



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:11 PM GMT

PDB ID : 3T6Z
Title : Crystal Structure of *Steccherinum ochraceum* Laccase obtained by multi-crystals composite data collection technique (60% dose)
Authors : Ferraroni, M.; Briganti, F.; Matera, I.; Kolomytseva, M.; Golovleva, L.; Scozzafava, A.; Chernykh, A.M.
Deposited on : 2011-07-29
Resolution : 2.15 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

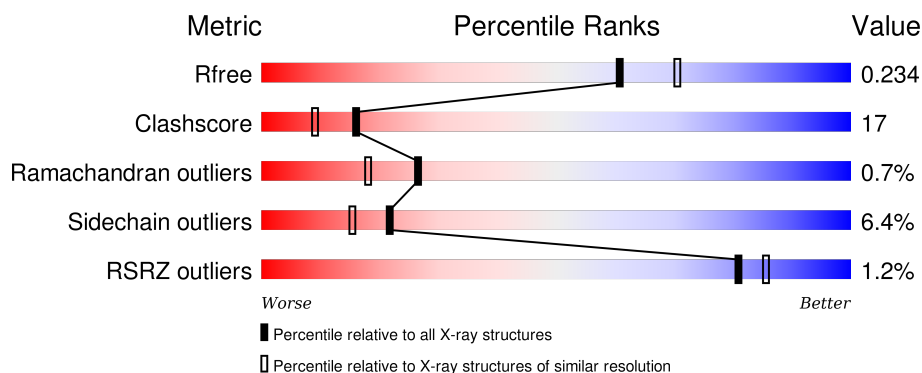
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	<div> <div>2%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	B	495	<div> <div>2%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	C	495	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	506	-	-	-	X
3	SO4	B	506	-	-	X	-
3	SO4	C	505	-	-	-	X
4	GOL	A	509	-	-	-	X
4	GOL	B	508	-	-	X	X
4	GOL	B	509	-	-	-	X
4	GOL	B	510	-	-	-	X
4	GOL	B	512	-	-	-	X
5	CBS	A	510	-	-	-	X
5	CBS	A	511	-	-	-	X
5	CBS	B	514	-	-	-	X
5	CBS	B	515	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12857 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 Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	5	0
			3736	2361	626	730	19			
1	B	495	Total	C	N	O	S	0	5	0
			3727	2356	628	725	18			
1	C	495	Total	C	N	O	S	0	4	0
			3733	2358	629	729	17			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Cu	0	0
			4	4		
2	A	4	Total	Cu	0	0
			4	4		
2	C	4	Total	Cu	0	0
			4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



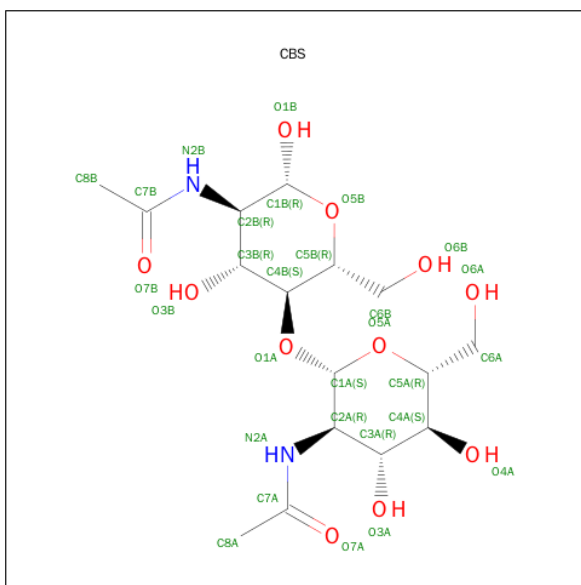
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SUGAR (DI(N-ACETYL-D-GLUCOSAMINE)) (three-letter code: CBS) (formula: C₁₆H₂₈N₂O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	16	2	10		
5	A	1	Total	C	N	O	0	0
			28	16	2	10		
5	B	1	Total	C	N	O	0	0
			28	16	2	10		
5	B	1	Total	C	N	O	0	0
			28	16	2	10		
5	C	1	Total	C	N	O	0	0
			28	16	2	10		

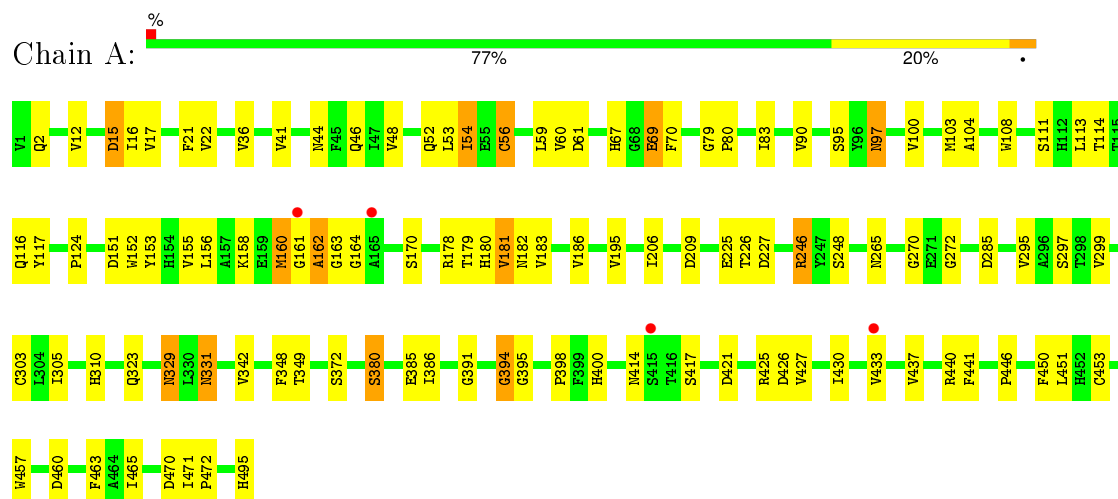
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	503	Total	O	0	0
			503	503		
6	B	453	Total	O	0	0
			453	453		
6	C	464	Total	O	0	0
			464	464		

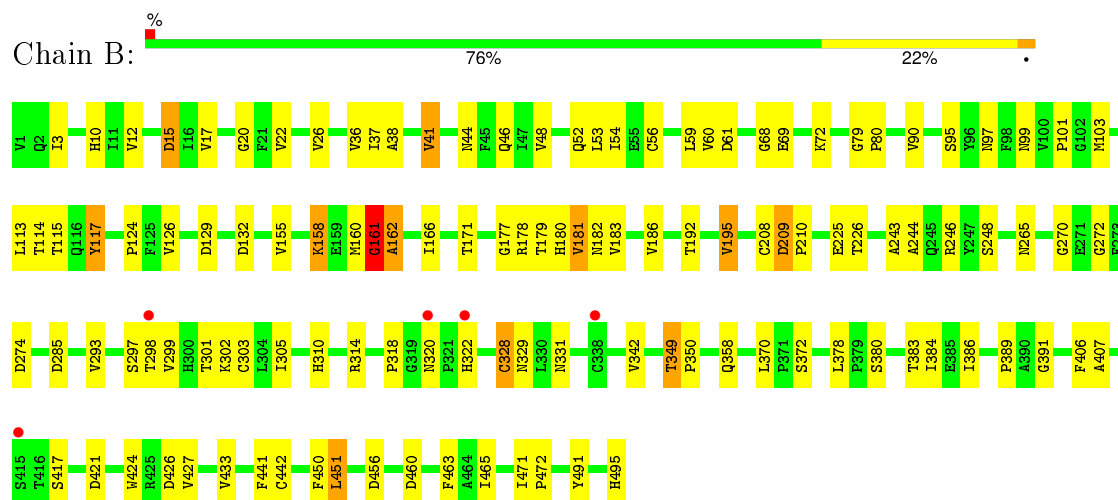
3 Residue-property plots

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

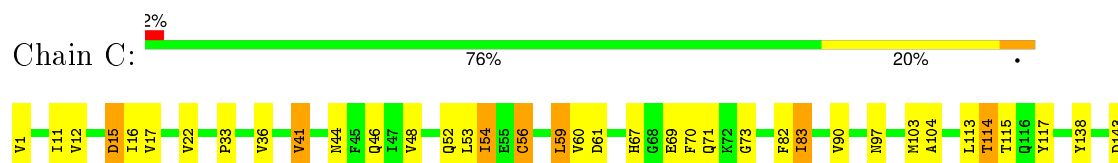
• Molecule 1: Laccase

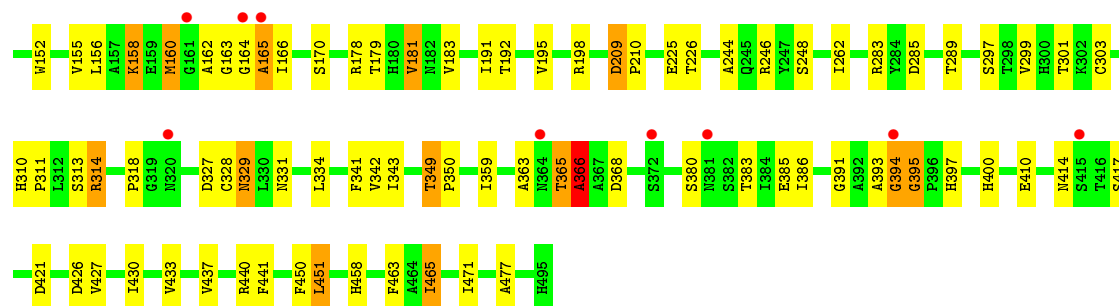


• Molecule 1: Laccase



• Molecule 1: Laccase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.51Å 140.04Å 172.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.15 19.80 – 2.15	Depositor EDS
% Data completeness (in resolution range)	90.5 (19.80-2.15) 90.6 (19.80-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.174 , 0.232 0.177 , 0.234	Depositor DCC
R_{free} test set	4418 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 88328 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12857	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.63	2/3859 (0.1%)	0.70	1/5299 (0.0%)
1	B	0.62	1/3850 (0.0%)	0.69	1/5287 (0.0%)
1	C	0.62	2/3855 (0.1%)	0.71	4/5294 (0.1%)
All	All	0.62	5/11564 (0.0%)	0.70	6/15880 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	CYS	CB-SG	-5.51	1.72	1.81
1	A	56[A]	CYS	CB-SG	-5.20	1.73	1.81
1	A	56[B]	CYS	CB-SG	-5.20	1.73	1.81
1	C	56[A]	CYS	CB-SG	-5.10	1.73	1.81
1	C	56[B]	CYS	CB-SG	-5.10	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	GLY	N-CA-C	-5.93	98.28	113.10
1	C	395	GLY	N-CA-C	-5.68	98.89	113.10
1	A	246	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	366	ALA	N-CA-C	-5.36	96.54	111.00
1	C	365	THR	N-CA-C	-5.27	96.76	111.00
1	C	394	GLY	N-CA-C	-5.14	100.24	113.10

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	3736	0	3510	116	0
1	B	3727	0	3498	124	0
1	C	3733	0	3510	124	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	6	0
3	C	5	0	0	0	0
4	A	12	0	16	3	0
4	B	36	0	48	15	0
4	C	6	0	8	1	0
5	A	56	0	52	5	0
5	B	56	0	52	11	0
5	C	28	0	26	2	0
6	A	503	0	0	40	0
6	B	453	0	0	32	0
6	C	464	0	0	33	0
All	All	12857	0	10720	374	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 17.

All (374) 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:A:414:ASN:ND2	5:A:510:CBS:C1B	1.68	1.53
1:C:414:ASN:HD21	5:C:507:CBS:C1B	1.18	1.50
1:C:365:THR:HB	1:C:366:ALA:CB	1.52	1.37
5:B:515:CBS:C8A	5:B:515:CBS:H1A	1.61	1.29
1:C:365:THR:CB	1:C:366:ALA:HB3	1.65	1.25
1:C:414:ASN:ND2	5:C:507:CBS:C1B	2.02	1.20
5:B:515:CBS:H83A	5:B:515:CBS:H1A	1.25	1.15
1:A:331:ASN:HB2	6:A:1088:HOH:O	1.41	1.15
1:A:161:GLY:HA2	1:A:162:ALA:CB	1.82	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HD11	1:C:114:THR:HG21	1.37	1.07
1:A:299:VAL:HB	6:A:997:HOH:O	1.56	1.05
1:A:161:GLY:HA2	1:A:162:ALA:HB3	1.40	1.04
1:C:329:ASN:ND2	1:C:329:ASN:H	1.56	1.04
5:B:515:CBS:C8A	5:B:515:CBS:C1A	2.30	1.03
1:C:365:THR:CB	1:C:366:ALA:CB	2.30	1.01
1:A:53:LEU:O	1:A:90:VAL:HG21	1.64	0.98
1:C:329:ASN:HD22	1:C:329:ASN:N	1.53	0.98
5:B:515:CBS:H82A	5:B:515:CBS:C1A	1.92	0.97
1:A:183:VAL:HG21	6:A:618:HOH:O	1.65	0.96
1:B:358:GLN:HE22	1:B:370:LEU:H	1.08	0.96
1:B:17:VAL:HG23	4:B:512:GOL:O2	1.67	0.95
1:B:265[A]:ASN:HD21	1:B:272:GLY:H	1.11	0.94
1:A:36:VAL:HG22	1:A:124:PRO:HG2	1.49	0.94
6:B:605:HOH:O	1:C:12:VAL:HG21	1.68	0.93
1:B:61:ASP:OD2	6:B:1033:HOH:O	1.88	0.90
1:A:60:VAL:HG23	6:A:661:HOH:O	1.72	0.89
1:B:161:GLY:N	1:B:162:ALA:HB2	1.87	0.89
1:B:303[A]:CYS:SG	6:B:707:HOH:O	2.30	0.89
1:B:72:LYS:H	4:B:508:GOL:H2	1.39	0.88
1:A:329:ASN:ND2	1:A:329:ASN:H	1.70	0.87
1:B:17:VAL:HG12	1:B:22:VAL:N	1.91	0.86
1:C:365:THR:HA	1:C:366:ALA:HB2	1.56	0.85
5:B:515:CBS:H82A	5:B:515:CBS:H1A	1.46	0.84
1:C:59:LEU:CD1	1:C:114:THR:HG21	2.06	0.84
1:C:365:THR:CA	1:C:366:ALA:CB	2.54	0.84
6:A:789:HOH:O	1:B:12:VAL:HG21	1.76	0.84
1:B:179:THR:O	1:B:183:VAL:HG22	1.78	0.84
1:C:365:THR:CA	1:C:366:ALA:HB2	2.07	0.84
4:B:513:GOL:C3	6:B:1053:HOH:O	2.24	0.83
1:B:36:VAL:HG22	1:B:124:PRO:HG2	1.59	0.83
1:A:44:ASN:ND2	1:A:46:GLN:HE21	1.76	0.83
1:A:310:HIS:HE1	6:A:843:HOH:O	1.61	0.83
1:A:70:PHE:H	1:A:103:MET:HE1	1.43	0.82
1:B:59:LEU:HD11	1:B:114:THR:HG21	1.61	0.82
1:A:17:VAL:HG12	1:A:22:VAL:N	1.95	0.80
1:C:48:VAL:HG23	6:C:684:HOH:O	1.81	0.80
1:B:161:GLY:N	1:B:162:ALA:CB	2.45	0.79
1:A:495:HIS:NE2	6:A:1090:HOH:O	2.16	0.79
1:B:53:LEU:O	1:B:90:VAL:HG21	1.82	0.79
1:A:60:VAL:HG21	6:A:971:HOH:O	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLY:HA2	1:C:165:ALA:HB3	1.62	0.79
1:A:17:VAL:HG22	3:B:506:SO4:O4	1.81	0.79
1:A:44:ASN:HD21	1:A:46:GLN:HE21	1.25	0.79
1:C:365:THR:O	1:C:368:ASP:HB2	1.82	0.79
1:C:179:THR:O	1:C:183:VAL:HG22	1.83	0.79
1:C:17:VAL:HG12	1:C:22:VAL:CA	2.13	0.79
1:C:53:LEU:O	1:C:90:VAL:HG21	1.83	0.79
1:A:17:VAL:HG12	1:A:22:VAL:CA	2.14	0.78
3:B:506:SO4:O2	1:C:17:VAL:HG22	1.83	0.78
1:A:161:GLY:CA	1:A:162:ALA:CB	2.62	0.78
1:A:59:LEU:HD11	1:A:114:THR:HG21	1.65	0.78
1:A:12:VAL:HG21	6:C:674:HOH:O	1.83	0.77
1:A:329:ASN:HD22	1:A:329:ASN:H	1.28	0.77
1:A:61:ASP:OD2	6:A:1090:HOH:O	2.01	0.77
1:B:17:VAL:HG23	4:B:512:GOL:HO2	1.48	0.76
1:A:17:VAL:HG23	4:A:508:GOL:O2	1.85	0.76
1:B:302:LYS:HD3	6:B:781:HOH:O	1.85	0.75
1:A:161:GLY:HA2	1:A:162:ALA:HB2	1.69	0.74
1:C:17:VAL:HG12	1:C:22:VAL:HA	1.69	0.74
1:A:12:VAL:HG22	6:A:811:HOH:O	1.86	0.74
1:A:195:VAL:HG23	6:A:675:HOH:O	1.87	0.74
1:A:329:ASN:N	1:A:329:ASN:HD22	1.84	0.74
1:B:342:VAL:HG23	6:B:754:HOH:O	1.87	0.73
1:C:451:LEU:HD12	1:C:465:ILE:HD11	1.69	0.73
1:B:195:VAL:HG11	6:B:987:HOH:O	1.87	0.73
1:A:195:VAL:HG22	6:A:960:HOH:O	1.86	0.73
1:C:209:ASP:HB3	1:C:210:PRO:CD	2.19	0.73
1:B:56[A]:CYS:SG	1:C:52:GLN:NE2	2.62	0.73
1:C:365:THR:HB	1:C:366:ALA:HB3	0.78	0.73
5:B:515:CBS:H82A	5:B:515:CBS:O1A	1.89	0.72
1:C:12:VAL:HG22	6:C:663:HOH:O	1.89	0.72
1:A:17:VAL:HG12	1:A:22:VAL:HA	1.70	0.72
1:A:90:VAL:HG22	6:A:784:HOH:O	1.88	0.72
1:A:59:LEU:CD1	1:A:114:THR:HG21	2.19	0.72
1:C:183:VAL:HG21	6:C:632:HOH:O	1.89	0.72
1:A:179:THR:O	1:A:183:VAL:HG22	1.91	0.71
1:A:470:ASP:OD2	6:A:1085:HOH:O	2.09	0.71
1:C:17:VAL:HG12	1:C:22:VAL:N	2.06	0.70
1:B:314:ARG:NH2	6:B:1034:HOH:O	2.24	0.70
1:C:155:VAL:HG23	6:C:873:HOH:O	1.91	0.70
1:C:365:THR:CB	1:C:366:ALA:HB2	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLN:NE2	1:B:370:LEU:H	1.86	0.69
1:A:53:LEU:O	1:A:90:VAL:CG2	2.39	0.69
1:C:359:ILE:HA	1:C:363:ALA:HB3	1.74	0.69
1:C:209:ASP:HB3	1:C:210:PRO:HD3	1.74	0.69
1:B:3:ILE:O	1:B:37:ILE:HA	1.93	0.68
1:C:17:VAL:CG1	1:C:22:VAL:HB	2.24	0.68
1:C:59:LEU:CD1	1:C:114:THR:CG2	2.71	0.68
1:B:101:PRO:HD2	4:B:508:GOL:H11	1.75	0.68
1:A:70:PHE:H	1:A:103:MET:CE	2.07	0.68
1:A:41:VAL:CG2	1:A:104:ALA:HB2	2.22	0.68
1:C:44:ASN:ND2	1:C:46:GLN:HE21	1.92	0.68
1:C:164:GLY:N	6:C:1049:HOH:O	2.28	0.67
1:B:17:VAL:HG22	3:B:506:SO4:O3	1.94	0.67
1:B:183:VAL:HG21	6:B:773:HOH:O	1.93	0.67
1:C:61:ASP:OD2	6:C:1048:HOH:O	2.12	0.66
4:B:508:GOL:H31	6:B:677:HOH:O	1.95	0.66
1:A:52:GLN:NE2	1:C:56[A]:CYS:SG	2.68	0.66
1:A:48:VAL:HG23	6:A:753:HOH:O	1.96	0.65
1:A:391:GLY:HA2	1:A:433:VAL:HG22	1.77	0.65
1:B:161:GLY:CA	1:B:162:ALA:HB2	2.25	0.65
1:A:265:ASN:ND2	6:A:771:HOH:O	2.29	0.65
1:C:160:MET:HE1	6:C:792:HOH:O	1.96	0.65
1:A:162:ALA:H	1:A:164:GLY:HA3	1.62	0.64
1:C:90:VAL:HG22	6:C:609:HOH:O	1.97	0.64
1:B:60:VAL:HG23	6:B:721:HOH:O	1.97	0.64
1:A:310:HIS:HD2	1:A:421:ASP:O	1.80	0.64
1:B:358:GLN:HE22	1:B:370:LEU:N	1.89	0.64
1:A:56[A]:CYS:SG	1:B:52:GLN:NE2	2.70	0.64
1:C:103:MET:CE	6:C:705:HOH:O	2.46	0.64
1:C:164:GLY:CA	1:C:165:ALA:HB3	2.26	0.64
1:B:451:LEU:HD12	1:B:465:ILE:HD11	1.78	0.63
1:A:182:ASN:ND2	1:B:192:THR:H	1.95	0.63
1:C:426:ASP:OD1	1:C:427:VAL:HG23	1.98	0.63
1:B:17:VAL:HG12	1:B:22:VAL:CA	2.28	0.63
1:A:182:ASN:HD21	1:B:192:THR:H	1.46	0.62
1:C:365:THR:HB	1:C:366:ALA:HB2	1.71	0.62
1:C:433:VAL:HG23	6:C:953:HOH:O	1.99	0.61
1:B:68:GLY:O	1:B:103:MET:HE1	2.00	0.61
1:B:72:LYS:H	4:B:508:GOL:C2	2.12	0.61
1:B:12:VAL:HG22	6:B:648:HOH:O	1.99	0.61
1:A:430:ILE:HA	1:A:437:VAL:HG21	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PRO:HB2	1:B:383:THR:HG23	1.82	0.61
1:C:310:HIS:HD2	1:C:421:ASP:O	1.84	0.61
1:B:378:LEU:HD22	1:B:384:ILE:HD12	1.82	0.61
1:B:59:LEU:HD21	1:B:158[B]:LYS:HE3	1.84	0.60
1:C:41:VAL:CG1	1:C:103:MET:O	2.49	0.60
1:A:17:VAL:CG2	3:B:506:SO4:O4	2.49	0.60
1:B:36:VAL:HG22	1:B:124:PRO:CG	2.32	0.60
1:C:103:MET:HE3	6:C:705:HOH:O	2.01	0.60
1:C:164:GLY:O	6:C:1013:HOH:O	2.17	0.59
1:A:451:LEU:HD23	1:A:465:ILE:HD11	1.84	0.59
1:A:158[B]:LYS:HE2	6:A:1010:HOH:O	2.01	0.59
1:C:162:ALA:HB3	6:C:859:HOH:O	2.02	0.59
1:B:46:GLN:HA	1:B:97:ASN:HD22	1.67	0.59
4:B:511:GOL:H11	6:B:808:HOH:O	2.03	0.59
1:B:59:LEU:CD1	1:B:114:THR:HG21	2.31	0.59
1:C:343:ILE:HG21	1:C:465:ILE:HG12	1.85	0.59
1:B:391:GLY:HA2	1:B:433:VAL:HG22	1.85	0.59
1:A:17:VAL:CG1	1:A:22:VAL:HA	2.32	0.59
1:A:69:GLU:HA	1:A:103:MET:HE1	1.84	0.58
1:B:17:VAL:CG2	3:B:506:SO4:O3	2.51	0.58
1:B:162:ALA:HB1	6:B:832:HOH:O	2.04	0.58
1:C:314:ARG:HH11	1:C:314:ARG:CG	2.16	0.58
1:A:97:ASN:HB2	6:A:683:HOH:O	2.02	0.58
1:B:155:VAL:HG21	6:C:866:HOH:O	2.04	0.57
1:A:414:ASN:CG	5:A:510:CBS:C1B	2.63	0.57
1:C:17:VAL:CG1	1:C:22:VAL:HA	2.35	0.57
1:B:114:THR:HG23	1:B:115:THR:N	2.19	0.57
1:C:225:GLU:HB3	1:C:248:SER:HB2	1.86	0.57
1:C:17:VAL:HG23	6:C:648:HOH:O	2.04	0.57
1:C:391:GLY:HA2	1:C:433:VAL:HG22	1.87	0.57
1:B:41:VAL:HG13	1:B:103:MET:O	2.03	0.57
1:A:113:LEU:HG	1:A:114:THR:HG22	1.87	0.56
1:B:114:THR:H	4:B:510:GOL:C3	2.19	0.56
4:A:509:GOL:H31	6:A:1103:HOH:O	2.05	0.56
1:C:329:ASN:HD22	1:C:329:ASN:H	0.74	0.56
1:B:114:THR:HG23	1:B:115:THR:H	1.71	0.56
1:A:170:SER:HB3	1:A:179:THR:HA	1.87	0.56
1:B:331:ASN:ND2	5:B:515:CBS:H3B	2.21	0.56
1:C:17:VAL:CG1	1:C:22:VAL:CA	2.84	0.56
1:B:161:GLY:H	1:B:162:ALA:CB	2.18	0.55
1:A:17:VAL:CG1	1:A:22:VAL:CA	2.84	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LEU:HG	1:C:114:THR:HG22	1.87	0.55
1:B:386:ILE:HD13	1:B:441:PHE:HE1	1.72	0.55
1:B:60:VAL:HG21	6:B:839:HOH:O	2.05	0.54
1:B:44:ASN:ND2	1:B:46:GLN:HE21	2.05	0.54
1:C:60:VAL:HG23	6:C:613:HOH:O	2.06	0.54
1:B:3:ILE:O	1:B:38:ALA:N	2.38	0.54
1:A:295:VAL:HG23	6:A:948:HOH:O	2.07	0.54
1:B:182:ASN:HD21	1:C:192:THR:H	1.54	0.54
1:C:334:LEU:HB2	6:C:916:HOH:O	2.07	0.54
1:B:195:VAL:CG1	6:B:987:HOH:O	2.52	0.53
1:C:70:PHE:H	1:C:103:MET:CE	2.20	0.53
1:A:95:SER:HB3	6:A:683:HOH:O	2.09	0.53
1:C:179:THR:HG22	6:C:618:HOH:O	2.09	0.52
1:A:41:VAL:HG22	1:A:104:ALA:HB2	1.90	0.52
1:C:70:PHE:H	1:C:103:MET:HE1	1.75	0.52
1:A:161:GLY:CA	1:A:162:ALA:HB2	2.32	0.52
1:B:114:THR:H	4:B:510:GOL:H31	1.73	0.52
1:B:155:VAL:HG23	6:B:770:HOH:O	2.09	0.52
1:B:310:HIS:HD2	1:B:421:ASP:O	1.91	0.52
1:B:22:VAL:CG2	6:C:640:HOH:O	2.57	0.52
1:A:181:VAL:CG1	6:A:762:HOH:O	2.57	0.52
1:B:426:ASP:OD1	1:B:427:VAL:HG23	2.09	0.52
5:B:515:CBS:H61B	6:B:607:HOH:O	2.10	0.51
1:A:386:ILE:CD1	1:A:441:PHE:HE1	2.23	0.51
1:B:158[B]:LYS:HE2	6:B:828:HOH:O	2.09	0.51
1:A:386:ILE:HD12	1:A:441:PHE:HE1	1.75	0.51
1:A:398:PRO:HD2	1:A:453:CYS:SG	2.50	0.51
1:A:15:ASP:OD2	1:A:22:VAL:HG22	2.10	0.51
1:A:299:VAL:HG12	6:A:1066:HOH:O	2.10	0.51
1:A:195:VAL:HG21	6:A:1060:HOH:O	2.09	0.51
1:C:36:VAL:HG21	1:C:143:ASP:OD2	2.09	0.51
1:A:426:ASP:OD1	1:A:427:VAL:HG23	2.10	0.51
1:B:15:ASP:OD2	1:B:22:VAL:HG22	2.11	0.51
1:A:400:HIS:HB2	1:A:427:VAL:HG22	1.92	0.51
1:B:179:THR:HG22	6:B:642:HOH:O	2.10	0.51
4:B:513:GOL:H31	6:B:1053:HOH:O	2.02	0.50
1:A:265:ASN:HD21	1:A:272:GLY:H	1.59	0.50
1:B:129:ASP:HB3	1:B:132:ASP:HB2	1.92	0.50
1:B:265[A]:ASN:HD21	1:B:272:GLY:N	1.94	0.50
1:C:162:ALA:HB2	1:C:166:ILE:HD11	1.93	0.50
4:B:508:GOL:C3	6:B:677:HOH:O	2.57	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:VAL:HG12	1:C:103:MET:O	2.12	0.50
1:A:155:VAL:HG13	6:A:696:HOH:O	2.12	0.50
1:C:318:PRO:HB2	1:C:383:THR:HG23	1.93	0.50
1:C:342:VAL:HG23	6:C:612:HOH:O	2.10	0.50
1:A:2:GLN:NE2	6:A:1058:HOH:O	2.44	0.50
5:A:511:CBS:C8A	6:A:1070:HOH:O	2.59	0.50
1:A:16:ILE:HD11	1:A:152:TRP:CH2	2.47	0.50
1:B:274:ASP:HB3	6:B:990:HOH:O	2.11	0.50
1:C:17:VAL:CG1	1:C:22:VAL:CB	2.90	0.49
1:B:180:HIS:O	4:B:509:GOL:H2	2.12	0.49
1:B:22:VAL:HG23	6:C:640:HOH:O	2.13	0.49
1:C:41:VAL:HG13	1:C:103:MET:O	2.13	0.49
1:B:491:TYR:CE1	1:B:495:HIS:CE1	3.01	0.49
1:B:95:SER:HB3	6:B:675:HOH:O	2.12	0.49
1:B:17:VAL:CG1	1:B:22:VAL:CA	2.91	0.49
1:A:70:PHE:N	1:A:103:MET:HE1	2.19	0.49
1:A:41:VAL:HG21	1:A:104:ALA:HB2	1.95	0.48
1:C:170:SER:HB2	1:C:178:ARG:O	2.13	0.48
1:C:301:THR:HG21	6:C:835:HOH:O	2.13	0.48
1:B:225:GLU:HB3	1:B:248:SER:HB2	1.94	0.48
1:C:60:VAL:HG21	6:C:1046:HOH:O	2.13	0.48
1:C:16:ILE:HD11	1:C:152:TRP:CH2	2.49	0.48
1:B:305:ILE:HD13	6:B:791:HOH:O	2.12	0.48
1:C:114:THR:OG1	1:C:115:THR:N	2.46	0.48
1:A:160:MET:O	1:A:162:ALA:HB2	2.13	0.48
1:C:327:ASP:HA	6:C:610:HOH:O	2.14	0.47
1:B:265[A]:ASN:ND2	1:B:272:GLY:H	1.94	0.47
1:C:400:HIS:HB2	1:C:427:VAL:HG22	1.97	0.47
1:B:320:ASN:HB3	1:B:322:HIS:CE1	2.49	0.47
1:C:301:THR:HB	6:C:760:HOH:O	2.14	0.47
1:A:108:TRP:CE3	1:A:206:ILE:HG22	2.49	0.47
1:B:243:ALA:O	1:B:244:ALA:HB3	2.14	0.47
1:B:331:ASN:HD22	5:B:515:CBS:H3B	1.79	0.47
1:B:59:LEU:HD21	1:B:158[B]:LYS:CE	2.44	0.47
1:A:181:VAL:HG13	6:A:762:HOH:O	2.15	0.47
1:A:181:VAL:HG13	6:A:884:HOH:O	2.14	0.47
1:B:178:ARG:HG2	1:B:186:VAL:HG22	1.97	0.47
1:B:48:VAL:HG23	6:B:620:HOH:O	2.15	0.47
1:C:341:PHE:HE1	1:C:393:ALA:O	1.98	0.47
1:C:410:GLU:O	1:C:437:VAL:HA	2.15	0.47
1:B:17:VAL:CG1	1:B:22:VAL:HA	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:HG12	1:B:22:VAL:HA	1.98	0.46
1:B:155:VAL:HG22	1:C:1:VAL:HG13	1.96	0.46
1:B:329:ASN:OD1	1:B:329:ASN:N	2.47	0.46
1:A:100:VAL:HG23	1:A:100:VAL:O	2.14	0.46
1:A:385:GLU:HG3	1:A:440:ARG:HG2	1.98	0.46
1:A:163:GLY:HA3	6:A:738:HOH:O	2.15	0.46
1:C:289:THR:HB	6:C:1052:HOH:O	2.15	0.46
3:B:506:SO4:O2	1:C:17:VAL:CG2	2.60	0.46
1:B:171:THR:O	1:B:177:GLY:HA3	2.16	0.46
1:A:79:GLY:N	1:A:80:PRO:HD2	2.30	0.46
1:C:310:HIS:CD2	1:C:421:ASP:O	2.67	0.46
1:B:181:VAL:HA	4:B:509:GOL:H2	1.97	0.46
1:B:38:ALA:HA	1:B:126:VAL:O	2.16	0.46
1:B:386:ILE:CD1	1:B:441:PHE:HE1	2.28	0.46
1:B:293:VAL:HG23	6:B:834:HOH:O	2.15	0.46
1:B:471:ILE:N	1:B:472:PRO:HD2	2.31	0.45
4:A:509:GOL:C3	6:A:1103:HOH:O	2.64	0.45
1:A:162:ALA:HB3	6:A:1025:HOH:O	2.16	0.45
1:C:329:ASN:ND2	1:C:329:ASN:N	2.27	0.45
1:C:54:ILE:HD13	6:C:628:HOH:O	2.17	0.45
1:A:178:ARG:HG2	1:A:186:VAL:HG22	1.99	0.45
1:A:17:VAL:CG1	1:A:22:VAL:HB	2.47	0.45
1:A:59:LEU:HD12	1:A:114:THR:HG21	1.98	0.45
1:C:181:VAL:HG13	6:C:664:HOH:O	2.17	0.45
1:A:162:ALA:H	1:A:163:GLY:HA2	1.82	0.45
1:B:386:ILE:CD1	1:B:441:PHE:CE1	3.00	0.45
1:C:209:ASP:CB	1:C:210:PRO:CD	2.90	0.45
1:C:385:GLU:HB2	1:C:440:ARG:HG2	1.99	0.45
1:C:451:LEU:HB3	1:C:465:ILE:HD12	1.99	0.44
1:B:181:VAL:HG13	6:B:829:HOH:O	2.18	0.44
1:C:103:MET:HE2	6:C:705:HOH:O	2.14	0.44
1:B:161:GLY:H	1:B:162:ALA:HB3	1.83	0.44
1:C:33:PRO:HB2	6:C:805:HOH:O	2.18	0.44
1:A:67:HIS:C	1:A:67:HIS:CD2	2.90	0.44
1:B:209:ASP:HB3	1:B:210:PRO:CD	2.47	0.44
1:C:163:GLY:HA2	1:C:164:GLY:HA3	1.76	0.44
1:B:389:PRO:HG3	5:B:515:CBS:H82B	2.00	0.44
1:A:111:SER:OG	1:A:116:GLN:HB3	2.18	0.44
1:B:79:GLY:N	1:B:80:PRO:HD2	2.32	0.44
1:A:446:PRO:HB3	1:A:470:ASP:HB3	2.00	0.44
1:C:394:GLY:O	1:C:458:HIS:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLY:HA2	1:C:477:ALA:O	2.18	0.43
1:B:113:LEU:O	1:B:114:THR:HG22	2.18	0.43
1:A:451:LEU:HB3	1:A:465:ILE:HD12	2.00	0.43
1:A:56[A]:CYS:SG	1:B:10:HIS:CD2	3.12	0.43
1:C:179:THR:HG23	1:C:183:VAL:HA	2.00	0.43
1:A:471:ILE:HB	1:A:472:PRO:HD3	2.01	0.43
1:C:191:ILE:HD12	1:C:262:ILE:HD13	1.99	0.43
1:A:160:MET:HG3	1:A:457:TRP:CH2	2.53	0.43
1:C:15:ASP:OD2	1:C:22:VAL:HG22	2.18	0.43
1:B:299:VAL:HG12	6:B:978:HOH:O	2.17	0.43
5:B:515:CBS:HO3B	5:B:515:CBS:C1A	2.32	0.43
1:A:36:VAL:CG2	1:A:124:PRO:HG2	2.34	0.43
1:C:183:VAL:HG23	4:C:506:GOL:O1	2.18	0.43
1:B:161:GLY:HA3	1:B:166:ILE:HD11	2.01	0.43
1:A:295:VAL:CG2	6:A:948:HOH:O	2.64	0.43
1:C:430:ILE:HA	1:C:437:VAL:HG21	2.01	0.43
1:C:341:PHE:CE1	1:C:393:ALA:O	2.73	0.42
1:C:394:GLY:HA2	1:C:395:GLY:HA3	1.77	0.42
1:C:386:ILE:HD13	1:C:441:PHE:HE1	1.83	0.42
5:A:511:CBS:H81A	6:A:1070:HOH:O	2.18	0.42
1:C:82:PHE:C	1:C:83:ILE:HD13	2.39	0.42
1:A:97:ASN:C	1:A:97:ASN:HD22	2.22	0.42
1:A:342:VAL:HG23	6:A:657:HOH:O	2.17	0.42
1:C:311:PRO:HB2	1:C:313:SER:O	2.19	0.42
1:A:17:VAL:HG12	1:A:21:PHE:C	2.37	0.42
1:A:225:GLU:HB3	1:A:248:SER:HB2	1.99	0.42
1:C:15:ASP:HB3	1:C:22:VAL:CG2	2.49	0.42
1:C:11:ILE:HG22	1:C:53:LEU:HD21	2.00	0.42
1:B:117:TYR:CE1	1:B:208:CYS:SG	3.12	0.42
1:C:83:ILE:N	1:C:83:ILE:HD13	2.34	0.42
1:C:471:ILE:HG13	6:C:762:HOH:O	2.19	0.42
1:A:83:ILE:HD11	1:A:348:PHE:CZ	2.54	0.42
1:A:180:HIS:CD2	1:A:270:GLY:H	2.38	0.42
5:A:511:CBS:H62B	5:A:511:CBS:H82A	2.02	0.42
1:A:16:ILE:HD11	1:A:152:TRP:CZ2	2.55	0.42
1:B:161:GLY:CA	1:B:162:ALA:CB	2.94	0.42
1:B:384:ILE:CG2	1:B:386:ILE:HD11	2.50	0.42
1:A:380:SER:HB3	6:A:1085:HOH:O	2.19	0.41
1:B:384:ILE:HG22	1:B:386:ILE:HD11	2.01	0.41
1:B:349:THR:HA	1:B:350:PRO:HD3	1.95	0.41
1:B:179:THR:HG23	1:B:183:VAL:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:PHE:O	1:B:424:TRP:HA	2.21	0.41
1:C:349:THR:HA	1:C:350:PRO:HD3	1.86	0.41
1:C:41:VAL:HG13	1:C:104:ALA:HB2	2.01	0.41
1:B:180:HIS:CD2	1:B:270:GLY:H	2.38	0.41
1:C:301:THR:CG2	6:C:835:HOH:O	2.69	0.41
1:C:138:TYR:HA	1:C:198:ARG:HB2	2.02	0.41
1:A:163:GLY:HA2	1:A:164:GLY:HA3	1.82	0.41
1:C:59:LEU:HD21	1:C:158[A]:LYS:HD2	2.02	0.41
1:A:151:ASP:OD2	1:A:153:TYR:OH	2.28	0.41
1:A:227:ASP:OD2	1:A:425:ARG:HB2	2.21	0.41
1:C:67:HIS:CE1	1:C:244:ALA:HB1	2.55	0.41
1:B:114:THR:OG1	1:B:158[A]:LYS:HE2	2.21	0.41
1:B:99:ASN:O	4:B:508:GOL:H11	2.21	0.41
1:A:59:LEU:HD12	1:A:114:THR:CG2	2.51	0.41
1:B:328:CYS:HB2	1:B:384:ILE:HD13	2.02	0.41
1:C:192:THR:HA	1:C:283:ARG:O	2.21	0.41
1:B:305:ILE:CD1	6:B:791:HOH:O	2.69	0.41
1:B:298:THR:HB	6:B:851:HOH:O	2.20	0.41
1:C:164:GLY:CA	1:C:165:ALA:CB	2.95	0.41
1:B:186:VAL:HG23	6:B:614:HOH:O	2.20	0.41
1:C:394:GLY:N	1:C:397:HIS:CE1	2.89	0.41
6:A:685:HOH:O	1:C:22:VAL:HG21	2.21	0.40
1:A:59:LEU:CD1	1:A:114:THR:CG2	2.95	0.40
1:A:394:GLY:HA2	1:A:395:GLY:HA3	1.73	0.40
1:B:384:ILE:HG22	1:B:386:ILE:CD1	2.51	0.40
1:C:394:GLY:O	1:C:458:HIS:CE1	2.74	0.40
1:B:17:VAL:CG1	1:B:22:VAL:HB	2.51	0.40
1:A:95:SER:HB3	6:A:922:HOH:O	2.20	0.40
1:B:182:ASN:HA	1:B:182:ASN:HD22	1.70	0.40
1:B:407:ALA:HB2	1:B:424:TRP:CE2	2.56	0.40
1:C:67:HIS:CD2	1:C:67:HIS:C	2.95	0.40
1:A:305:ILE:HD13	6:A:1049:HOH:O	2.20	0.40
1:B:26:VAL:HG13	1:B:53:LEU:HD21	2.03	0.40
1:A:54:ILE:HD13	6:A:692:HOH:O	2.22	0.40
1:C:164:GLY:HA2	1:C:165:ALA:CB	2.35	0.40
1:B:20:GLY:HA3	1:B:186:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/495 (101%)	476 (96%)	19 (4%)	3 (1%)	30	21
1	B	497/495 (100%)	471 (95%)	23 (5%)	3 (1%)	30	21
1	C	497/495 (100%)	468 (94%)	25 (5%)	4 (1%)	24	15
All	All	1492/1485 (100%)	1415 (95%)	67 (4%)	10 (1%)	26	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ALA
1	B	162	ALA
1	C	366	ALA
1	A	209	ASP
1	A	394	GLY
1	B	209	ASP
1	C	209	ASP
1	B	161	GLY
1	C	59	LEU
1	C	165	ALA

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	409/406 (101%)	386 (94%)	23 (6%)	26	20
1	B	406/406 (100%)	381 (94%)	25 (6%)	23	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	408/406 (100%)	376 (92%)	32 (8%)	16 9
All	All	1223/1218 (100%)	1143 (94%)	80 (6%)	22 15

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	54	ILE
1	A	69	GLU
1	A	97	ASN
1	A	117	TYR
1	A	156	LEU
1	A	160	MET
1	A	181	VAL
1	A	226	THR
1	A	246	ARG
1	A	285	ASP
1	A	297	SER
1	A	303	CYS
1	A	323	GLN
1	A	329	ASN
1	A	331	ASN
1	A	349	THR
1	A	372	SER
1	A	380	SER
1	A	417	SER
1	A	450	PHE
1	A	460	ASP
1	A	463	PHE
1	B	15	ASP
1	B	41	VAL
1	B	54	ILE
1	B	69	GLU
1	B	117	TYR
1	B	158[A]	LYS
1	B	158[B]	LYS
1	B	160	MET
1	B	181	VAL
1	B	195	VAL
1	B	226	THR
1	B	246	ARG
1	B	285	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	297	SER
1	B	301	THR
1	B	328	CYS
1	B	349	THR
1	B	372	SER
1	B	380	SER
1	B	417	SER
1	B	450	PHE
1	B	451	LEU
1	B	456	ASP
1	B	460	ASP
1	B	463	PHE
1	C	15	ASP
1	C	41	VAL
1	C	54	ILE
1	C	69	GLU
1	C	71	GLN
1	C	83	ILE
1	C	97	ASN
1	C	114	THR
1	C	117	TYR
1	C	156	LEU
1	C	158[A]	LYS
1	C	158[B]	LYS
1	C	160	MET
1	C	181	VAL
1	C	195	VAL
1	C	226	THR
1	C	246	ARG
1	C	285	ASP
1	C	297	SER
1	C	299	VAL
1	C	303	CYS
1	C	314	ARG
1	C	328	CYS
1	C	329	ASN
1	C	331	ASN
1	C	349	THR
1	C	380	SER
1	C	417	SER
1	C	450	PHE
1	C	451	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	463	PHE
1	C	465	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	44	ASN
1	A	52	GLN
1	A	71	GLN
1	A	85	GLN
1	A	92	ASN
1	A	97	ASN
1	A	136	ASN
1	A	180	HIS
1	A	182	ASN
1	A	265	ASN
1	A	310	HIS
1	A	320	ASN
1	A	329	ASN
1	A	486	ASN
1	B	44	ASN
1	B	52	GLN
1	B	92	ASN
1	B	97	ASN
1	B	116	GLN
1	B	180	HIS
1	B	182	ASN
1	B	232	GLN
1	B	255	GLN
1	B	310	HIS
1	B	320	ASN
1	B	322	HIS
1	B	358	GLN
1	B	364	ASN
1	B	486	ASN
1	C	2	GLN
1	C	44	ASN
1	C	52	GLN
1	C	71	GLN
1	C	92	ASN
1	C	180	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	232	GLN
1	C	310	HIS
1	C	320	ASN
1	C	329	ASN
1	C	331	ASN
1	C	364	ASN
1	C	486	ASN

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 ⓘ

Of 33 ligands modelled in this entry, 12 are monoatomic - leaving 21 for Mogul analysis.

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	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.28	0
3	SO4	A	506	-	4,4,4	0.21	0	6,6,6	0.11	0
3	SO4	A	507	-	4,4,4	0.35	0	6,6,6	0.25	0
4	GOL	A	508	-	5,5,5	0.27	0	5,5,5	0.41	0
4	GOL	A	509	-	5,5,5	0.22	0	5,5,5	0.50	0
5	CBS	A	510	-	29,29,30	1.15	3 (10%)	36,41,43	2.59	11 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CBS	A	511	-	29,29,30	0.82	0	36,41,43	2.33	10 (27%)
3	SO4	B	505	-	4,4,4	0.94	0	6,6,6	0.38	0
3	SO4	B	506	-	4,4,4	0.82	0	6,6,6	0.64	0
3	SO4	B	507	-	4,4,4	0.28	0	6,6,6	0.22	0
4	GOL	B	508	-	5,5,5	0.47	0	5,5,5	0.79	0
4	GOL	B	509	-	5,5,5	0.26	0	5,5,5	0.46	0
4	GOL	B	510	-	5,5,5	0.13	0	5,5,5	0.48	0
4	GOL	B	511	-	5,5,5	0.40	0	5,5,5	0.60	0
4	GOL	B	512	-	5,5,5	0.14	0	5,5,5	0.34	0
4	GOL	B	513	-	5,5,5	0.19	0	5,5,5	0.45	0
5	CBS	B	514	1	29,29,30	0.64	0	36,41,43	2.43	9 (25%)
5	CBS	B	515	1	29,29,30	0.99	2 (6%)	36,41,43	2.18	11 (30%)
3	SO4	C	505	-	4,4,4	0.17	0	6,6,6	0.19	0
4	GOL	C	506	-	5,5,5	0.16	0	5,5,5	0.39	0
5	CBS	C	507	-	29,29,30	2.43	4 (13%)	36,41,43	2.97	13 (36%)

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	SO4	A	505	-	-	0/0/0/0	0/0/0/0
3	SO4	A	506	-	-	0/0/0/0	0/0/0/0
3	SO4	A	507	-	-	0/0/0/0	0/0/0/0
4	GOL	A	508	-	-	0/4/4/4	0/0/0/0
4	GOL	A	509	-	-	0/4/4/4	0/0/0/0
5	CBS	A	510	-	-	0/16/53/56	0/2/2/2
5	CBS	A	511	-	-	0/16/53/56	0/2/2/2
3	SO4	B	505	-	-	0/0/0/0	0/0/0/0
3	SO4	B	506	-	-	0/0/0/0	0/0/0/0
3	SO4	B	507	-	-	0/0/0/0	0/0/0/0
4	GOL	B	508	-	-	0/4/4/4	0/0/0/0
4	GOL	B	509	-	-	0/4/4/4	0/0/0/0
4	GOL	B	510	-	-	0/4/4/4	0/0/0/0
4	GOL	B	511	-	-	0/4/4/4	0/0/0/0
4	GOL	B	512	-	-	0/4/4/4	0/0/0/0
4	GOL	B	513	-	-	0/4/4/4	0/0/0/0
5	CBS	B	514	1	-	0/16/53/56	0/2/2/2
5	CBS	B	515	1	-	1/16/53/56	0/2/2/2
3	SO4	C	505	-	-	0/0/0/0	0/0/0/0
4	GOL	C	506	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CBS	C	507	-	-	2/16/53/56	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	510	CBS	C2A-N2A	-2.96	1.40	1.45
5	B	515	CBS	C2B-N2B	-2.80	1.41	1.46
5	B	515	CBS	O5B-C1B	-2.59	1.39	1.43
5	A	510	CBS	O5B-C1B	-2.22	1.40	1.43
5	A	510	CBS	O7B-C7B	-2.15	1.18	1.23
5	C	507	CBS	C7A-N2A	2.16	1.42	1.34
5	C	507	CBS	C7B-N2B	3.10	1.46	1.34
5	C	507	CBS	O7B-C7B	8.16	1.42	1.23
5	C	507	CBS	O7A-C7A	8.69	1.43	1.23

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	507	CBS	O7B-C7B-C8B	-8.05	107.29	122.06
5	C	507	CBS	O7A-C7A-N2A	-7.32	106.94	121.86
5	A	511	CBS	C4A-C3A-C2A	-7.11	100.57	110.43
5	A	510	CBS	C3A-C2A-N2A	-6.92	96.34	110.66
5	C	507	CBS	C3A-C2A-N2A	-6.16	97.91	110.66
5	B	514	CBS	C3A-C2A-N2A	-5.55	99.17	110.66
5	B	514	CBS	C6A-C5A-C4A	-5.48	99.49	113.02
5	B	515	CBS	O3B-C3B-C4B	-5.43	97.03	109.87
5	C	507	CBS	O7A-C7A-C8A	-5.16	112.60	122.06
5	C	507	CBS	O7B-C7B-N2B	-4.86	111.96	121.86
5	C	507	CBS	C8A-C7A-N2A	-4.66	107.19	116.11
5	A	510	CBS	C8A-C7A-N2A	-3.71	109.00	116.11
5	B	515	CBS	C6A-C5A-C4A	-3.49	104.41	113.02
5	A	511	CBS	O5A-C1A-C2A	-3.46	103.25	110.78
5	A	510	CBS	C6A-C5A-C4A	-3.10	105.36	113.02
5	B	515	CBS	C8B-C7B-N2B	-3.03	110.30	116.11
5	B	515	CBS	O3A-C3A-C4A	-2.85	103.92	110.34
5	C	507	CBS	C8B-C7B-N2B	-2.69	110.95	116.11
5	A	511	CBS	C6B-C5B-C4B	-2.69	105.41	113.25
5	C	507	CBS	C6B-C5B-C4B	-2.31	106.52	113.25
5	B	514	CBS	O3B-C3B-C4B	-2.20	104.66	109.87
5	C	507	CBS	C6A-C5A-C4A	-2.14	107.75	113.02
5	A	510	CBS	O7B-C7B-C8B	-2.03	118.34	122.06
5	A	511	CBS	O6A-C6A-C5A	2.01	117.96	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	514	CBS	O5A-C5A-C6A	2.11	111.68	106.36
5	B	515	CBS	O4A-C4A-C5A	2.26	115.24	109.24
5	A	510	CBS	C4A-C3A-C2A	2.38	113.72	110.43
5	B	515	CBS	O7B-C7B-N2B	2.44	126.85	121.86
5	C	507	CBS	C4B-C3B-C2B	2.46	115.92	109.74
5	A	511	CBS	O3B-C3B-C2B	2.55	114.16	109.11
5	B	515	CBS	C1B-O5B-C5B	2.66	115.63	112.25
5	A	510	CBS	O7A-C7A-C8A	2.76	127.13	122.06
5	A	511	CBS	C3A-C2A-N2A	2.84	116.54	110.66
5	A	510	CBS	C3A-C4A-C5A	2.95	115.35	110.20
5	B	515	CBS	O1A-C1A-O5A	3.05	118.40	110.68
5	A	510	CBS	O5B-C5B-C4B	3.08	115.61	110.01
5	B	514	CBS	O5A-C5A-C4A	3.17	115.63	109.68
5	A	511	CBS	O5A-C5A-C4A	3.19	115.66	109.68
5	C	507	CBS	O5B-C5B-C4B	3.26	115.93	110.01
5	A	511	CBS	C1A-O5A-C5A	3.33	120.21	113.75
5	C	507	CBS	C1B-O5B-C5B	3.39	116.55	112.25
5	B	514	CBS	C4B-C3B-C2B	3.52	118.60	109.74
5	B	514	CBS	C3A-C4A-C5A	3.59	116.45	110.20
5	B	515	CBS	C3A-C2A-N2A	3.74	118.41	110.66
5	A	510	CBS	C1A-O5A-C5A	3.75	121.01	113.75
5	A	510	CBS	O5A-C5A-C4A	4.02	117.22	109.68
5	B	515	CBS	C1A-O1A-C4B	4.34	129.36	118.01
5	A	511	CBS	C1B-O5B-C5B	4.62	118.11	112.25
5	B	514	CBS	C4A-C3A-C2A	4.65	116.87	110.43
5	C	507	CBS	C4A-C3A-C2A	4.69	116.94	110.43
5	B	515	CBS	C4A-C3A-C2A	5.29	117.77	110.43
5	A	511	CBS	C1A-C2A-N2A	5.65	121.65	111.01
5	B	514	CBS	C1B-O5B-C5B	7.85	122.21	112.25
5	A	510	CBS	C1B-O5B-C5B	8.64	123.22	112.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	507	CBS	O7A-C7A-N2A-C2A
5	C	507	CBS	O7B-C7B-N2B-C2B
5	B	515	CBS	C1A-C2A-N2A-C7A

There are no ring outliers.

14 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	508	GOL	1	0
4	A	509	GOL	2	0
5	A	510	CBS	2	0
5	A	511	CBS	3	0
3	B	506	SO4	6	0
4	B	508	GOL	6	0
4	B	509	GOL	2	0
4	B	510	GOL	2	0
4	B	511	GOL	1	0
4	B	512	GOL	2	0
4	B	513	GOL	2	0
5	B	515	CBS	11	0
4	C	506	GOL	1	0
5	C	507	CBS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/495 (100%)	-0.52	4 (0%) 87 90	10, 18, 32, 42	0
1	B	495/495 (100%)	-0.40	5 (1%) 84 88	11, 21, 37, 54	0
1	C	495/495 (100%)	-0.40	9 (1%) 71 79	11, 21, 37, 50	0
All	All	1485/1485 (100%)	-0.44	18 (1%) 81 85	10, 20, 36, 54	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	SER	4.2
1	B	320	ASN	4.1
1	A	165	ALA	3.5
1	C	381	ASN	2.9
1	C	165	ALA	2.9
1	C	415	SER	2.8
1	B	298	THR	2.5
1	A	415	SER	2.5
1	A	161	GLY	2.4
1	C	320	ASN	2.4
1	C	161	GLY	2.3
1	B	338	CYS	2.3
1	C	394	GLY	2.2
1	C	364	ASN	2.1
1	A	433	VAL	2.1
1	C	164	GLY	2.1
1	C	372	SER	2.1
1	B	322	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	B	508	6/6	0.93	0.26	9.86	32,37,38,39	0
4	GOL	B	509	6/6	0.91	0.14	5.73	32,34,36,37	0
3	SO4	C	505	5/5	0.74	0.33	5.64	35,36,37,37	5
3	SO4	A	506	5/5	0.98	0.15	3.95	59,59,59,60	0
4	GOL	A	509	6/6	0.85	0.15	2.69	40,45,46,46	0
5	CBS	B	514	28/29	0.70	0.25	2.59	67,70,72,73	0
5	CBS	B	515	28/29	0.61	0.27	2.45	62,70,75,76	0
5	CBS	A	511	28/29	0.75	0.21	2.22	43,50,56,56	0
5	CBS	A	510	28/29	0.85	0.19	2.13	35,44,51,52	0
4	GOL	B	510	6/6	0.87	0.15	2.05	39,39,39,41	0
4	GOL	B	512	6/6	0.95	0.12	2.03	23,26,27,28	0
3	SO4	A	505	5/5	0.98	0.10	1.81	45,47,47,48	0
5	CBS	C	507	28/29	0.77	0.20	1.75	58,62,66,67	0
4	GOL	A	508	6/6	0.95	0.09	0.96	30,31,32,33	0
4	GOL	C	506	6/6	0.94	0.10	0.62	31,32,34,37	0
4	GOL	B	511	6/6	0.95	0.09	0.54	26,29,31,31	0
3	SO4	B	506	5/5	0.99	0.08	-0.10	24,27,29,29	0
3	SO4	B	505	5/5	0.99	0.06	-0.85	16,20,23,24	0
2	CU	B	504	1/1	0.99	0.06	-1.11	20,20,20,20	0
2	CU	C	504	1/1	1.00	0.06	-1.35	18,18,18,18	0
2	CU	C	501	1/1	1.00	0.04	-1.49	20,20,20,20	0
2	CU	A	504	1/1	1.00	0.05	-1.66	15,15,15,15	0
2	CU	B	501	1/1	1.00	0.04	-1.76	19,19,19,19	0
2	CU	C	502	1/1	0.99	0.05	-1.77	17,17,17,17	0
2	CU	A	501	1/1	1.00	0.04	-2.12	18,18,18,18	0
2	CU	C	503	1/1	1.00	0.05	-2.20	16,16,16,16	0
2	CU	B	503	1/1	1.00	0.04	-2.60	17,17,17,17	0
2	CU	A	503	1/1	0.99	0.04	-3.72	18,18,18,18	0
2	CU	A	502	1/1	1.00	0.03	-4.29	14,14,14,14	0
2	CU	B	502	1/1	1.00	0.03	-5.45	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	A	507	5/5	0.95	0.12	-	15,16,18,18	5
4	GOL	B	513	6/6	0.90	0.21	-	31,34,36,37	0
3	SO4	B	507	5/5	0.93	0.14	-	21,21,22,23	5

6.5 Other polymers [i](#)

There are no such residues in this entry.