



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:55 am GMT

PDB ID : 3T6X  
Title : Crystal Structure of *Steccherinum ochraceum* Laccase obtained by multi-crystals composite data collection technique (20% dose)  
Authors : Ferraroni, M.; Briganti, F.; Matera, I.; Kolomytseva, M.; Golovleva, L.; Scoz-zafava, 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](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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949



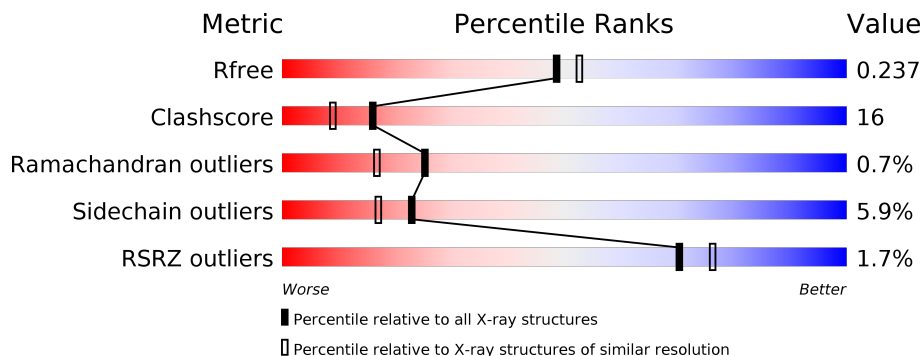
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	495	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
1	C	495	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>21%</div> <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	505	-	-	-	X
3	SO4	B	506	-	-	X	-
3	SO4	C	505	-	-	X	X
4	GOL	A	508	-	-	X	X
4	GOL	B	508	-	-	X	X
4	GOL	B	510	-	-	-	X
4	GOL	C	506	-	-	X	X
5	CBS	A	510	-	-	-	X
5	CBS	A	511	-	-	-	X
5	CBS	B	512	-	-	-	X
5	CBS	B	513	-	-	-	X
5	CBS	C	508	-	-	-	X
6	PER	A	512	-	-	-	X
6	PER	C	510	-	-	-	X



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12916 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.

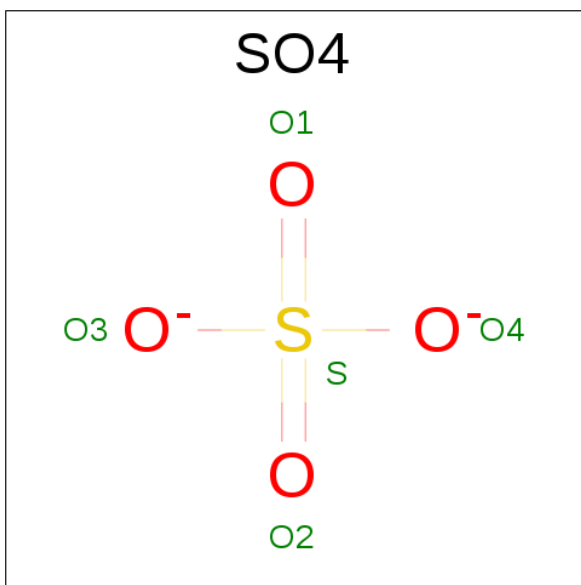
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	5	0
			3734	2360	626	729	19			
1	B	495	Total	C	N	O	S	0	5	0
			3728	2357	629	724	18			
1	C	495	Total	C	N	O	S	0	3	0
			3725	2354	629	725	17			

- 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: O<sub>4</sub>S).

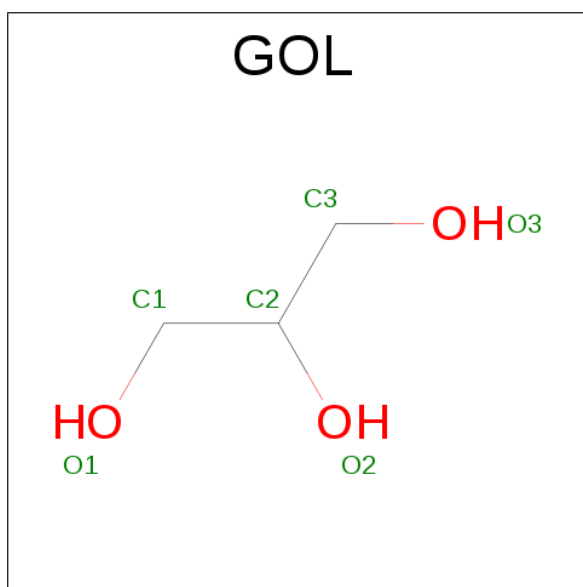




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

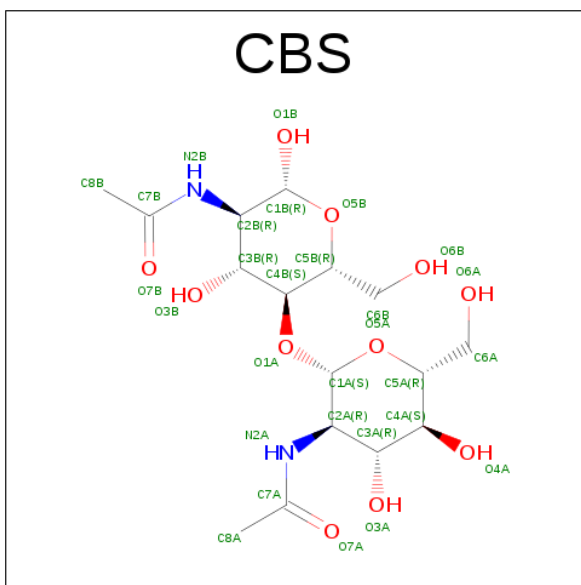




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SUGAR (DI(N-ACETYL-D-GLUCOSAMINE)) (three-letter code: CBS) (formula: C<sub>16</sub>H<sub>28</sub>N<sub>2</sub>O<sub>11</sub>).

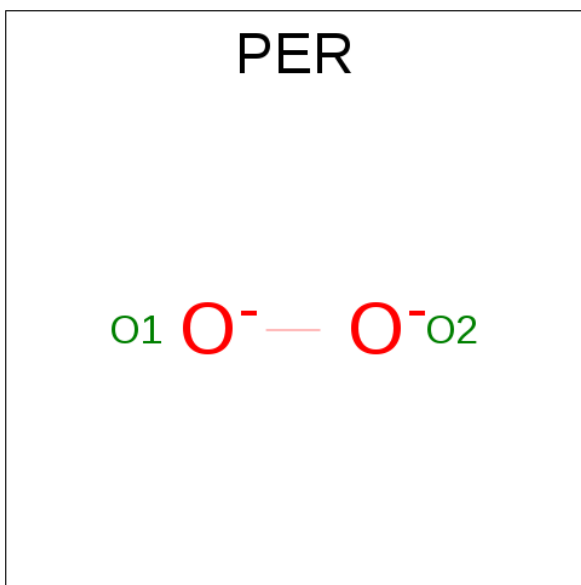




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	16	2	10		
5	A	1	Total	C	N	O	0	0
			28	16	2	10		
5	B	1	Total	C	N	O	0	0
			28	16	2	10		
5	B	1	Total	C	N	O	0	0
			28	16	2	10		
5	C	1	Total	C	N	O	0	0
			28	16	2	10		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	C	1	Total O 2 2	0	0

- Molecule 7 is water.

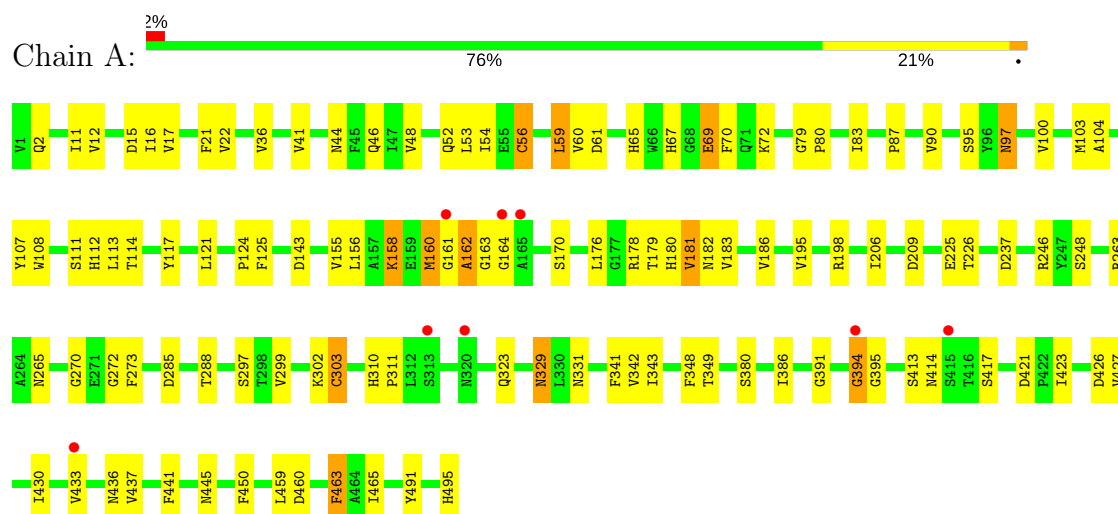
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	531	Total O 531 531	0	0
7	B	465	Total O 465 465	0	0
7	C	478	Total O 478 478	0	0



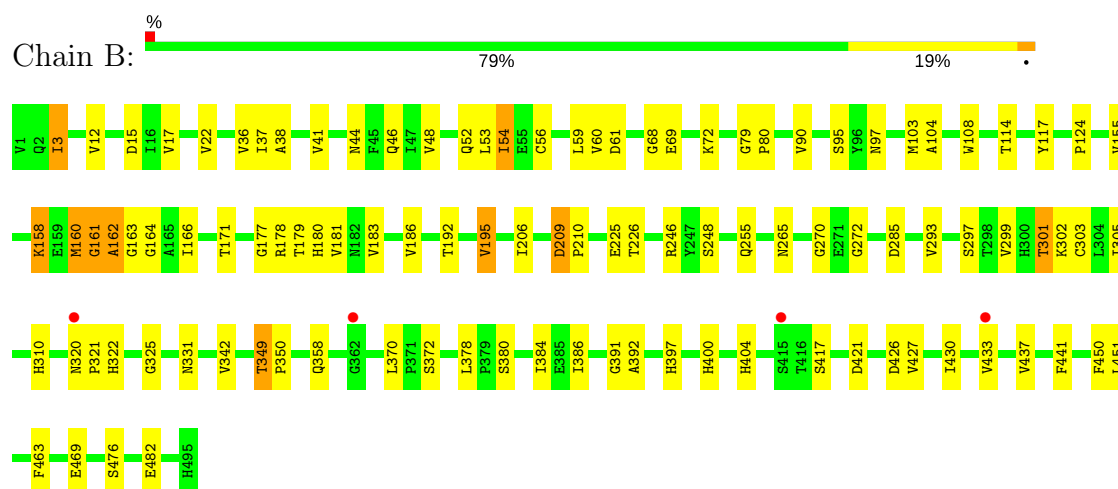
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

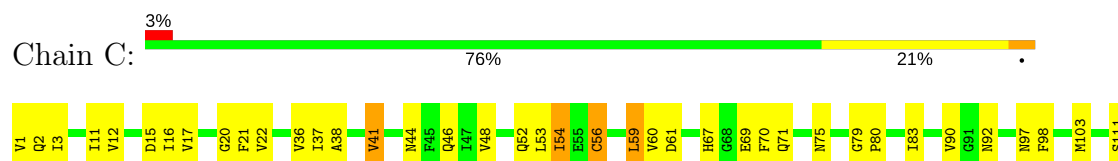
#### • Molecule 1: Laccase



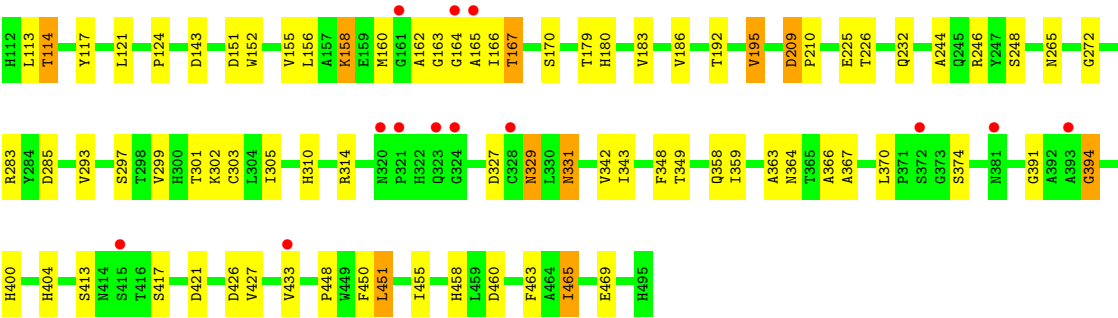
#### • Molecule 1: Laccase



#### • Molecule 1: Laccase









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.51Å 140.04Å 172.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.15 19.87 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.6 (19.87-2.15) 94.7 (19.87-2.15)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.176 , 0.236 0.178 , 0.237	Depositor DCC
$R_{free}$ test set	4626 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CU, SO4, PER, 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	0.67	3/3857 (0.1%)	0.72	1/5296 (0.0%)
1	B	0.63	0/3851	0.69	1/5288 (0.0%)
1	C	0.63	2/3844 (0.1%)	0.71	1/5279 (0.0%)
All	All	0.64	5/11552 (0.0%)	0.71	3/15863 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56[A]	CYS	CB-SG	-5.46	1.73	1.81
1	C	56[B]	CYS	CB-SG	-5.46	1.73	1.81
1	A	56[A]	CYS	CB-SG	-5.24	1.73	1.81
1	A	56[B]	CYS	CB-SG	-5.24	1.73	1.81
1	A	303	CYS	CB-SG	-5.12	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	394	GLY	N-CA-C	-5.67	98.94	113.10
1	A	237	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	3	ILE	N-CA-C	-5.10	97.22	111.00

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	3734	0	3513	126	0
1	B	3728	0	3501	111	0
1	C	3725	0	3502	122	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	5	0
3	C	5	0	0	2	0
4	A	12	0	16	6	0
4	B	24	0	32	9	0
4	C	12	0	16	7	0
5	A	56	0	52	11	0
5	B	56	0	52	1	0
5	C	42	0	38	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	1	0
7	A	531	0	0	35	1
7	B	465	0	0	32	1
7	C	478	0	0	32	0
All	All	12916	0	10722	360	1

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 16.

All (360) 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:HD21	5:A:510:CBS:C1B	0.90	1.51
1:A:414:ASN:ND2	5:A:510:CBS:C1B	1.72	1.42
1:A:436:ASN:ND2	5:A:511:CBS:C1B	1.84	1.41
1:A:436:ASN:HD21	5:A:511:CBS:C1B	1.31	1.38
1:A:161:GLY:HA2	1:A:162:ALA:CB	1.77	1.14
1:C:17:VAL:HG12	1:C:22:VAL:HA	1.38	1.06
1:B:161:GLY:CA	1:B:162:ALA:HB2	1.86	1.05
1:C:162:ALA:HB2	1:C:166:ILE:HD11	1.42	1.01
1:C:162:ALA:HB2	1:C:166:ILE:CD1	1.91	1.00
1:C:358:GLN:HE22	1:C:370:LEU:H	1.03	1.00
1:C:59:LEU:HD11	1:C:114:THR:HG21	1.44	0.99

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD11	1:B:114:THR:HG21	1.45	0.98
1:C:17:VAL:HG12	1:C:22:VAL:CA	1.92	0.98
1:B:358:GLN:HE22	1:B:370:LEU:H	1.12	0.98
1:C:329:ASN:HD22	1:C:329:ASN:N	1.58	0.97
1:C:329:ASN:ND2	1:C:329:ASN:H	1.61	0.96
1:B:161:GLY:N	1:B:162:ALA:HB2	1.81	0.96
1:B:161:GLY:HA3	1:B:162:ALA:HB2	1.48	0.95
1:B:161:GLY:N	1:B:162:ALA:CB	2.30	0.95
1:A:331:ASN:HB2	7:A:1055:HOH:O	1.66	0.94
1:B:41:VAL:HG13	1:B:103:MET:O	1.66	0.94
1:A:112:HIS:HD1	4:A:508:GOL:H32	1.31	0.94
1:A:161:GLY:HA2	1:A:162:ALA:HB3	1.46	0.94
1:C:20:GLY:O	4:C:506:GOL:H31	1.67	0.94
1:B:265[A]:ASN:HD21	1:B:272:GLY:H	1.16	0.94
1:C:179:THR:O	1:C:183:VAL:HG22	1.69	0.93
1:C:48:VAL:HG23	7:C:686:HOH:O	1.68	0.93
1:B:36:VAL:HG22	1:B:124:PRO:HG2	1.48	0.92
4:C:506:GOL:H11	7:C:666:HOH:O	1.68	0.92
1:A:195:VAL:HG23	7:A:681:HOH:O	1.67	0.92
1:B:195:VAL:HG11	7:B:1004:HOH:O	1.70	0.92
1:B:342:VAL:HG23	7:B:761:HOH:O	1.69	0.92
1:C:164:GLY:HA2	1:C:165:ALA:HB3	1.52	0.91
1:A:59:LEU:CD1	1:A:114:THR:HG21	2.01	0.91
1:A:161:GLY:HA2	1:A:162:ALA:HB2	1.53	0.89
1:A:41:VAL:HB	7:A:1062:HOH:O	1.71	0.89
1:B:302:LYS:HD3	7:B:788:HOH:O	1.72	0.89
1:A:17:VAL:HG23	4:C:506:GOL:O1	1.73	0.88
1:A:310:HIS:HE1	7:A:856:HOH:O	1.58	0.87
1:A:59:LEU:HD11	1:A:114:THR:HG21	1.58	0.86
1:C:12:VAL:HG22	7:C:665:HOH:O	1.75	0.86
1:A:299:VAL:HB	7:A:1002:HOH:O	1.75	0.86
1:A:183:VAL:HG21	7:A:619:HOH:O	1.75	0.85
1:A:53:LEU:O	1:A:90:VAL:HG21	1.76	0.85
1:B:293:VAL:HG23	7:B:841:HOH:O	1.75	0.84
7:B:605:HOH:O	1:C:12:VAL:HG21	1.76	0.84
1:A:48:VAL:HG23	7:A:761:HOH:O	1.77	0.84
1:B:53:LEU:O	1:B:90:VAL:HG21	1.76	0.84
1:C:44:ASN:ND2	1:C:46:GLN:HE21	1.75	0.84
1:A:12:VAL:HG21	7:C:677:HOH:O	1.77	0.83
1:A:436:ASN:CG	5:A:511:CBS:C1B	2.47	0.83
5:A:511:CBS:H2A	7:A:1131:HOH:O	1.79	0.83

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:O	1:C:90:VAL:HG21	1.79	0.83
1:B:161:GLY:H	1:B:162:ALA:HB3	1.45	0.82
1:C:17:VAL:CG1	1:C:22:VAL:HA	2.10	0.81
1:B:12:VAL:HG22	7:B:646:HOH:O	1.79	0.81
1:A:44:ASN:HD21	1:A:46:GLN:HE21	1.29	0.80
1:A:112:HIS:ND1	4:A:508:GOL:H32	1.96	0.80
7:A:797:HOH:O	1:B:12:VAL:HG21	1.80	0.80
1:A:56[A]:CYS:SG	1:B:52:GLN:NE2	2.55	0.80
1:B:56[A]:CYS:SG	1:C:52:GLN:NE2	2.55	0.79
1:B:3:ILE:O	1:B:37:ILE:HA	1.82	0.79
1:A:329:ASN:ND2	1:A:329:ASN:H	1.81	0.79
1:A:160:MET:O	1:A:162:ALA:HB2	1.83	0.78
1:C:209:ASP:HB3	1:C:210:PRO:HD3	1.65	0.78
1:B:59:LEU:CD1	1:B:114:THR:HG21	2.14	0.78
1:A:161:GLY:CA	1:A:162:ALA:CB	2.61	0.78
1:A:17:VAL:HG12	1:A:22:VAL:N	1.98	0.78
1:A:162:ALA:H	1:A:163:GLY:HA2	1.48	0.77
1:B:179:THR:O	1:B:183:VAL:HG22	1.83	0.77
1:C:209:ASP:HB3	1:C:210:PRO:CD	2.14	0.77
1:C:61:ASP:OD2	7:C:1075:HOH:O	2.01	0.77
4:A:509:GOL:O2	1:B:17:VAL:HG23	1.85	0.77
1:C:451:LEU:HD12	1:C:465:ILE:HD11	1.66	0.77
1:B:72:LYS:N	4:B:508:GOL:H12	1.99	0.76
1:A:329:ASN:N	1:A:329:ASN:ND2	2.33	0.76
1:C:17:VAL:HG12	1:C:22:VAL:N	2.00	0.76
1:C:60:VAL:HG21	7:C:617:HOH:O	1.85	0.75
1:C:3:ILE:O	1:C:37:ILE:HA	1.87	0.75
1:A:52:GLN:NE2	1:C:56[A]:CYS:SG	2.60	0.75
1:C:155:VAL:HG23	7:C:871:HOH:O	1.87	0.74
1:C:70:PHE:H	1:C:103:MET:HE1	1.52	0.73
1:A:12:VAL:HG22	7:A:818:HOH:O	1.89	0.73
1:C:17:VAL:HG21	4:C:506:GOL:H2	1.69	0.73
1:A:36:VAL:HG22	1:A:124:PRO:HG2	1.71	0.73
1:C:59:LEU:HD11	1:C:114:THR:CG2	2.18	0.72
1:C:367:ALA:HA	7:C:1043:HOH:O	1.87	0.72
1:A:60:VAL:HG23	7:A:666:HOH:O	1.88	0.72
1:A:265:ASN:HD21	1:A:272:GLY:H	1.38	0.72
1:A:414:ASN:CG	5:A:510:CBS:C1B	2.57	0.72
1:B:68:GLY:O	1:B:103:MET:HE1	1.90	0.72
1:B:160:MET:O	7:B:1054:HOH:O	2.08	0.71
1:A:17:VAL:HG12	1:A:22:VAL:CA	2.20	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:CG1	1:C:22:VAL:CA	2.68	0.71
1:A:459:LEU:HD21	4:A:508:GOL:H31	1.73	0.70
1:C:265[B]:ASN:HD21	1:C:272:GLY:H	1.37	0.70
1:A:170:SER:HB3	1:A:179:THR:HA	1.73	0.70
1:B:183:VAL:HG21	7:B:782:HOH:O	1.92	0.70
1:B:90:VAL:HG22	7:B:707:HOH:O	1.93	0.69
5:C:508:CBS:N2B	7:C:735:HOH:O	2.24	0.69
1:C:329:ASN:HD22	1:C:329:ASN:H	0.79	0.69
1:A:329:ASN:N	1:A:329:ASN:HD22	1.90	0.69
1:A:342:VAL:HG23	7:A:662:HOH:O	1.93	0.69
1:A:60:VAL:HG21	7:A:978:HOH:O	1.93	0.69
1:B:60:VAL:HG23	7:B:726:HOH:O	1.93	0.68
1:C:162:ALA:HB1	1:C:163:GLY:HA2	1.75	0.68
1:A:323:GLN:OE1	7:A:1127:HOH:O	2.11	0.68
1:C:162:ALA:CB	1:C:166:ILE:HD11	2.21	0.68
3:B:506:SO4:O2	1:C:17:VAL:HG22	1.93	0.68
1:C:162:ALA:HB2	1:C:166:ILE:HD12	1.75	0.68
1:A:95:SER:HB3	7:A:689:HOH:O	1.95	0.67
1:B:161:GLY:CA	1:B:162:ALA:CB	2.56	0.67
1:A:17:VAL:CG2	3:B:506:SO4:O4	2.43	0.67
1:A:17:VAL:HG22	3:B:506:SO4:O4	1.95	0.67
1:A:310:HIS:HD2	1:A:421:ASP:O	1.78	0.67
1:A:426:ASP:OD1	1:A:427:VAL:HG23	1.94	0.67
1:C:426:ASP:OD1	1:C:427:VAL:HG23	1.94	0.67
1:B:161:GLY:H	1:B:162:ALA:CB	1.98	0.66
1:A:17:VAL:HG23	4:C:506:GOL:HO1	1.61	0.66
1:B:358:GLN:NE2	1:B:370:LEU:H	1.89	0.66
1:C:59:LEU:HD21	1:C:158[B]:LYS:HE3	1.76	0.66
1:A:69:GLU:HA	1:A:103:MET:HE1	1.78	0.66
1:C:17:VAL:HG23	7:C:650:HOH:O	1.94	0.66
1:A:386:ILE:CD1	1:A:441:PHE:HE1	2.09	0.66
1:B:61:ASP:OD2	7:B:1038:HOH:O	2.12	0.66
1:C:36:VAL:HG21	1:C:143:ASP:OD2	1.96	0.66
1:C:90:VAL:HG22	7:C:611:HOH:O	1.96	0.66
1:C:59:LEU:CD1	1:C:114:THR:CG2	2.75	0.65
1:B:72:LYS:H	4:B:508:GOL:H12	1.60	0.65
5:A:511:CBS:H81B	7:A:1063:HOH:O	1.95	0.65
1:B:301:THR:HB	7:B:1014:HOH:O	1.96	0.65
1:A:59:LEU:HD12	1:A:114:THR:HG21	1.76	0.65
1:B:161:GLY:N	1:B:162:ALA:HB3	2.05	0.65
1:C:164:GLY:N	7:C:1076:HOH:O	2.30	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:H	1:A:103:MET:HE2	1.61	0.65
1:C:179:THR:HG22	7:C:621:HOH:O	1.97	0.65
1:B:17:VAL:HG12	1:B:22:VAL:N	2.12	0.64
1:A:90:VAL:HG22	7:A:792:HOH:O	1.96	0.64
1:C:164:GLY:CA	1:C:165:ALA:HB3	2.25	0.64
1:C:413:SER:HB2	7:C:1021:HOH:O	1.98	0.64
1:C:17:VAL:CG1	1:C:22:VAL:HB	2.27	0.64
1:C:36:VAL:HG22	1:C:124:PRO:HG2	1.78	0.64
1:B:162:ALA:HB1	7:B:839:HOH:O	1.98	0.63
1:A:158[B]:LYS:HE2	7:A:1016:HOH:O	1.98	0.63
1:B:378:LEU:HD22	1:B:384:ILE:HD12	1.81	0.62
1:C:374:SER:O	1:C:465:ILE:HG22	1.99	0.62
1:C:400:HIS:HB2	1:C:427:VAL:HG22	1.80	0.62
1:A:17:VAL:HG12	1:A:22:VAL:HA	1.80	0.62
1:C:60:VAL:HG23	7:C:614:HOH:O	1.98	0.62
1:B:426:ASP:OD1	1:B:427:VAL:HG23	1.98	0.62
1:A:161:GLY:CA	1:A:162:ALA:HB2	2.25	0.62
1:B:41:VAL:HG22	1:B:104:ALA:HB2	1.81	0.61
1:A:414:ASN:HD21	5:A:510:CBS:C2B	1.96	0.61
1:A:391:GLY:HA2	1:A:433:VAL:HG22	1.81	0.61
1:A:288:THR:HG22	7:A:655:HOH:O	2.00	0.61
1:C:358:GLN:HE22	1:C:370:LEU:N	1.86	0.61
1:C:59:LEU:CD1	1:C:114:THR:HG21	2.25	0.60
1:A:386:ILE:HD11	1:A:441:PHE:HE1	1.66	0.60
1:B:36:VAL:HG23	7:B:867:HOH:O	2.01	0.60
1:C:359:ILE:HA	1:C:363:ALA:HB3	1.83	0.60
1:A:265:ASN:ND2	7:A:781:HOH:O	2.34	0.60
1:B:72:LYS:H	4:B:508:GOL:H2	1.67	0.60
1:B:255:GLN:NE2	7:B:892:HOH:O	2.34	0.59
1:A:41:VAL:HG22	1:A:103:MET:O	2.02	0.59
1:C:451:LEU:HD12	1:C:465:ILE:CD1	2.31	0.59
1:A:430:ILE:HA	1:A:437:VAL:HG21	1.85	0.59
1:B:293:VAL:HG22	7:B:983:HOH:O	2.00	0.59
1:A:41:VAL:HG13	1:A:103:MET:O	2.02	0.59
1:C:170:SER:HB3	1:C:179:THR:HA	1.85	0.59
1:B:358:GLN:HE22	1:B:370:LEU:N	1.93	0.58
1:C:54:ILE:HD13	7:C:629:HOH:O	2.02	0.58
1:C:167:THR:HG23	7:C:773:HOH:O	2.04	0.58
1:C:451:LEU:HB3	1:C:465:ILE:HD12	1.86	0.57
1:C:70:PHE:H	1:C:103:MET:CE	2.17	0.57
1:A:53:LEU:O	1:A:90:VAL:CG2	2.49	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HG22	1:B:124:PRO:CG	2.28	0.57
1:A:113:LEU:HG	1:A:114:THR:HG22	1.87	0.57
1:B:186:VAL:HG23	7:B:613:HOH:O	2.04	0.57
1:A:70:PHE:H	1:A:103:MET:CE	2.17	0.57
1:A:181:VAL:HG13	7:A:770:HOH:O	2.05	0.57
1:A:41:VAL:HG21	1:A:104:ALA:HB2	1.87	0.57
1:B:391:GLY:HA2	1:B:433:VAL:HG22	1.87	0.57
1:B:59:LEU:HD21	1:B:158[B]:LYS:HE3	1.88	0.56
1:B:265[A]:ASN:ND2	1:B:272:GLY:H	1.97	0.56
1:B:46:GLN:HA	1:B:97:ASN:HD22	1.71	0.56
1:A:413:SER:HB2	7:A:740:HOH:O	2.06	0.56
1:A:17:VAL:CG1	1:A:22:VAL:HA	2.36	0.56
1:A:195:VAL:HG22	7:A:965:HOH:O	2.06	0.55
1:A:225:GLU:HB3	1:A:248:SER:HB2	1.87	0.55
1:B:183:VAL:HG23	4:B:509:GOL:O3	2.07	0.55
1:A:11:ILE:HG22	1:A:53:LEU:HD21	1.89	0.55
1:A:112:HIS:HD1	4:A:508:GOL:C3	2.12	0.55
1:A:386:ILE:HD11	1:A:441:PHE:CE1	2.42	0.55
1:A:61:ASP:OD2	7:A:1082:HOH:O	2.18	0.54
1:C:3:ILE:O	1:C:38:ALA:N	2.40	0.54
1:A:17:VAL:CG1	1:A:22:VAL:CA	2.85	0.54
1:B:48:VAL:HG23	7:B:622:HOH:O	2.07	0.54
1:A:41:VAL:CG2	1:A:104:ALA:HB2	2.37	0.54
1:A:59:LEU:HD12	1:A:114:THR:CG2	2.37	0.54
1:B:44:ASN:ND2	1:B:46:GLN:HE21	2.05	0.54
1:B:17:VAL:HG12	1:B:22:VAL:CA	2.37	0.54
1:B:293:VAL:CG2	7:B:983:HOH:O	2.55	0.54
1:A:178:ARG:HG2	1:A:186:VAL:HG22	1.89	0.54
1:C:17:VAL:CG1	1:C:22:VAL:CB	2.85	0.54
1:A:162:ALA:H	1:A:164:GLY:HA3	1.73	0.53
1:A:343:ILE:HG21	1:A:465:ILE:HG12	1.90	0.53
1:A:179:THR:O	1:A:183:VAL:HG22	2.07	0.53
1:B:171:THR:O	1:B:177:GLY:HA3	2.09	0.53
4:B:511:GOL:H11	7:B:814:HOH:O	2.07	0.53
1:A:17:VAL:HG12	1:A:21:PHE:C	2.28	0.53
1:A:495:HIS:NE2	7:A:1082:HOH:O	1.96	0.53
1:B:320:ASN:HB2	1:B:325:GLY:HA3	1.91	0.53
1:B:3:ILE:O	1:B:38:ALA:N	2.42	0.53
1:B:59:LEU:CD1	1:B:114:THR:CG2	2.84	0.53
1:C:265[B]:ASN:ND2	1:C:272:GLY:H	2.05	0.53
1:A:59:LEU:CD1	1:A:114:THR:CG2	2.83	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:CG2	1:B:124:PRO:HG2	2.31	0.52
1:A:182:ASN:HD21	1:B:192:THR:H	1.57	0.52
1:A:112:HIS:CE1	4:A:508:GOL:H32	2.45	0.52
1:C:343:ILE:HD12	1:C:465:ILE:HG13	1.92	0.52
1:C:83:ILE:HD11	1:C:348:PHE:CZ	2.44	0.52
1:A:83:ILE:HD11	1:A:348:PHE:CZ	2.45	0.52
1:B:179:THR:HG23	1:B:183:VAL:HA	1.92	0.51
1:B:72:LYS:H	4:B:508:GOL:C1	2.23	0.51
1:C:293:VAL:HG21	7:C:1061:HOH:O	2.09	0.51
1:C:83:ILE:HD11	1:C:348:PHE:HZ	1.75	0.51
1:A:17:VAL:CG1	1:A:22:VAL:HB	2.41	0.51
1:B:225:GLU:HB3	1:B:248:SER:HB2	1.93	0.51
1:C:391:GLY:HA2	1:C:433:VAL:HG22	1.92	0.51
1:B:114:THR:H	4:B:510:GOL:C3	2.24	0.51
1:C:11:ILE:HG22	1:C:53:LEU:HD21	1.92	0.51
1:B:331:ASN:ND2	5:B:513:CBS:H3B	2.25	0.51
1:C:183:VAL:HG21	7:C:634:HOH:O	2.11	0.51
1:B:17:VAL:HG22	3:B:506:SO4:O3	2.11	0.51
1:B:386:ILE:HD13	1:B:441:PHE:HE1	1.76	0.51
1:C:192:THR:HA	1:C:283:ARG:O	2.11	0.51
1:C:41:VAL:CG1	1:C:103:MET:O	2.59	0.51
1:C:225:GLU:HB3	1:C:248:SER:HB2	1.94	0.50
1:A:176:LEU:HD21	4:C:506:GOL:H32	1.93	0.50
1:C:17:VAL:HG11	1:C:22:VAL:HB	1.92	0.50
1:A:103:MET:HE3	7:A:935:HOH:O	2.11	0.50
1:C:342:VAL:HG23	7:C:612:HOH:O	2.11	0.50
1:A:178:ARG:HG2	1:A:186:VAL:CG2	2.41	0.50
1:B:79:GLY:N	1:B:80:PRO:HD2	2.27	0.50
1:C:305:ILE:HD13	7:C:841:HOH:O	2.10	0.50
1:A:302:LYS:HD3	7:A:1068:HOH:O	2.11	0.50
1:C:374:SER:C	1:C:465:ILE:HG22	2.32	0.49
1:B:195:VAL:HB	7:B:956:HOH:O	2.12	0.49
1:B:209:ASP:HB3	1:B:210:PRO:CD	2.42	0.49
1:B:72:LYS:H	4:B:508:GOL:C2	2.26	0.49
1:B:108:TRP:CE3	1:B:206:ILE:HG22	2.48	0.49
1:B:103:MET:HE3	7:B:875:HOH:O	2.12	0.49
3:B:506:SO4:O1	7:B:1039:HOH:O	2.18	0.48
1:C:44:ASN:HD21	1:C:46:GLN:HE21	1.57	0.48
1:C:67:HIS:CE1	1:C:244:ALA:HB1	2.48	0.48
1:B:310:HIS:HD2	1:B:421:ASP:O	1.96	0.48
1:B:320:ASN:HB3	1:B:322:HIS:CE1	2.49	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:HG23	4:C:507:GOL:O1	2.14	0.48
1:B:179:THR:CG2	1:B:183:VAL:HA	2.44	0.48
1:C:394:GLY:O	1:C:458:HIS:HE1	1.97	0.48
1:A:111:SER:HB2	1:A:121:LEU:HD13	1.96	0.48
4:B:511:GOL:H12	7:B:760:HOH:O	2.13	0.47
1:B:54:ILE:HG13	7:C:603:HOH:O	2.14	0.47
1:B:155:VAL:HG22	1:C:1:VAL:CG1	2.43	0.47
1:C:366:ALA:HB3	3:C:505:SO4:O3	2.14	0.47
1:B:59:LEU:HD21	1:B:158[B]:LYS:CE	2.43	0.47
1:A:2:GLN:NE2	7:A:1091:HOH:O	2.47	0.47
1:A:163:GLY:HA3	7:A:746:HOH:O	2.14	0.47
1:C:364:ASN:HB2	7:C:946:HOH:O	2.14	0.47
1:B:180:HIS:CD2	1:B:270:GLY:H	2.33	0.47
1:B:209:ASP:HB3	1:B:210:PRO:HD3	1.97	0.47
1:B:482:GLU:HG2	7:B:608:HOH:O	2.15	0.47
1:C:162:ALA:CB	1:C:163:GLY:HA2	2.37	0.47
1:B:178:ARG:HG2	1:B:186:VAL:HG22	1.96	0.47
1:C:179:THR:HG23	1:C:183:VAL:HA	1.97	0.46
1:A:65:HIS:NE2	1:A:67:HIS:HA	2.30	0.46
1:A:103:MET:CE	7:A:935:HOH:O	2.63	0.46
1:A:436:ASN:OD1	5:A:511:CBS:C1B	2.64	0.46
1:C:301:THR:HB	7:C:755:HOH:O	2.16	0.46
1:A:155:VAL:HG13	7:A:702:HOH:O	2.15	0.46
1:A:198:ARG:HD3	7:A:1073:HOH:O	2.16	0.46
1:C:164:GLY:HA2	1:C:165:ALA:CB	2.27	0.46
1:C:2:GLN:HG2	1:C:36:VAL:HB	1.96	0.46
1:A:386:ILE:HD12	1:A:441:PHE:HE1	1.79	0.46
1:A:394:GLY:HA2	1:A:395:GLY:HA3	1.65	0.46
1:B:301:THR:HG21	7:B:927:HOH:O	2.17	0.45
1:A:36:VAL:HG21	1:A:143:ASP:OD2	2.16	0.45
1:A:100:VAL:HG23	1:A:100:VAL:O	2.16	0.45
1:A:323:GLN:HG2	7:A:1129:HOH:O	2.16	0.45
1:B:53:LEU:O	1:B:90:VAL:CG2	2.58	0.45
1:A:107:TYR:HB2	1:A:125:PHE:HB3	1.99	0.45
1:A:108:TRP:CE3	1:A:206:ILE:HG22	2.52	0.45
1:B:320:ASN:O	1:B:322:HIS:N	2.40	0.45
1:B:430:ILE:HA	1:B:437:VAL:HG21	1.99	0.45
5:A:511:CBS:H62B	7:A:1055:HOH:O	2.17	0.44
1:C:53:LEU:O	1:C:90:VAL:CG2	2.59	0.44
1:B:68:GLY:O	1:B:103:MET:CE	2.62	0.44
1:C:366:ALA:HB3	3:C:505:SO4:S	2.57	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ALA:CB	1:C:166:ILE:CD1	2.81	0.44
1:B:392:ALA:O	1:B:397:HIS:HE1	2.00	0.44
1:A:97:ASN:C	1:A:97:ASN:HD22	2.21	0.44
1:B:60:VAL:HG21	7:B:846:HOH:O	2.17	0.44
1:C:41:VAL:HG13	1:C:103:MET:O	2.18	0.44
1:B:342:VAL:CG2	7:B:761:HOH:O	2.47	0.43
1:B:158[B]:LYS:HE2	7:B:834:HOH:O	2.17	0.43
1:A:263:ARG:HB3	1:A:273:PHE:CE1	2.54	0.43
1:C:92:ASN:ND2	7:C:989:HOH:O	2.51	0.43
1:A:59:LEU:HD11	1:A:158[A]:LYS:HE2	2.00	0.43
1:C:111:SER:HB2	1:C:121:LEU:HD13	2.00	0.43
1:A:67:HIS:C	1:A:67:HIS:CD2	2.92	0.43
1:B:163:GLY:HA2	1:B:164:GLY:HA3	1.81	0.43
1:B:305:ILE:HD13	7:B:796:HOH:O	2.19	0.43
1:C:170:SER:HA	1:C:180:HIS:CE1	2.54	0.43
1:C:232:GLN:NE2	1:C:310:HIS:HB2	2.33	0.43
1:C:400:HIS:CD2	6:C:510:PER:O1	2.72	0.43
1:C:113:LEU:HG	1:C:114:THR:HG22	2.00	0.43
1:C:17:VAL:HG12	1:C:21:PHE:C	2.38	0.43
1:C:195:VAL:HG11	7:C:703:HOH:O	2.19	0.43
1:C:331:ASN:OD1	5:C:509:CBS:H5B	2.19	0.42
1:A:79:GLY:N	1:A:80:PRO:HD2	2.34	0.42
1:B:17:VAL:HG12	1:B:22:VAL:HA	2.01	0.42
1:C:79:GLY:N	1:C:80:PRO:CD	2.82	0.42
1:B:22:VAL:CG2	7:C:642:HOH:O	2.67	0.42
1:B:303[A]:CYS:SG	7:B:706:HOH:O	2.48	0.42
1:C:186:VAL:HG23	7:C:714:HOH:O	2.20	0.42
1:C:209:ASP:HA	1:C:455:ILE:HG23	2.00	0.42
1:B:349:THR:HA	1:B:350:PRO:HD3	1.88	0.42
1:A:180:HIS:CD2	1:A:270:GLY:H	2.38	0.42
1:A:87:PRO:HG2	1:A:491:TYR:CE1	2.55	0.42
1:C:394:GLY:O	1:C:458:HIS:CE1	2.73	0.42
1:C:151:ASP:OD1	1:C:151:ASP:N	2.53	0.41
1:C:41:VAL:HG11	7:C:978:HOH:O	2.21	0.41
1:B:209:ASP:C	1:B:209:ASP:OD1	2.58	0.41
1:A:83:ILE:HD11	1:A:348:PHE:HZ	1.83	0.41
1:C:162:ALA:HA	1:C:164:GLY:HA3	2.03	0.41
1:C:16:ILE:HD11	1:C:152:TRP:CH2	2.55	0.41
1:C:75:ASN:OD1	1:C:448:PRO:HD2	2.20	0.41
1:A:162:ALA:HB3	7:A:1034:HOH:O	2.21	0.41
1:C:299:VAL:HG12	7:C:1026:HOH:O	2.19	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:MET:CE	1:A:160:MET:HA	2.51	0.41
1:B:178:ARG:HG2	1:B:186:VAL:CG2	2.51	0.41
1:B:400:HIS:HB2	1:B:427:VAL:HG22	2.03	0.41
1:C:164:GLY:CA	7:C:1076:HOH:O	2.66	0.41
1:B:386:ILE:CD1	1:B:441:PHE:HE1	2.34	0.41
1:B:95:SER:HB3	7:B:675:HOH:O	2.21	0.41
1:A:16:ILE:HG22	1:C:22:VAL:HG21	2.03	0.41
1:B:404:HIS:NE2	1:B:469:GLU:OE1	2.48	0.41
1:C:404:HIS:NE2	1:C:469:GLU:OE1	2.51	0.41
1:C:310:HIS:HD2	1:C:421:ASP:O	2.03	0.40
1:A:341:PHE:HB3	1:A:463:PHE:CD1	2.55	0.40
1:A:72:LYS:HA	1:A:445:ASN:OD1	2.21	0.40
1:A:160:MET:HE3	1:A:160:MET:HA	2.03	0.40
1:B:155:VAL:HG22	1:C:1:VAL:HG13	2.02	0.40
1:B:161:GLY:HA3	1:B:166:ILE:HD11	2.03	0.40
1:C:71:GLN:HE22	1:C:98:PHE:CB	2.34	0.40
1:A:311:PRO:HD3	1:A:423:ILE:HA	2.03	0.40
1:C:195:VAL:CG1	7:C:703:HOH:O	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:719:HOH:O	7:B:1004:HOH:O[1_655]	2.17	0.03

## 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%)	474 (95%)	20 (4%)	4 (1%)	22	14
1	B	497/495 (100%)	473 (95%)	20 (4%)	4 (1%)	22	14

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	496/495 (100%)	473 (95%)	20 (4%)	3 (1%)	28	20
All	All	1491/1485 (100%)	1420 (95%)	60 (4%)	11 (1%)	25	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ALA
1	B	162	ALA
1	A	394	GLY
1	C	209	ASP
1	A	209	ASP
1	B	161	GLY
1	B	209	ASP
1	C	327	ASP
1	A	59	LEU
1	B	321	PRO
1	C	59	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/406 (101%)	387 (95%)	22 (5%)	26	20
1	B	406/406 (100%)	383 (94%)	23 (6%)	24	18
1	C	406/406 (100%)	377 (93%)	29 (7%)	17	11
All	All	1221/1218 (100%)	1147 (94%)	74 (6%)	23	16

All (74) 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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	117	TYR
1	A	156	LEU
1	A	158[A]	LYS
1	A	158[B]	LYS
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	329	ASN
1	A	349	THR
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	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
1	B	297	SER
1	B	299	VAL
1	B	301	THR
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	463	PHE
1	B	476	SER
1	C	15	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	41	VAL
1	C	54	ILE
1	C	69	GLU
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	167	THR
1	C	195	VAL
1	C	226	THR
1	C	246	ARG
1	C	285	ASP
1	C	297	SER
1	C	302	LYS
1	C	303	CYS
1	C	314	ARG
1	C	329	ASN
1	C	331	ASN
1	C	349	THR
1	C	417	SER
1	C	450	PHE
1	C	451	LEU
1	C	460	ASP
1	C	463	PHE
1	C	465	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) 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	92	ASN
1	A	97	ASN
1	A	180	HIS
1	A	182	ASN
1	A	265	ASN
1	A	310	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	320	ASN
1	A	323	GLN
1	A	329	ASN
1	A	414	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	255	GLN
1	B	310	HIS
1	B	358	GLN
1	B	397	HIS
1	B	486	ASN
1	C	2	GLN
1	C	44	ASN
1	C	52	GLN
1	C	71	GLN
1	C	85	GLN
1	C	92	ASN
1	C	136	ASN
1	C	180	HIS
1	C	232	GLN
1	C	310	HIS
1	C	329	ASN
1	C	358	GLN
1	C	473	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	0.12	0	6,6,6	0.42	0
3	SO4	A	506	-	4,4,4	0.19	0	6,6,6	0.19	0
3	SO4	A	507	-	4,4,4	0.15	0	6,6,6	0.29	0
4	GOL	A	508	-	5,5,5	0.28	0	5,5,5	0.58	0
4	GOL	A	509	-	5,5,5	0.26	0	5,5,5	0.54	0
5	CBS	A	510	-	29,29,30	1.18	2 (6%)	36,41,43	2.04	10 (27%)
5	CBS	A	511	-	29,29,30	1.08	3 (10%)	36,41,43	1.61	8 (22%)
6	PER	A	512	2	0,1,1	0.00	-	0,0,0	0.00	-
3	SO4	B	505	-	4,4,4	0.24	0	6,6,6	0.30	0
3	SO4	B	506	-	4,4,4	0.26	0	6,6,6	0.35	0
3	SO4	B	507	-	4,4,4	0.20	0	6,6,6	0.20	0
4	GOL	B	508	-	5,5,5	0.58	0	5,5,5	0.97	0
4	GOL	B	509	-	5,5,5	0.18	0	5,5,5	0.73	0
4	GOL	B	510	-	5,5,5	0.23	0	5,5,5	0.43	0
4	GOL	B	511	-	5,5,5	0.21	0	5,5,5	0.61	0
5	CBS	B	512	1	29,29,30	0.66	0	36,41,43	2.32	9 (25%)
5	CBS	B	513	-	29,29,30	1.01	2 (6%)	36,41,43	2.11	12 (33%)
6	PER	B	514	2	0,1,1	0.00	-	0,0,0	0.00	-
3	SO4	C	505	-	4,4,4	0.16	0	6,6,6	0.41	0
4	GOL	C	506	-	5,5,5	0.24	0	5,5,5	0.61	0
4	GOL	C	507	-	5,5,5	0.11	0	5,5,5	0.37	0
5	CBS	C	508	1	29,29,30	2.55	5 (17%)	36,41,43	2.59	10 (27%)
5	CBS	C	509	1	14,14,30	0.87	0	15,19,43	1.67	5 (33%)
6	PER	C	510	2	0,1,1	0.00	-	0,0,0	0.00	-

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
6	PER	A	512	2	-	0/0/0/0	0/0/0/0
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
5	CBS	B	512	1	-	0/16/53/56	0/2/2/2
5	CBS	B	513	-	-	0/16/53/56	0/2/2/2
6	PER	B	514	2	-	0/0/0/0	0/0/0/0
3	SO4	C	505	-	-	0/0/0/0	0/0/0/0
4	GOL	C	506	-	-	0/4/4/4	0/0/0/0
4	GOL	C	507	-	-	0/4/4/4	0/0/0/0
5	CBS	C	508	1	-	1/16/53/56	0/2/2/2
5	CBS	C	509	1	-	0/6/23/56	0/1/1/2
6	PER	C	510	2	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	510	CBS	O5B-C1B	-3.29	1.38	1.43
5	B	513	CBS	C2A-N2A	-2.49	1.41	1.45
5	A	511	CBS	O7B-C7B	-2.46	1.17	1.23
5	A	511	CBS	C2B-N2B	-2.29	1.42	1.46
5	A	511	CBS	O5B-C1B	-2.25	1.40	1.43
5	A	510	CBS	C2A-N2A	-2.14	1.42	1.45
5	C	508	CBS	O5A-C5A	-2.10	1.39	1.44
5	B	513	CBS	O1A-C4B	-2.01	1.39	1.43
5	C	508	CBS	C8A-C7A	2.08	1.55	1.50
5	C	508	CBS	C7B-N2B	2.62	1.44	1.34
5	C	508	CBS	O7A-C7A	8.43	1.43	1.23
5	C	508	CBS	O7B-C7B	8.98	1.44	1.23



All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	508	CBS	C3A-C2A-N2A	-9.89	91.67	110.61
5	B	512	CBS	C6A-C5A-C4A	-6.83	97.01	113.00
5	A	511	CBS	C3A-C2A-N2A	-4.16	102.65	110.61
5	B	513	CBS	C8A-C7A-N2A	-3.83	109.19	116.11
5	B	512	CBS	O5B-C1B-C2B	-3.74	106.27	111.47
5	B	513	CBS	O3B-C3B-C4B	-3.72	101.41	109.87
5	C	508	CBS	C3A-C4A-C5A	-3.70	103.69	110.22
5	B	513	CBS	O1A-C4B-C3B	-3.69	98.30	107.19
5	B	512	CBS	O3A-C3A-C4A	-3.63	102.45	110.36
5	A	510	CBS	C2A-N2A-C7A	-3.47	114.41	123.19
5	C	508	CBS	O3A-C3A-C2A	-3.44	102.64	109.61
5	B	512	CBS	C3A-C2A-N2A	-3.36	104.16	110.61
5	A	511	CBS	C1A-C2A-N2A	-3.32	105.42	111.03
5	B	513	CBS	O1A-C1A-C2A	-2.93	102.51	108.23
5	A	510	CBS	O1A-C4B-C5B	-2.83	102.38	109.34
5	C	508	CBS	O7A-C7A-N2A	-2.60	116.92	121.92
5	B	513	CBS	O4A-C4A-C3A	-2.50	104.93	110.36
5	C	508	CBS	O5A-C1A-C2A	-2.43	105.68	110.65
5	A	510	CBS	O4A-C4A-C3A	-2.38	105.18	110.36
5	C	509	CBS	C6B-C5B-C4B	-2.34	107.53	113.00
5	B	513	CBS	C8B-C7B-N2B	-2.27	112.01	116.11
5	A	511	CBS	C6B-C5B-C4B	-2.24	107.12	113.24
5	A	511	CBS	O3A-C3A-C4A	-2.20	105.58	110.36
5	A	510	CBS	O5A-C5A-C6A	-2.18	101.18	106.41
5	A	511	CBS	O1A-C1A-O5A	-2.11	105.57	110.70
5	C	509	CBS	O3B-C3B-C2B	-2.06	104.98	109.39
5	A	510	CBS	C2B-N2B-C7B	-2.01	120.02	122.94
5	A	511	CBS	C8B-C7B-N2B	2.08	119.86	116.11
5	C	509	CBS	O5B-C1B-C2B	2.14	114.45	111.47
5	B	513	CBS	O3A-C3A-C2A	2.16	114.00	109.61
5	B	513	CBS	O3B-C3B-C2B	2.25	114.20	109.39
5	A	511	CBS	C4A-C3A-C2A	2.25	113.66	110.33
5	C	509	CBS	O3B-C3B-C4B	2.27	115.31	110.36
5	A	510	CBS	O5B-C5B-C4B	2.44	114.41	109.98
5	B	512	CBS	O5A-C5A-C6A	2.53	112.48	106.41
5	A	511	CBS	C3A-C4A-C5A	2.55	114.72	110.22
5	C	508	CBS	O1A-C4B-C3B	2.63	113.51	107.19
5	B	513	CBS	O7A-C7A-N2A	2.63	126.98	121.92
5	B	512	CBS	O1A-C4B-C3B	2.91	114.19	107.19
5	B	512	CBS	C3A-C4A-C5A	2.97	115.45	110.22
5	C	508	CBS	O5B-C5B-C4B	2.97	115.39	109.98
5	A	510	CBS	C1A-O5A-C5A	3.15	119.64	113.72

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	510	CBS	C3A-C4A-C5A	3.34	116.10	110.22
5	B	513	CBS	C2B-N2B-C7B	3.52	128.09	122.94
5	B	513	CBS	C1B-O5B-C5B	3.59	117.11	112.17
5	C	508	CBS	C1A-C2A-N2A	3.86	117.56	111.03
5	C	508	CBS	C4A-C3A-C2A	3.94	116.17	110.33
5	B	512	CBS	C1A-O5A-C5A	4.15	121.53	113.72
5	B	513	CBS	C2A-N2A-C7A	4.18	133.77	123.19
5	C	509	CBS	C1B-O5B-C5B	4.22	117.98	112.17
5	C	508	CBS	C1B-O5B-C5B	4.68	118.61	112.17
5	A	510	CBS	C4A-C3A-C2A	4.70	117.30	110.33
5	A	510	CBS	C1B-O5B-C5B	5.22	119.36	112.17
5	B	512	CBS	O5A-C5A-C4A	6.12	120.92	109.66

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	508	CBS	O7B-C7B-N2B-C2B

There are no ring outliers.

16 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	508	GOL	5	0
4	A	509	GOL	1	0
5	A	510	CBS	4	0
5	A	511	CBS	7	0
3	B	506	SO4	5	0
4	B	508	GOL	5	0
4	B	509	GOL	1	0
4	B	510	GOL	1	0
4	B	511	GOL	2	0
5	B	513	CBS	1	0
3	C	505	SO4	2	0
4	C	506	GOL	6	0
4	C	507	GOL	1	0
5	C	508	CBS	1	0
5	C	509	CBS	1	0
6	C	510	PER	1	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	495/495 (100%)	-0.52	8 (1%) 72 77	10, 18, 32, 44	0
1	B	495/495 (100%)	-0.40	4 (0%) 86 89	11, 21, 38, 53	0
1	C	495/495 (100%)	-0.36	13 (2%) 56 64	11, 22, 38, 53	0
All	All	1485/1485 (100%)	-0.42	25 (1%) 70 76	10, 20, 36, 53	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	415	SER	3.7
1	B	320	ASN	3.6
1	C	328	CYS	3.2
1	C	164	GLY	3.0
1	B	415	SER	2.9
1	C	433	VAL	2.9
1	C	165	ALA	2.9
1	C	321	PRO	2.6
1	C	381	ASN	2.6
1	A	164	GLY	2.5
1	C	320	ASN	2.5
1	A	320	ASN	2.5
1	A	415	SER	2.4
1	C	393	ALA	2.4
1	A	394	GLY	2.3
1	B	433	VAL	2.2
1	A	161	GLY	2.1
1	B	362	GLY	2.1
1	C	161	GLY	2.1
1	C	324	GLY	2.1
1	A	313	SER	2.1
1	A	433	VAL	2.1
1	C	372	SER	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	165	ALA	2.0
1	C	323	GLN	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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	508	6/6	0.90	0.33	18.00	38,40,42,43	0
3	SO4	C	505	5/5	0.80	0.33	10.04	34,35,35,36	5
5	CBS	A	510	28/29	0.86	0.18	8.38	38,45,53,55	0
4	GOL	C	506	6/6	0.79	0.25	7.86	41,44,47,49	0
5	CBS	B	512	28/29	0.64	0.28	5.85	76,79,80,80	0
4	GOL	B	510	6/6	0.90	0.16	3.49	39,40,41,43	0
6	PER	A	512	2/2	0.99	0.11	3.27	30,30,30,33	0
4	GOL	A	508	6/6	0.83	0.18	3.05	40,41,42,42	0
5	CBS	A	511	28/29	0.71	0.24	2.88	41,55,63,63	0
5	CBS	B	513	28/29	0.64	0.28	2.54	52,65,73,73	0
5	CBS	C	508	28/29	0.77	0.22	2.49	57,62,65,66	0
3	SO4	A	505	5/5	0.96	0.11	2.44	41,42,43,43	0
6	PER	C	510	2/2	1.00	0.08	2.31	18,18,18,20	0
4	GOL	C	507	6/6	0.91	0.14	2.00	27,29,32,36	0
3	SO4	A	506	5/5	0.98	0.15	1.77	53,53,53,54	0
6	PER	B	514	2/2	0.99	0.08	1.11	36,36,36,37	0
5	CBS	C	509	14/29	0.83	0.18	0.61	58,60,61,63	0
4	GOL	A	509	6/6	0.97	0.08	0.17	21,26,26,28	0
4	GOL	B	511	6/6	0.97	0.08	0.14	22,25,26,27	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	C	503	1/1	1.00	0.07	-0.26	15,15,15,15	0
2	CU	C	504	1/1	0.99	0.07	-0.58	19,19,19,19	0
2	CU	C	502	1/1	1.00	0.07	-0.62	20,20,20,20	0
4	GOL	B	509	6/6	0.94	0.08	-0.70	27,31,32,32	0
3	SO4	B	506	5/5	0.99	0.06	-1.18	24,25,28,28	0
2	CU	A	503	1/1	1.00	0.06	-1.42	14,14,14,14	0
2	CU	A	502	1/1	0.99	0.06	-1.65	18,18,18,18	0
2	CU	B	501	1/1	1.00	0.06	-1.79	17,17,17,17	0
2	CU	B	502	1/1	1.00	0.05	-1.84	21,21,21,21	0
2	CU	C	501	1/1	1.00	0.04	-2.05	22,22,22,22	0
2	CU	A	504	1/1	1.00	0.04	-2.42	16,16,16,16	0
2	CU	B	503	1/1	1.00	0.05	-2.70	18,18,18,18	0
2	CU	A	501	1/1	1.00	0.04	-2.93	18,18,18,18	0
3	SO4	B	505	5/5	0.99	0.04	-2.97	16,21,23,23	0
2	CU	B	504	1/1	0.99	0.05	-3.10	20,20,20,20	0
3	SO4	A	507	5/5	0.95	0.10	-	18,20,20,21	5
3	SO4	B	507	5/5	0.93	0.13	-	25,25,26,26	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.