319:LEU:N	1:B:2319:LEU:HD23	2.23	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:LEU:HD13	6:A:102:TCH:C16	2.38	0.53
1:B:2355:PHE:CE1	1:B:2360:PRO:HG3	2.43	0.53
1:A:1353:GLN:O	1:A:1467:ASP:HA	2.09	0.53
1:B:2029:VAL:HG23	1:B:2204:ASN:OD1	2.09	0.53
1:C:3086:MET:CE	1:C:3110:LEU:HB2	2.38	0.53
1:C:3217:ILE:HD12	1:C:3227:VAL:HG13	1.91	0.53
1:B:2338:GLU:CG	1:B:2340:ASN:H	2.21	0.53
1:B:2338:GLU:HG2	1:B:2339:ARG:N	2.23	0.53
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.24	0.53
1:B:2086:MET:CE	1:B:2110:LEU:HD12	2.38	0.53
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.24	0.53
1:B:2190:GLY:O	1:B:2194:GLN:HG3	2.08	0.53
1:B:2395:LEU:HB3	1:B:2550:LEU:HD11	1.91	0.53
1:C:3349:GLY:HA3	1:C:3447:TYR:CE1	2.44	0.53
1:B:2359:ILE:HG13	7:B:7162:HOH:O	2.09	0.52
1:B:2089:GLN:OE1	1:B:2146:VAL:HB	2.09	0.52
1:C:3447:TYR:HB3	1:C:3517:TRP:CZ2	2.44	0.52
1:C:3343:THR:HA	7:C:7250:HOH:O	2.07	0.52
1:C:3526:TYR:CD2	1:C:3539:LEU:HB2	2.44	0.52
1:B:2359:ILE:CD1	6:B:202:TCH:O7	2.58	0.52
1:C:3414:LYS:HZ2	6:C:301:TCH:H4A	1.74	0.52
1:C:3318:LEU:HD23	1:C:3318:LEU:N	2.25	0.52
1:A:1338:GLU:HG2	1:A:1339:ARG:N	2.24	0.52
1:C:3338:GLU:CG	1:C:3340:ASN:H	2.21	0.52
1:C:3338:GLU:HG2	1:C:3339:ARG:N	2.23	0.52
1:C:3353:GLN:O	1:C:3467:ASP:HA	2.10	0.52
1:C:3319:LEU:N	1:C:3319:LEU:HD23	2.24	0.52
1:C:3272:ALA:O	1:C:3289:LYS:HE3	2.09	0.52
1:A:1405:GLY:HA2	7:A:7235:HOH:O	2.09	0.52
1:A:1355:PHE:CE1	1:A:1360:PRO:HG3	2.45	0.52
1:C:3089:GLN:HB2	1:C:3146:VAL:HG12	1.91	0.52
1:A:1312:PRO:HG2	1:A:1383:TRP:CD1	2.45	0.52
1:C:3105:LYS:HD2	1:C:3106:GLU:H	1.74	0.52
1:C:3304:LEU:O	1:C:3364:MET:HE2	2.09	0.52
1:C:3439:ASP:HA	7:C:7206:HOH:O	2.10	0.52
1:B:2495:MET:HE3	1:B:2533:THR:CB	2.40	0.51
1:A:1447:TYR:HB3	1:A:1517:TRP:CZ2	2.45	0.51
1:A:1319:LEU:HD23	1:A:1319:LEU:N	2.25	0.51
1:B:2526:TYR:CD2	1:B:2539:LEU:HB2	2.45	0.51
1:B:2363:LEU:HA	6:B:202:TCH:H25	1.90	0.51
1:A:1338:GLU:CG	1:A:1340:ASN:H	2.23	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:ALA:O	1:A:1289:LYS:HE3	2.10	0.51
1:B:2359:ILE:HG21	6:B:202:TCH:H7	1.93	0.51
1:A:1414:LYS:HZ2	6:A:101:TCH:H4A	1.73	0.51
1:B:2257:LYS:HB2	1:B:2322:VAL:HG12	1.91	0.51
1:A:1417:PHE:O	1:A:1420:LEU:HB3	2.11	0.50
1:B:2232:LEU:HB3	1:B:2335:LEU:HD13	1.93	0.50
1:A:1199:ARG:HB3	1:A:1199:ARG:NH1	2.12	0.50
1:A:1199:ARG:HH11	1:A:1199:ARG:CB	2.11	0.50
1:C:3190:GLY:O	1:C:3194:GLN:HG3	2.12	0.50
1:B:2426:PHE:CE2	6:B:202:TCH:C4	2.93	0.50
1:B:2266:GLU:O	1:B:2270:ILE:HG13	2.11	0.50
1:C:3304:LEU:HD22	6:C:302:TCH:H18B	1.93	0.50
1:B:2447:TYR:C	1:B:2447:TYR:CD2	2.84	0.50
1:C:3132:ARG:HD3	7:C:7123:HOH:O	2.12	0.50
1:C:3355:PHE:CD1	1:C:3360:PRO:HG3	2.47	0.50
1:C:3026:VAL:CG1	1:C:3207:SER:HB3	2.42	0.50
1:C:3301:MET:HB2	1:C:3303:PHE:CE1	2.41	0.50
1:B:2272:ALA:O	1:B:2289:LYS:HE3	2.11	0.50
1:C:3395:LEU:HB3	1:C:3550:LEU:HD11	1.92	0.50
1:C:3304:LEU:HD22	6:C:302:TCH:C22	2.35	0.50
1:A:1526:TYR:CD2	1:A:1539:LEU:HB2	2.46	0.50
1:C:3227:VAL:O	1:C:3231:VAL:HG23	2.11	0.50
1:B:2343:THR:HB	1:B:2442:ALA:HB2	1.93	0.50
1:B:2199:ARG:HB3	1:B:2199:ARG:NH1	2.12	0.49
1:A:1227:VAL:O	1:A:1231:VAL:HG23	2.12	0.49
1:B:2445:TYR:CE1	1:B:2519:GLU:HA	2.47	0.49
1:C:3304:LEU:CG	1:C:3364:MET:HG2	2.42	0.49
1:A:1318:LEU:HD23	1:A:1318:LEU:N	2.28	0.49
1:B:2105:LYS:HD2	1:B:2106:GLU:H	1.77	0.49
1:A:1236:ALA:O	1:A:1237:LYS:C	2.50	0.49
1:C:3079:ASN:HB2	3:C:382:SIA:O2	2.12	0.49
1:A:1445:TYR:CE1	1:A:1519:GLU:HA	2.47	0.49
1:B:2160:HIS:HE1	7:B:7101:HOH:O	1.96	0.49
1:C:3304:LEU:HG	1:C:3364:MET:HG2	1.93	0.49
1:A:1254:VAL:CG1	1:A:1255:LEU:N	2.76	0.49
1:C:3417:PHE:O	1:C:3420:LEU:HB3	2.13	0.49
1:A:1364:MET:CE	1:A:1388:LEU:HD11	2.42	0.49
1:B:2417:PHE:O	1:B:2420:LEU:HB3	2.12	0.49
1:A:1349:GLY:HA3	1:A:1447:TYR:CZ	2.48	0.49
1:C:3526:TYR:CE2	1:C:3539:LEU:HB2	2.47	0.49
1:B:2349:GLY:HA3	1:B:2447:TYR:CE1	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:LYS:HB3	1:A:1541:ASP:HB2	1.93	0.49
6:B:202:TCH:H26	7:B:7246:HOH:O	2.12	0.49
1:C:3257:LYS:HB2	1:C:3322:VAL:HG12	1.95	0.49
1:C:3343:THR:HB	1:C:3442:ALA:HB2	1.95	0.48
1:B:2353:GLN:O	1:B:2467:ASP:HA	2.13	0.48
1:B:2132:ARG:HD3	7:B:7131:HOH:O	2.14	0.48
1:B:2176:GLY:HA2	1:B:2189:TRP:HB2	1.95	0.48
1:A:1343:THR:HB	1:A:1442:ALA:HB2	1.95	0.48
1:A:1143:GLY:CA	6:A:102:TCH:H11A	2.40	0.48
1:A:1089:GLN:HB2	1:A:1146:VAL:HG12	1.94	0.48
1:B:2538:LYS:HB3	1:B:2541:ASP:HB2	1.96	0.48
1:A:1341:PHE:HZ	7:A:7015:HOH:O	1.97	0.48
1:A:1173:GLY:HA3	7:A:7079:HOH:O	2.12	0.48
1:B:2236:ALA:O	1:B:2237:LYS:C	2.50	0.48
1:B:2201:VAL:HG13	1:B:2205:ILE:HB	1.95	0.48
1:B:2508:ASN:HB3	7:B:7173:HOH:O	2.13	0.48
1:C:3176:GLY:HA2	1:C:3189:TRP:HB2	1.96	0.48
1:C:3369:SER:HB2	6:C:301:TCH:H18B	1.95	0.48
1:C:3355:PHE:CE1	1:C:3360:PRO:HG3	2.49	0.48
1:B:2221:SER:OG	6:B:202:TCH:H1A	2.14	0.48
1:A:1231:VAL:HG12	1:A:1231:VAL:O	2.14	0.48
1:C:3236:ALA:O	1:C:3237:LYS:C	2.51	0.48
1:C:3268:ILE:HD11	1:C:3319:LEU:HD13	1.96	0.48
1:B:2364:MET:HE1	1:B:2388:LEU:HD11	1.96	0.47
1:A:1257:LYS:HB2	1:A:1322:VAL:HG12	1.95	0.47
1:C:3445:TYR:CE1	1:C:3519:GLU:HA	2.49	0.47
1:A:1373:LEU:HD11	1:A:1377:THR:HG21	1.96	0.47
1:A:1086:MET:CE	1:A:1110:LEU:HD12	2.40	0.47
1:A:1447:TYR:C	1:A:1447:TYR:CD2	2.87	0.47
1:C:3538:LYS:HB3	1:C:3541:ASP:HB2	1.96	0.47
1:B:2373:LEU:HD11	1:B:2377:THR:HG21	1.96	0.47
1:B:2420:LEU:CD2	1:B:2547:TRP:HZ2	2.26	0.47
1:C:3290:THR:HA	5:C:185:SO4:O4	2.13	0.47
1:A:1176:GLY:HA2	1:A:1189:TRP:HB2	1.97	0.47
1:A:1478:ALA:HB3	1:A:1479:PRO:HD3	1.96	0.47
1:B:2039:SER:OG	1:B:2046:PRO:HB3	2.15	0.47
1:A:1146:VAL:CG2	6:A:102:TCH:H21	2.45	0.47
1:C:3231:VAL:HG12	1:C:3231:VAL:O	2.14	0.47
1:B:2227:VAL:O	1:B:2231:VAL:HG23	2.14	0.47
1:A:1319:LEU:O	1:A:1319:LEU:HG	2.14	0.47
1:B:2478:ALA:HB3	1:B:2479:PRO:HD3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:GLY:HA3	1:A:1146:VAL:O	2.15	0.47
1:C:3414:LYS:HD2	6:C:301:TCH:H19A	1.96	0.47
1:C:3495:MET:HE3	1:C:3533:THR:CB	2.45	0.47
1:C:3349:GLY:HA3	1:C:3447:TYR:CZ	2.50	0.47
1:C:3120:ASN:HB2	1:C:3167:THR:OG1	2.15	0.47
1:B:2120:ASN:HB2	1:B:2167:THR:OG1	2.15	0.47
1:B:2403:TYR:CE2	1:B:2420:LEU:HA	2.50	0.47
1:C:3142:GLY:HA3	1:C:3146:VAL:O	2.15	0.47
1:B:2526:TYR:CE2	1:B:2539:LEU:HB2	2.50	0.47
1:C:3373:LEU:HD11	1:C:3377:THR:HG21	1.95	0.46
1:A:1363:LEU:CD1	6:A:102:TCH:C16	2.94	0.46
1:A:1363:LEU:CD1	6:A:102:TCH:H16A	2.44	0.46
1:B:2422:ALA:HB1	7:B:7164:HOH:O	2.15	0.46
1:B:2304:LEU:HD13	6:B:202:TCH:O24	2.15	0.46
1:A:1262:LYS:HZ1	3:C:382:SIA:H111	1.79	0.46
1:B:2268:ILE:HD11	1:B:2319:LEU:HD13	1.97	0.46
1:A:1341:PHE:HB3	7:A:7043:HOH:O	2.15	0.46
1:C:3241:HIS:HD2	7:C:7221:HOH:O	1.98	0.46
1:C:3233:SER:HA	1:C:3234:PRO:HD3	1.85	0.46
1:C:3241:HIS:C	1:C:3242:ARG:HG3	2.35	0.46
1:B:2349:GLY:HA3	1:B:2447:TYR:CZ	2.50	0.46
1:B:2414:LYS:HZ1	6:B:201:TCH:H4A	1.80	0.45
1:B:2354:GLU:O	1:B:2359:ILE:HD12	2.16	0.45
1:C:3403:TYR:CE2	1:C:3420:LEU:HA	2.51	0.45
1:B:2264:LEU:HD22	1:B:2268:ILE:HG13	1.98	0.45
1:C:3319:LEU:HG	1:C:3319:LEU:O	2.16	0.45
1:C:3103:ASN:ND2	1:C:3476:PHE:HB3	2.32	0.45
1:C:3323:ILE:HG21	1:C:3330:LYS:HA	1.98	0.45
1:B:2064:ARG:HG2	1:B:2065:PHE:CD2	2.51	0.45
1:A:1241:HIS:C	1:A:1242:ARG:HG3	2.36	0.45
1:C:3232:LEU:HB3	1:C:3335:LEU:HD13	1.98	0.45
1:A:1190:GLY:O	1:A:1194:GLN:HG3	2.17	0.45
1:C:3304:LEU:CD2	6:C:302:TCH:H18B	2.47	0.45
1:B:2363:LEU:CA	6:B:202:TCH:H25	2.46	0.45
1:A:1526:TYR:CE2	1:A:1539:LEU:HB2	2.51	0.45
1:B:2385:SER:O	1:B:2389:VAL:HG22	2.17	0.45
1:B:2369:SER:HB2	6:B:201:TCH:H18B	1.99	0.45
1:C:3420:LEU:CD2	1:C:3547:TRP:HZ2	2.30	0.45
1:A:1266:GLU:O	1:A:1270:ILE:HG13	2.16	0.45
1:A:1402:LYS:HE3	7:A:7028:HOH:O	2.16	0.45
1:A:1495:MET:HE3	1:A:1533:THR:CB	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:LEU:HD22	1:A:1268:ILE:HG13	1.99	0.45
1:B:2359:ILE:HD13	6:B:202:TCH:O7	2.16	0.45
1:B:2217:ILE:CD1	1:B:2227:VAL:HG13	2.47	0.45
1:C:3366:TYR:HA	1:C:3367:PRO:HD3	1.80	0.45
1:A:1304:LEU:HD22	6:A:102:TCH:C23	2.46	0.45
1:B:2373:LEU:HD11	1:B:2377:THR:HG22	1.98	0.45
1:C:3447:TYR:C	1:C:3447:TYR:CD2	2.89	0.45
1:A:1064:ARG:HG2	1:A:1065:PHE:CD2	2.52	0.45
1:B:2304:LEU:CD1	6:B:202:TCH:C24	2.93	0.44
1:B:2420:LEU:HD22	1:B:2547:TRP:HZ2	1.82	0.44
1:A:1403:TYR:CE2	1:A:1420:LEU:HA	2.52	0.44
1:C:3264:LEU:HD22	1:C:3268:ILE:HG13	1.99	0.44
1:B:2359:ILE:CG2	6:B:202:TCH:H7	2.46	0.44
1:C:3373:LEU:HD11	1:C:3377:THR:HG22	1.98	0.44
1:A:1420:LEU:CD2	1:A:1547:TRP:HZ2	2.28	0.44
1:C:3199:ARG:HB3	1:C:3199:ARG:NH1	2.13	0.44
1:C:3399:ALA:HB2	1:C:3550:LEU:HD21	2.00	0.44
1:B:2551:PHE:C	1:B:2553:LYS:H	2.21	0.44
1:A:1078:LYS:HD3	7:A:7041:HOH:O	2.18	0.44
1:B:2359:ILE:HA	6:B:202:TCH:C15	2.46	0.44
2:A:179:NAG:H2	7:A:7086:HOH:O	2.17	0.44
1:B:2319:LEU:O	1:B:2319:LEU:HG	2.18	0.44
1:A:1232:LEU:HB3	1:A:1335:LEU:HD13	2.00	0.44
1:A:1318:LEU:HB2	7:A:7042:HOH:O	2.17	0.44
1:B:2142:GLY:HA3	1:B:2146:VAL:O	2.18	0.44
1:B:2495:MET:HE3	1:B:2533:THR:CG2	2.48	0.44
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.81	0.43
1:A:1330:LYS:HG3	1:A:1335:LEU:HG	2.00	0.43
1:C:3199:ARG:HD2	7:C:7186:HOH:O	2.19	0.43
1:B:2303:PHE:O	1:B:2317:PRO:O	2.36	0.43
1:C:3241:HIS:CD2	7:C:7221:HOH:O	2.71	0.43
1:C:3478:ALA:HB3	1:C:3479:PRO:HD3	1.99	0.43
1:B:2045:GLN:HG3	7:B:7081:HOH:O	2.18	0.43
1:B:2361:MET:HA	7:B:7062:HOH:O	2.18	0.43
1:A:1255:LEU:CD1	6:A:102:TCH:H2	2.45	0.43
1:C:3301:MET:CB	1:C:3303:PHE:CE2	3.02	0.43
1:A:1373:LEU:HD11	1:A:1377:THR:HG22	1.98	0.43
1:A:1420:LEU:HD22	1:A:1547:TRP:HZ2	1.83	0.43
1:A:1262:LYS:HZ3	3:C:382:SIA:H111	1.84	0.43
1:B:2323:ILE:HG21	1:B:2330:LYS:HA	2.01	0.43
1:B:2399:ALA:HB2	1:B:2550:LEU:HD21	2.01	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:ASN:ND2	1:A:1476:PHE:HB3	2.33	0.43
1:B:2358:LEU:O	1:B:2363:LEU:HG	2.19	0.43
1:B:2086:MET:CE	1:B:2110:LEU:HB2	2.46	0.43
1:B:2119:LEU:C	1:B:2119:LEU:HD12	2.39	0.43
1:A:1251:LEU:O	1:A:1253:SER:N	2.52	0.43
1:B:2040:LEU:HD11	7:B:7056:HOH:O	2.17	0.43
1:A:1385:SER:O	1:A:1389:VAL:HG22	2.18	0.43
1:B:2233:SER:HA	1:B:2234:PRO:HD3	1.85	0.43
1:B:2098:SER:O	1:B:2102:THR:HB	2.19	0.43
1:C:3098:SER:O	1:C:3102:THR:HB	2.19	0.43
1:B:2304:LEU:CD1	6:B:202:TCH:O24	2.67	0.43
1:B:2393:LYS:HA	1:B:2396:ILE:HG12	2.00	0.43
1:C:3495:MET:HE3	1:C:3533:THR:CG2	2.48	0.43
1:A:1495:MET:HE3	1:A:1533:THR:CG2	2.48	0.43
1:C:3304:LEU:CD2	6:C:302:TCH:C18	2.97	0.42
1:A:1201:VAL:HG13	1:A:1205:ILE:HB	2.00	0.42
1:C:3364:MET:O	1:C:3365:SER:HB2	2.19	0.42
1:A:1120:ASN:HB2	1:A:1167:THR:OG1	2.20	0.42
1:C:3304:LEU:HD12	1:C:3304:LEU:HA	1.53	0.42
1:C:3216:THR:HG23	1:C:3242:ARG:HB2	2.01	0.42
1:C:3107:ASN:HD22	1:C:3108:ILE:N	2.17	0.42
1:A:1217:ILE:CD1	1:A:1227:VAL:HG13	2.48	0.42
1:C:3301:MET:O	1:C:3302:LYS:HB2	2.18	0.42
1:A:1255:LEU:HG	6:A:102:TCH:H2A	2.02	0.42
1:A:1105:LYS:NZ	1:A:1106:GLU:HG2	2.34	0.42
1:B:2363:LEU:HD22	6:B:202:TCH:HN24	1.85	0.42
1:B:2409:ASP:HB3	1:B:2412:LYS:CG	2.49	0.42
1:A:1414:LYS:O	1:A:1418:LEU:HG	2.20	0.42
1:A:1086:MET:CE	1:A:1110:LEU:HB2	2.48	0.42
1:B:2251:LEU:O	1:B:2253:SER:N	2.53	0.42
1:C:3096:LEU:HD11	1:C:3100:LEU:HD11	2.02	0.42
1:A:1039:SER:OG	1:A:1046:PRO:HB3	2.19	0.42
1:A:1130:LYS:HD3	7:A:7252:HOH:O	2.19	0.42
1:A:1304:LEU:CD1	1:A:1364:MET:HG2	2.50	0.42
1:A:1355:PHE:HE2	1:A:1425:MET:HE1	1.83	0.42
1:C:3393:LYS:HA	1:C:3396:ILE:HG12	2.02	0.42
1:A:1399:ALA:HB2	1:A:1550:LEU:HD21	2.02	0.42
1:C:3139:ILE:HG12	1:C:3168:ILE:HD11	2.02	0.42
1:B:2125:ALA:HA	7:B:7151:HOH:O	2.18	0.42
1:C:3262:LYS:HE2	7:C:7023:HOH:O	2.19	0.42
1:B:2312:PRO:HG2	1:B:2383:TRP:NE1	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2359:ILE:HG13	1:B:2359:ILE:H	1.72	0.41
1:C:3420:LEU:HD22	1:C:3547:TRP:HZ2	1.85	0.41
1:C:3428:VAL:HG13	1:C:3544:VAL:HA	2.02	0.41
1:A:1149:ALA:HB1	1:A:1167:THR:HB	2.02	0.41
1:B:2426:PHE:CD1	1:B:2426:PHE:N	2.88	0.41
1:A:1058:PRO:HA	1:A:1059:PRO:HD2	1.93	0.41
1:B:2363:LEU:O	6:B:202:TCH:C26	2.68	0.41
1:B:2359:ILE:HB	1:B:2360:PRO:CD	2.44	0.41
1:C:3403:TYR:CD1	1:C:3420:LEU:HD23	2.56	0.41
1:A:1393:LYS:HA	1:A:1396:ILE:HG12	2.02	0.41
1:A:1098:SER:O	1:A:1102:THR:HB	2.20	0.41
1:B:2096:LEU:HD11	1:B:2100:LEU:HD11	2.02	0.41
1:A:1255:LEU:HD23	1:A:1318:LEU:HD11	2.02	0.41
1:C:3330:LYS:HG3	1:C:3335:LEU:HG	2.01	0.41
1:A:1551:PHE:C	1:A:1553:LYS:H	2.23	0.41
1:A:1409:ASP:HB3	1:A:1412:LYS:CG	2.49	0.41
1:B:2359:ILE:CG1	6:B:202:TCH:H15	2.25	0.41
1:A:1023:PRO:HA	1:A:1024:PRO:HD3	1.90	0.41
1:B:2253:SER:O	1:B:2254:VAL:C	2.59	0.41
1:B:2392:ALA:O	1:B:2396:ILE:HG12	2.20	0.41
1:C:3392:ALA:O	1:C:3396:ILE:HG12	2.21	0.41
1:C:3312:PRO:HG2	1:C:3383:TRP:NE1	2.35	0.41
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.83	0.41
1:B:2136:MET:HB3	1:B:2218:PHE:CE1	2.55	0.41
1:C:3144:LEU:HD12	1:C:3255:LEU:HD22	2.02	0.41
1:A:1146:VAL:CG2	6:A:102:TCH:C21	2.99	0.41
1:B:2359:ILE:CB	1:B:2360:PRO:HD3	2.46	0.41
1:A:1323:ILE:HG21	1:A:1330:LYS:HA	2.02	0.41
1:A:1136:MET:HB3	1:A:1218:PHE:CE1	2.55	0.41
1:C:3483:GLU:HB2	7:C:7046:HOH:O	2.19	0.41
1:C:3064:ARG:HG2	1:C:3065:PHE:CD2	2.55	0.41
1:A:1038:VAL:HG21	1:A:1049:ILE:HD12	2.03	0.41
1:B:2114:GLU:HG3	1:B:2291:GLU:OE2	2.21	0.41
1:C:3136:MET:HB3	1:C:3218:PHE:CE1	2.55	0.41
1:C:3058:PRO:HA	1:C:3059:PRO:HD2	1.95	0.41
1:B:2414:LYS:O	1:B:2418:LEU:HG	2.20	0.41
1:B:2023:PRO:CB	1:B:2034:LEU:HD21	2.47	0.41
1:B:2393:LYS:HA	1:B:2396:ILE:CG1	2.51	0.41
1:A:1264:LEU:HG	1:A:1316:GLN:HG2	2.02	0.41
1:C:3385:SER:O	1:C:3389:VAL:HG22	2.20	0.41
1:C:3114:GLU:HG3	1:C:3291:GLU:OE2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2426:PHE:C	1:B:2429:PRO:HD2	2.41	0.41
1:A:1242:ARG:HD3	1:A:1503:PHE:O	2.21	0.41
1:A:1392:ALA:O	1:A:1396:ILE:HG12	2.21	0.41
1:A:1262:LYS:NZ	3:C:382:SIA:C11	2.83	0.41
1:B:2231:VAL:O	1:B:2231:VAL:HG12	2.19	0.41
1:B:2330:LYS:HG3	1:B:2335:LEU:HG	2.03	0.41
1:B:2551:PHE:HD2	1:B:2551:PHE:HA	1.78	0.41
1:A:1052:GLY:O	3:A:182:SIA:H91	2.21	0.41
1:B:2221:SER:O	1:B:2224:GLY:N	2.53	0.41
1:C:3201:VAL:HG13	1:C:3205:ILE:HB	2.03	0.41
1:C:3205:ILE:HA	1:C:3205:ILE:HD12	1.94	0.41
1:C:3425:MET:HE1	6:C:302:TCH:H6	1.98	0.40
1:C:3368:LEU:HB2	7:C:7218:HOH:O	2.22	0.40
1:B:2099:GLU:O	1:B:2102:THR:HG22	2.21	0.40
3:A:182:SIA:H8	7:A:7041:HOH:O	2.21	0.40
1:B:2355:PHE:HE2	1:B:2425:MET:CE	2.34	0.40
3:B:282:SIA:C11	1:C:3262:LYS:NZ	2.69	0.40
1:C:3107:ASN:HD22	1:C:3108:ILE:H	1.69	0.40
1:A:1304:LEU:HD11	1:A:1364:MET:HG2	2.02	0.40
1:A:1107:ASN:HD22	1:A:1108:ILE:N	2.20	0.40
1:C:3217:ILE:CD1	1:C:3227:VAL:HG13	2.50	0.40
1:B:2231:VAL:O	1:B:2341:PHE:CE2	2.75	0.40
1:C:3301:MET:HB3	1:C:3303:PHE:CE2	2.56	0.40
1:C:3086:MET:HE2	1:C:3110:LEU:CB	2.42	0.40
1:C:3086:MET:HE2	1:C:3110:LEU:CD1	2.48	0.40
1:B:2252:THR:HG22	1:B:2254:VAL:HG12	2.02	0.40
1:A:1026:VAL:HG12	1:A:1027:ASP:N	2.37	0.40
1:A:1268:ILE:HD11	1:A:1319:LEU:HD13	2.04	0.40
1:B:2064:ARG:O	1:B:2065:PHE:HB2	2.21	0.40
1:C:3364:MET:CE	1:C:3388:LEU:HD11	2.51	0.40
1:A:1304:LEU:O	1:A:1364:MET:HE2	2.21	0.40
1:B:2242:ARG:HD3	1:B:2503:PHE:O	2.22	0.40
1:A:1086:MET:HE2	1:A:1110:LEU:CD1	2.47	0.40
1:A:1428:VAL:HG13	1:A:1544:VAL:HA	2.02	0.40
1:B:2428:VAL:HG13	1:B:2544:VAL:HA	2.04	0.40
1:B:2480:PHE:HZ	1:B:2494:LYS:HG3	1.86	0.40
1:B:2149:ALA:HB1	1:B:2167:THR:HB	2.03	0.40
1:A:1205:ILE:HA	1:A:1205:ILE:HD12	1.93	0.40
1:B:2409:ASP:HB3	1:B:2412:LYS:HG3	2.04	0.40
1:B:2239:LEU:HA	1:B:2239:LEU:HD23	1.93	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	530/542 (98%)	473 (89%)	54 (10%)	3 (1%)	30	75
1	B	530/542 (98%)	473 (89%)	53 (10%)	4 (1%)	24	69
1	C	530/542 (98%)	467 (88%)	60 (11%)	3 (1%)	30	75
All	All	1590/1626 (98%)	1413 (89%)	167 (10%)	10 (1%)	30	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3302	LYS
1	B	2185	SER
1	C	3185	SER
1	C	3304	LEU
1	A	1185	SER
1	B	2252	THR
1	B	2368	LEU
1	A	1252	THR
1	A	1368	LEU
1	B	2237	LYS

### 5.3.2 Protein sidechains [i](#)

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	448/457 (98%)	423 (94%)	25 (6%)	26	68
1	B	448/457 (98%)	426 (95%)	22 (5%)	31	72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	448/457 (98%)	425 (95%)	23 (5%)	29	70
All	All	1344/1371 (98%)	1274 (95%)	70 (5%)	29	69

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1027	ASP
1	A	1069	GLN
1	A	1104	ARG
1	A	1105	LYS
1	A	1106	GLU
1	A	1107	ASN
1	A	1132	ARG
1	A	1151	THR
1	A	1199	ARG
1	A	1218	PHE
1	A	1225	GLU
1	A	1242	ARG
1	A	1264	LEU
1	A	1303	PHE
1	A	1304	LEU
1	A	1338	GLU
1	A	1339	ARG
1	A	1355	PHE
1	A	1361	MET
1	A	1366	TYR
1	A	1381	LEU
1	A	1450	GLN
1	A	1500	TRP
1	A	1523	LYS
1	A	1551	PHE
1	B	2027	ASP
1	B	2069	GLN
1	B	2104	ARG
1	B	2105	LYS
1	B	2106	GLU
1	B	2107	ASN
1	B	2132	ARG
1	B	2151	THR
1	B	2199	ARG
1	B	2225	GLU
1	B	2242	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	2264	LEU
1	B	2304	LEU
1	B	2338	GLU
1	B	2339	ARG
1	B	2355	PHE
1	B	2366	TYR
1	B	2381	LEU
1	B	2450	GLN
1	B	2500	TRP
1	B	2523	LYS
1	B	2551	PHE
1	C	3027	ASP
1	C	3066	THR
1	C	3069	GLN
1	C	3104	ARG
1	C	3105	LYS
1	C	3106	GLU
1	C	3107	ASN
1	C	3132	ARG
1	C	3151	THR
1	C	3199	ARG
1	C	3218	PHE
1	C	3225	GLU
1	C	3242	ARG
1	C	3264	LEU
1	C	3338	GLU
1	C	3339	ARG
1	C	3355	PHE
1	C	3366	TYR
1	C	3381	LEU
1	C	3450	GLN
1	C	3500	TRP
1	C	3523	LYS
1	C	3551	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	C	3030	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 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	$\# Z  > 2$
6	TCH	A	101	-	37,38,38	2.62	17 (45%)	59,60,60	3.92	34 (57%)
6	TCH	A	102	-	37,38,38	2.94	17 (45%)	59,60,60	11.49	40 (67%)
2	NAG	A	179	1	14,14,15	0.60	0	15,19,21	0.77	1 (6%)
3	SIA	A	182	-	17,21,21	0.86	0	19,31,31	1.00	2 (10%)
5	SO4	A	184	-	4,4,4	0.22	0	6,6,6	0.14	0
5	SO4	A	284	-	4,4,4	0.44	0	6,6,6	0.21	0
6	TCH	B	201	-	37,38,38	2.69	19 (51%)	59,60,60	3.90	32 (54%)
6	TCH	B	202	-	37,38,38	2.98	15 (40%)	59,60,60	11.42	40 (67%)
2	NAG	B	279	1	14,14,15	0.84	1 (7%)	15,19,21	0.70	0
3	SIA	B	282	-	17,21,21	0.90	1 (5%)	19,31,31	1.02	0
5	SO4	B	285	-	4,4,4	0.40	0	6,6,6	0.16	0
5	SO4	B	385	-	4,4,4	0.39	0	6,6,6	0.28	0
5	SO4	C	185	-	4,4,4	0.43	0	6,6,6	0.17	0
6	TCH	C	301	-	37,38,38	2.70	17 (45%)	59,60,60	3.92	36 (61%)
6	TCH	C	302	-	37,38,38	3.31	18 (48%)	59,60,60	11.40	41 (69%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NDG	C	379	1	14,14,15	0.75	0	15,19,21	0.88	1 (6%)
3	SIA	C	382	-	17,21,21	0.99	1 (5%)	19,31,31	0.91	2 (10%)
5	SO4	C	384	-	4,4,4	0.37	0	6,6,6	0.21	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
6	TCH	A	101	-	4/4/13/14	2/16/81/81	0/4/4/4
6	TCH	A	102	-	4/4/13/14	0/16/81/81	0/4/4/4
2	NAG	A	179	1	-	0/6/23/26	0/1/1/1
3	SIA	A	182	-	-	0/14/38/38	0/1/1/1
5	SO4	A	184	-	-	0/0/0/0	0/0/0/0
5	SO4	A	284	-	-	0/0/0/0	0/0/0/0
6	TCH	B	201	-	4/4/13/14	2/16/81/81	0/4/4/4
6	TCH	B	202	-	4/4/13/14	0/16/81/81	0/4/4/4
2	NAG	B	279	1	-	0/6/23/26	0/1/1/1
3	SIA	B	282	-	-	0/14/38/38	0/1/1/1
5	SO4	B	285	-	-	0/0/0/0	0/0/0/0
5	SO4	B	385	-	-	0/0/0/0	0/0/0/0
5	SO4	C	185	-	-	0/0/0/0	0/0/0/0
6	TCH	C	301	-	4/4/13/14	1/16/81/81	0/4/4/4
6	TCH	C	302	-	4/4/13/14	0/16/81/81	0/4/4/4
4	NDG	C	379	1	-	0/6/23/26	0/1/1/1
3	SIA	C	382	-	-	1/14/38/38	0/1/1/1
5	SO4	C	384	-	-	0/0/0/0	0/0/0/0

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	202	TCH	O3S-S26	-7.04	1.28	1.46
6	C	302	TCH	O3S-S26	-6.74	1.29	1.46
6	A	102	TCH	O3S-S26	-6.70	1.29	1.46
6	B	202	TCH	C25-N24	-5.00	1.34	1.46
6	C	302	TCH	C6-C5	-4.74	1.45	1.53
6	A	102	TCH	C25-N24	-4.66	1.35	1.46
6	A	102	TCH	C6-C5	-4.49	1.46	1.53
6	B	202	TCH	C11-C9	-3.63	1.47	1.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	202	TCH	C6-C5	-3.60	1.47	1.53
6	A	101	TCH	C6-C5	-3.51	1.47	1.53
6	B	201	TCH	C6-C5	-3.06	1.48	1.53
6	A	102	TCH	C21-C20	-3.06	1.45	1.53
6	C	301	TCH	C6-C5	-3.03	1.48	1.53
6	A	101	TCH	C11-C9	-2.82	1.49	1.53
6	A	102	TCH	C11-C9	-2.63	1.49	1.53
6	C	301	TCH	C11-C9	-2.57	1.49	1.53
6	C	302	TCH	C11-C9	-2.51	1.49	1.53
6	C	302	TCH	C21-C20	-2.38	1.47	1.53
6	B	202	TCH	C21-C20	-2.37	1.47	1.53
6	B	201	TCH	C11-C9	-2.27	1.50	1.53
6	A	102	TCH	C13-C14	2.01	1.59	1.55
6	A	101	TCH	O2S-S26	2.01	1.51	1.45
6	B	201	TCH	C23-C24	2.07	1.55	1.51
6	B	201	TCH	C15-C14	2.09	1.59	1.54
6	C	301	TCH	C4-C3	2.10	1.55	1.51
6	A	101	TCH	C10-C9	2.10	1.60	1.56
6	C	301	TCH	C8-C14	2.11	1.58	1.53
6	B	202	TCH	C13-C14	2.12	1.59	1.55
3	B	282	SIA	C7-C6	2.13	1.55	1.52
6	B	201	TCH	O2S-S26	2.14	1.52	1.45
6	C	302	TCH	C4-C3	2.18	1.56	1.51
6	B	201	TCH	C8-C14	2.22	1.58	1.53
6	C	302	TCH	C8-C14	2.30	1.58	1.53
6	B	201	TCH	C4-C3	2.30	1.56	1.51
6	A	102	TCH	C13-C17	2.33	1.59	1.55
6	B	201	TCH	C22-C23	2.35	1.60	1.52
6	A	101	TCH	C23-C24	2.35	1.55	1.51
6	C	301	TCH	C22-C23	2.36	1.60	1.52
6	C	301	TCH	C22-C20	2.43	1.61	1.54
6	A	101	TCH	C4-C3	2.46	1.56	1.51
6	B	202	TCH	C13-C17	2.47	1.59	1.55
6	B	201	TCH	C10-C9	2.47	1.61	1.56
6	A	101	TCH	C22-C20	2.49	1.61	1.54
6	A	101	TCH	C22-C23	2.50	1.61	1.52
6	A	102	TCH	O1S-S26	2.53	1.53	1.45
6	C	301	TCH	O2S-S26	2.53	1.53	1.45
3	C	382	SIA	C3-C2	2.56	1.55	1.51
6	B	201	TCH	C22-C20	2.56	1.61	1.54
6	A	102	TCH	C24-N24	2.70	1.39	1.33
6	A	102	TCH	C22-C20	2.72	1.62	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	279	NAG	C1-C2	2.75	1.56	1.52
6	A	101	TCH	C13-C14	2.77	1.60	1.55
6	C	301	TCH	C10-C9	2.79	1.61	1.56
6	C	302	TCH	C13-C17	2.79	1.60	1.55
6	B	201	TCH	C13-C17	2.93	1.60	1.55
6	A	101	TCH	C13-C17	3.03	1.60	1.55
6	A	102	TCH	C8-C7	3.10	1.58	1.53
6	C	301	TCH	C13-C14	3.11	1.61	1.55
6	C	301	TCH	C13-C17	3.20	1.61	1.55
6	B	201	TCH	C13-C14	3.26	1.61	1.55
6	C	301	TCH	O24-C24	3.32	1.30	1.23
6	C	302	TCH	C8-C7	3.36	1.59	1.53
6	B	202	TCH	C20-C17	3.37	1.60	1.54
6	A	102	TCH	C8-C9	3.41	1.60	1.53
6	A	101	TCH	O24-C24	3.45	1.30	1.23
6	B	201	TCH	O24-C24	3.63	1.30	1.23
6	A	101	TCH	C8-C7	3.68	1.59	1.53
6	A	102	TCH	C13-C12	3.69	1.60	1.54
6	C	302	TCH	C22-C23	3.74	1.65	1.52
6	C	302	TCH	C8-C9	3.79	1.61	1.53
6	C	301	TCH	C8-C7	3.94	1.59	1.53
6	B	202	TCH	C8-C7	4.05	1.60	1.53
6	C	302	TCH	C13-C12	4.11	1.61	1.54
6	B	202	TCH	C23-C24	4.21	1.59	1.51
6	C	302	TCH	O1S-S26	4.29	1.58	1.45
6	B	201	TCH	C8-C7	4.29	1.60	1.53
6	C	302	TCH	C22-C20	4.29	1.66	1.54
6	A	102	TCH	C20-C17	4.30	1.62	1.54
6	B	202	TCH	C8-C9	4.38	1.62	1.53
6	C	302	TCH	C24-N24	4.38	1.43	1.33
6	A	101	TCH	C8-C9	4.48	1.62	1.53
6	C	301	TCH	C20-C17	4.51	1.62	1.54
6	A	102	TCH	C23-C24	4.59	1.60	1.51
6	B	201	TCH	C20-C17	4.61	1.63	1.54
6	B	202	TCH	C13-C12	4.83	1.62	1.54
6	A	101	TCH	C18-C13	4.85	1.62	1.54
6	C	302	TCH	O24-C24	4.87	1.33	1.23
6	A	101	TCH	C11-C12	4.91	1.62	1.53
6	C	301	TCH	C18-C13	4.92	1.62	1.54
6	B	202	TCH	C11-C12	4.94	1.62	1.53
6	C	302	TCH	C20-C17	4.94	1.63	1.54
6	A	101	TCH	C20-C17	4.96	1.63	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	201	TCH	C18-C13	5.04	1.62	1.54
6	B	201	TCH	C11-C12	5.14	1.62	1.53
6	B	201	TCH	C8-C9	5.19	1.64	1.53
6	C	301	TCH	C8-C9	5.22	1.64	1.53
6	C	302	TCH	C11-C12	5.46	1.63	1.53
6	B	202	TCH	O24-C24	5.66	1.35	1.23
6	B	202	TCH	C18-C13	5.68	1.63	1.54
6	A	102	TCH	C11-C12	5.69	1.63	1.53
6	C	301	TCH	C11-C12	5.72	1.63	1.53
6	A	101	TCH	C13-C12	6.13	1.64	1.54
6	C	301	TCH	C13-C12	6.36	1.64	1.54
6	B	201	TCH	C13-C12	6.40	1.64	1.54
6	A	102	TCH	O24-C24	7.19	1.38	1.23
6	C	302	TCH	C23-C24	9.53	1.69	1.51

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	302	TCH	O1S-S26-C26	-21.96	88.17	106.91
6	A	102	TCH	O1S-S26-C26	-21.26	88.76	106.91
6	B	202	TCH	O1S-S26-C26	-20.22	89.66	106.91
6	A	102	TCH	O3S-S26-O2S	-13.68	79.78	111.61
6	C	302	TCH	O3S-S26-O2S	-13.56	80.06	111.61
6	B	202	TCH	O3S-S26-O2S	-12.94	81.50	111.61
6	C	302	TCH	O24-C24-C23	-12.07	101.16	121.98
6	B	202	TCH	O24-C24-C23	-11.48	102.19	121.98
6	A	102	TCH	O24-C24-C23	-10.29	104.22	121.98
6	C	302	TCH	C9-C11-C12	-8.15	104.06	114.36
6	A	102	TCH	C9-C11-C12	-7.99	104.27	114.36
6	B	202	TCH	C9-C11-C12	-7.87	104.42	114.36
6	A	101	TCH	C9-C11-C12	-7.31	105.13	114.36
6	C	301	TCH	C17-C13-C14	-7.21	92.77	100.05
6	C	301	TCH	C9-C11-C12	-7.15	105.33	114.36
6	C	302	TCH	O24-C24-N24	-7.12	108.81	122.94
6	B	201	TCH	C9-C11-C12	-7.09	105.40	114.36
6	B	202	TCH	C17-C13-C14	-7.06	92.91	100.05
6	B	201	TCH	O24-C24-N24	-6.90	109.25	122.94
6	A	101	TCH	O24-C24-N24	-6.87	109.30	122.94
6	A	101	TCH	C17-C13-C14	-6.84	93.14	100.05
6	B	201	TCH	C17-C13-C14	-6.82	93.16	100.05
6	C	301	TCH	O24-C24-N24	-6.82	109.41	122.94
6	B	202	TCH	C4-C3-C2	-6.74	101.93	110.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	302	TCH	C4-C3-C2	-6.70	101.99	110.52
6	C	302	TCH	C25-N24-C24	-6.57	109.87	122.79
6	C	302	TCH	O2S-S26-O1S	-6.33	90.43	113.48
6	C	302	TCH	C17-C13-C14	-6.08	93.91	100.05
6	A	102	TCH	O2S-S26-O1S	-6.04	91.48	113.48
6	A	102	TCH	C17-C13-C14	-5.95	94.04	100.05
6	A	102	TCH	C5-C6-C7	-5.90	107.86	114.44
6	A	102	TCH	C4-C3-C2	-5.90	103.01	110.52
6	C	302	TCH	C5-C6-C7	-5.68	108.10	114.44
6	C	302	TCH	O3S-S26-O1S	-5.65	98.47	111.61
6	C	301	TCH	O24-C24-C23	-5.54	112.42	121.98
6	C	301	TCH	C4-C3-C2	-5.46	103.56	110.52
6	B	201	TCH	C4-C3-C2	-5.35	103.71	110.52
6	A	101	TCH	O24-C24-C23	-5.29	112.85	121.98
6	B	201	TCH	O24-C24-C23	-5.28	112.87	121.98
6	A	101	TCH	C5-C6-C7	-5.27	108.56	114.44
6	A	101	TCH	C4-C3-C2	-5.20	103.89	110.52
6	C	302	TCH	C18-C13-C14	-5.10	103.16	111.22
6	B	202	TCH	C5-C6-C7	-5.02	108.84	114.44
6	B	202	TCH	O2S-S26-O1S	-4.93	95.50	113.48
6	B	201	TCH	C5-C6-C7	-4.68	109.22	114.44
6	C	301	TCH	C5-C6-C7	-4.63	109.28	114.44
6	C	302	TCH	C13-C14-C8	-4.32	109.19	114.75
6	C	301	TCH	O1S-S26-C26	-4.25	103.28	106.91
6	C	302	TCH	O12-C12-C13	-4.20	104.31	111.11
6	B	202	TCH	C13-C14-C8	-4.11	109.45	114.75
6	B	202	TCH	O24-C24-N24	-4.03	114.93	122.94
6	B	201	TCH	C18-C13-C14	-4.01	104.89	111.22
6	A	102	TCH	C13-C14-C8	-4.01	109.58	114.75
6	C	302	TCH	C6-C5-C10	-3.95	108.30	112.66
6	A	101	TCH	C13-C14-C8	-3.94	109.67	114.75
6	C	301	TCH	C18-C13-C14	-3.89	105.08	111.22
6	C	301	TCH	C13-C14-C8	-3.87	109.75	114.75
6	A	102	TCH	O3S-S26-O1S	-3.84	102.67	111.61
6	B	201	TCH	C13-C14-C8	-3.81	109.83	114.75
6	A	101	TCH	C18-C13-C14	-3.81	105.21	111.22
6	B	202	TCH	C18-C13-C14	-3.76	105.29	111.22
6	A	102	TCH	C18-C13-C14	-3.62	105.51	111.22
6	A	102	TCH	O12-C12-C13	-3.55	105.35	111.11
6	B	202	TCH	C4-C5-C10	-3.43	108.87	112.66
6	C	302	TCH	C5-C4-C3	-3.43	107.81	112.91
6	A	102	TCH	C6-C5-C10	-3.39	108.92	112.66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	302	TCH	C19-C10-C9	-3.32	106.21	111.18
6	B	202	TCH	C25-N24-C24	-3.29	116.32	122.79
6	B	202	TCH	O12-C12-C13	-3.29	105.78	111.11
4	C	379	NDG	C2-N2-C7	-3.06	119.11	123.04
6	C	301	TCH	O12-C12-C13	-2.91	106.39	111.11
6	A	102	TCH	C19-C10-C9	-2.90	106.83	111.18
6	B	201	TCH	O12-C12-C13	-2.89	106.43	111.11
6	A	102	TCH	C16-C15-C14	-2.82	99.45	105.12
6	A	102	TCH	O24-C24-N24	-2.81	117.35	122.94
6	B	202	TCH	O3S-S26-O1S	-2.79	105.11	111.61
6	C	302	TCH	C16-C17-C20	-2.75	107.14	112.05
6	A	102	TCH	C21-C20-C17	-2.75	108.38	112.96
6	A	101	TCH	O12-C12-C13	-2.74	106.67	111.11
6	B	201	TCH	C6-C5-C10	-2.73	109.65	112.66
6	A	101	TCH	C6-C5-C10	-2.72	109.65	112.66
6	B	201	TCH	C16-C15-C14	-2.65	99.79	105.12
6	B	202	TCH	C6-C5-C10	-2.64	109.74	112.66
6	A	102	TCH	C25-N24-C24	-2.62	117.64	122.79
6	B	201	TCH	O1S-S26-C26	-2.57	104.72	106.91
6	C	301	TCH	C16-C15-C14	-2.54	100.01	105.12
6	B	202	TCH	C5-C4-C3	-2.53	109.15	112.91
6	C	301	TCH	C6-C5-C10	-2.51	109.89	112.66
3	C	382	SIA	C7-C6-C5	-2.51	110.52	114.32
6	A	101	TCH	C16-C15-C14	-2.50	100.09	105.12
6	A	102	TCH	C16-C17-C20	-2.41	107.76	112.05
6	A	101	TCH	C19-C10-C9	-2.37	107.63	111.18
6	B	201	TCH	C4-C5-C10	-2.33	110.08	112.66
6	C	301	TCH	C19-C10-C1	-2.32	104.29	108.20
6	C	302	TCH	C16-C15-C14	-2.29	100.51	105.12
6	B	202	TCH	C16-C17-C20	-2.29	107.97	112.05
6	A	102	TCH	C5-C4-C3	-2.26	109.55	112.91
2	A	179	NAG	C2-N2-C7	-2.26	120.14	123.04
6	B	202	TCH	C19-C10-C9	-2.26	107.80	111.18
3	A	182	SIA	C9-C8-C7	-2.24	107.22	112.48
6	A	101	TCH	C4-C5-C10	-2.23	110.20	112.66
6	C	301	TCH	C4-C5-C10	-2.21	110.22	112.66
6	A	101	TCH	O1S-S26-C26	-2.21	105.02	106.91
6	C	302	TCH	C21-C20-C17	-2.17	109.34	112.96
6	C	301	TCH	C21-C20-C17	-2.11	109.44	112.96
6	C	301	TCH	C5-C4-C3	-2.08	109.82	112.91
6	B	201	TCH	C19-C10-C1	-2.07	104.72	108.20
3	A	182	SIA	C7-C6-C5	-2.07	111.19	114.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	101	TCH	C5-C4-C3	-2.05	109.86	112.91
3	C	382	SIA	C9-C8-C7	-2.01	107.75	112.48
6	A	101	TCH	C16-C17-C13	2.02	105.61	103.60
6	C	301	TCH	O3-C3-C2	2.04	115.81	110.05
6	B	202	TCH	C22-C20-C17	2.05	114.54	110.24
6	C	301	TCH	C17-C13-C12	2.05	119.49	117.68
6	C	302	TCH	O7-C7-C6	2.06	115.11	110.06
6	A	101	TCH	O3-C3-C2	2.09	115.97	110.05
6	B	202	TCH	C19-C10-C5	2.14	114.03	110.25
6	B	202	TCH	C15-C16-C17	2.14	109.44	105.12
6	A	102	TCH	C14-C13-C12	2.16	109.32	107.39
6	B	202	TCH	C18-C13-C17	2.19	114.67	111.22
6	B	202	TCH	C6-C7-C8	2.20	113.80	111.47
6	C	301	TCH	C16-C17-C13	2.29	105.88	103.60
6	B	201	TCH	C6-C7-C8	2.31	113.92	111.47
6	B	202	TCH	O3-C3-C2	2.31	116.59	110.05
6	C	301	TCH	C6-C7-C8	2.32	113.93	111.47
6	B	201	TCH	C19-C10-C5	2.33	114.37	110.25
6	B	201	TCH	C16-C17-C13	2.34	105.93	103.60
6	A	101	TCH	C19-C10-C5	2.35	114.41	110.25
6	C	301	TCH	C15-C16-C17	2.49	110.14	105.12
6	A	102	TCH	C18-C13-C12	2.53	111.56	109.09
6	A	101	TCH	C15-C16-C17	2.58	110.33	105.12
6	C	301	TCH	C22-C20-C17	2.60	115.71	110.24
6	C	302	TCH	C15-C16-C17	2.62	110.40	105.12
6	A	101	TCH	C22-C20-C17	2.64	115.78	110.24
6	A	101	TCH	C6-C7-C8	2.64	114.27	111.47
6	B	201	TCH	C15-C16-C17	2.66	110.48	105.12
6	C	301	TCH	C19-C10-C5	2.67	114.97	110.25
6	B	201	TCH	C22-C20-C17	2.69	115.90	110.24
6	B	202	TCH	C16-C17-C13	2.70	106.29	103.60
6	A	102	TCH	C6-C7-C8	2.78	114.42	111.47
6	C	301	TCH	C14-C8-C7	2.83	115.66	111.74
6	C	302	TCH	C14-C8-C7	2.83	115.66	111.74
6	A	102	TCH	C19-C10-C5	2.83	115.25	110.25
6	C	302	TCH	C14-C13-C12	2.86	109.95	107.39
6	A	102	TCH	C17-C13-C12	2.87	120.23	117.68
6	A	102	TCH	C14-C8-C7	2.95	115.83	111.74
6	C	302	TCH	C19-C10-C5	2.96	115.48	110.25
6	B	202	TCH	C13-C17-C20	2.99	123.15	119.50
6	A	101	TCH	C14-C8-C7	3.04	115.96	111.74
6	A	102	TCH	C15-C16-C17	3.06	111.30	105.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	102	TCH	C13-C17-C20	3.19	123.39	119.50
6	A	102	TCH	C22-C20-C17	3.21	116.98	110.24
6	B	201	TCH	C14-C8-C7	3.34	116.38	111.74
6	B	202	TCH	C14-C8-C7	3.43	116.50	111.74
6	B	201	TCH	C13-C17-C20	3.47	123.72	119.50
6	A	101	TCH	C13-C17-C20	3.67	123.97	119.50
6	C	302	TCH	C22-C23-C24	3.67	121.99	113.27
6	C	301	TCH	C13-C17-C20	3.69	124.00	119.50
6	B	201	TCH	C23-C22-C20	3.76	121.28	114.48
6	C	302	TCH	C22-C20-C17	3.78	118.18	110.24
6	C	302	TCH	C17-C13-C12	3.87	121.11	117.68
6	C	301	TCH	C23-C22-C20	3.91	121.55	114.48
6	A	101	TCH	C23-C22-C20	3.95	121.62	114.48
6	A	102	TCH	C11-C12-C13	4.00	115.26	111.20
6	C	301	TCH	C26-C25-N24	4.12	123.93	111.27
6	B	201	TCH	C26-C25-N24	4.15	124.01	111.27
6	C	302	TCH	C18-C13-C12	4.18	113.17	109.09
6	A	101	TCH	C26-C25-N24	4.19	124.13	111.27
6	A	101	TCH	O3-C3-C4	4.24	118.30	109.86
6	C	301	TCH	C18-C13-C12	4.29	113.28	109.09
6	B	201	TCH	O3-C3-C4	4.30	118.41	109.86
6	C	301	TCH	O3-C3-C4	4.36	118.54	109.86
6	C	302	TCH	C13-C17-C20	4.40	124.86	119.50
6	B	202	TCH	C11-C12-C13	4.52	115.79	111.20
6	A	102	TCH	O3-C3-C4	4.52	118.85	109.86
6	A	101	TCH	C11-C12-C13	4.58	115.85	111.20
6	C	301	TCH	C11-C12-C13	4.61	115.88	111.20
6	B	202	TCH	O3-C3-C4	4.64	119.08	109.86
6	A	101	TCH	C18-C13-C12	4.68	113.65	109.09
6	B	202	TCH	C18-C13-C12	4.73	113.70	109.09
6	B	201	TCH	C11-C12-C13	4.85	116.12	111.20
6	B	201	TCH	C18-C13-C12	4.85	113.82	109.09
6	A	102	TCH	C6-C5-C4	4.98	116.61	111.05
6	A	101	TCH	C6-C5-C4	5.35	117.02	111.05
6	B	202	TCH	C6-C5-C4	5.35	117.02	111.05
6	B	201	TCH	O12-C12-C11	5.38	120.08	109.06
6	C	302	TCH	C15-C14-C13	5.39	108.96	103.60
6	A	101	TCH	O12-C12-C11	5.39	120.09	109.06
6	C	301	TCH	C6-C5-C4	5.39	117.07	111.05
6	C	302	TCH	C11-C12-C13	5.41	116.69	111.20
6	C	302	TCH	O3-C3-C4	5.45	120.70	109.86
6	B	201	TCH	C6-C5-C4	5.52	117.21	111.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	302	TCH	C23-C22-C20	5.55	124.51	114.48
6	C	301	TCH	O12-C12-C11	5.67	120.66	109.06
6	B	202	TCH	C23-C22-C20	5.71	124.81	114.48
6	B	202	TCH	O12-C12-C11	5.82	120.97	109.06
6	A	102	TCH	C23-C22-C20	5.84	125.05	114.48
6	C	302	TCH	C6-C5-C4	5.90	117.64	111.05
6	C	302	TCH	O12-C12-C11	5.99	121.33	109.06
6	B	202	TCH	C15-C14-C13	6.19	109.76	103.60
6	A	102	TCH	O12-C12-C11	6.29	121.94	109.06
6	A	102	TCH	C15-C14-C13	6.45	110.01	103.60
6	C	301	TCH	C15-C14-C13	6.56	110.12	103.60
6	A	101	TCH	C15-C14-C13	6.64	110.20	103.60
6	B	201	TCH	C15-C14-C13	6.73	110.30	103.60
6	C	302	TCH	C10-C9-C8	7.55	120.17	111.88
6	A	102	TCH	C10-C9-C8	7.72	120.35	111.88
6	B	201	TCH	C10-C9-C8	8.04	120.70	111.88
6	A	101	TCH	C10-C9-C8	8.09	120.76	111.88
6	B	202	TCH	C10-C9-C8	8.12	120.80	111.88
6	C	301	TCH	C10-C9-C8	8.23	120.91	111.88
6	C	302	TCH	C26-C25-N24	8.43	137.17	111.27
6	A	102	TCH	C23-C24-N24	8.52	131.27	116.46
6	A	102	TCH	C26-C25-N24	8.87	138.51	111.27
6	A	102	TCH	C11-C9-C8	9.68	124.49	110.73
6	C	302	TCH	C11-C9-C8	9.89	124.79	110.73
6	B	202	TCH	C23-C24-N24	9.95	133.74	116.46
6	C	301	TCH	C11-C9-C8	9.98	124.92	110.73
6	B	202	TCH	C11-C9-C8	10.07	125.04	110.73
6	B	202	TCH	C26-C25-N24	10.18	142.55	111.27
6	A	101	TCH	C11-C9-C8	10.20	125.24	110.73
6	B	201	TCH	C11-C9-C8	10.33	125.41	110.73
6	C	302	TCH	C23-C24-N24	11.23	135.97	116.46
6	C	301	TCH	O2S-S26-C26	11.66	116.85	106.91
6	B	201	TCH	O2S-S26-C26	11.72	116.91	106.91
6	A	101	TCH	O2S-S26-C26	12.21	117.32	106.91
6	C	302	TCH	O2S-S26-C26	75.58	171.39	106.91
6	B	202	TCH	O2S-S26-C26	77.57	173.09	106.91
6	A	102	TCH	O2S-S26-C26	78.41	173.81	106.91

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	302	TCH	C5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atom
6	C	302	TCH	C3
6	C	302	TCH	C20
6	C	302	TCH	C9
6	B	201	TCH	C5
6	B	201	TCH	C3
6	B	201	TCH	C20
6	B	201	TCH	C9
6	C	301	TCH	C5
6	C	301	TCH	C3
6	C	301	TCH	C20
6	C	301	TCH	C9
6	A	102	TCH	C5
6	A	102	TCH	C3
6	A	102	TCH	C20
6	A	102	TCH	C9
6	A	101	TCH	C5
6	A	101	TCH	C3
6	A	101	TCH	C20
6	A	101	TCH	C9
6	B	202	TCH	C5
6	B	202	TCH	C3
6	B	202	TCH	C20
6	B	202	TCH	C9

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	382	SIA	O10-C10-N5-C5
6	A	101	TCH	C23-C24-N24-C25
6	B	201	TCH	C23-C24-N24-C25
6	C	301	TCH	S26-C26-C25-N24
6	A	101	TCH	S26-C26-C25-N24
6	B	201	TCH	S26-C26-C25-N24

There are no ring outliers.

11 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	101	TCH	5	0
6	A	102	TCH	26	0
2	A	179	NAG	1	0
3	A	182	SIA	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	201	TCH	5	0
6	B	202	TCH	34	0
3	B	282	SIA	6	0
5	C	185	SO4	1	0
6	C	301	TCH	7	0
6	C	302	TCH	41	0
3	C	382	SIA	5	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](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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