



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 11:29 pm BST

PDB ID : 3RQ1  
Title : Crystal Structure of Aminotransferase Class I and II from *Veillonella parvula*  
Authors : Kim, Y.; Hatzos-Skintges, C.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2011-04-27  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

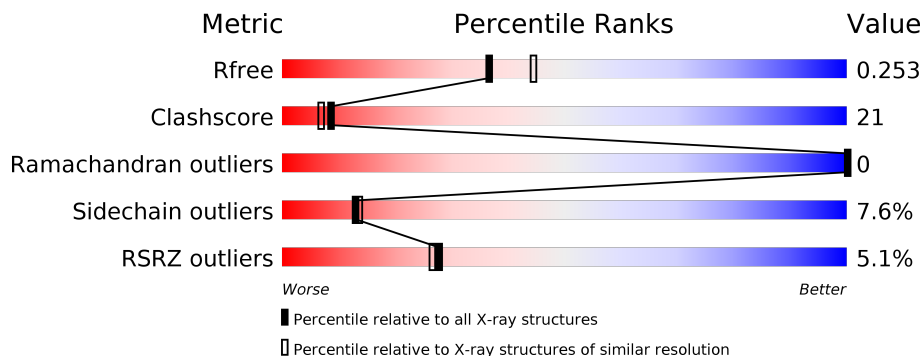
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. 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	418	
1	B	418	
1	C	418	
1	D	418	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	424	-	-	X	-
2	GOL	C	424	-	-	X	-
2	GOL	C	426	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13495 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 Aminotransferase class I and II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	414	3310	2090	572	630	11	7	0	9	0
1	B	414	3239	2051	554	617	10	7	0	1	0
1	C	413	3291	2078	565	631	10	7	0	8	0
1	D	392	3109	1974	527	593	9	6	0	5	0

There are 12 discrepancies between the modelled and reference sequences:

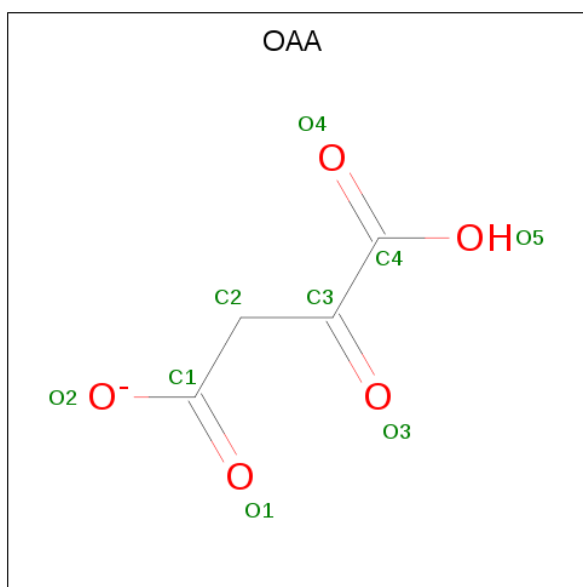
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP D1BN29
A	-1	ASN	-	EXPRESSION TAG	UNP D1BN29
A	0	ALA	-	EXPRESSION TAG	UNP D1BN29
B	-2	SER	-	EXPRESSION TAG	UNP D1BN29
B	-1	ASN	-	EXPRESSION TAG	UNP D1BN29
B	0	ALA	-	EXPRESSION TAG	UNP D1BN29
C	-2	SER	-	EXPRESSION TAG	UNP D1BN29
C	-1	ASN	-	EXPRESSION TAG	UNP D1BN29
C	0	ALA	-	EXPRESSION TAG	UNP D1BN29
D	-2	SER	-	EXPRESSION TAG	UNP D1BN29
D	-1	ASN	-	EXPRESSION TAG	UNP D1BN29
D	0	ALA	-	EXPRESSION TAG	UNP D1BN29

- Molecule 2 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
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 12 6 6	0	1

- Molecule 3 is OXALOACETATE ION (three-letter code: OAA) (formula:  $C_4H_3O_5$ ).

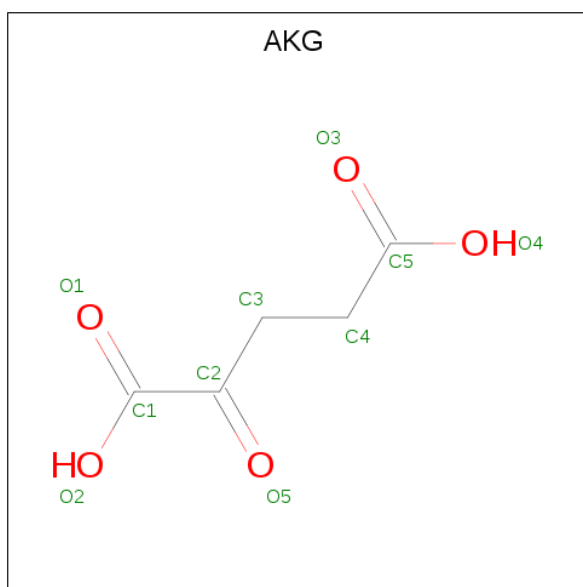


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 4 5	0	0
3	B	1	Total C O 9 4 5	0	0
3	C	1	Total C O 9 4 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	5	5		

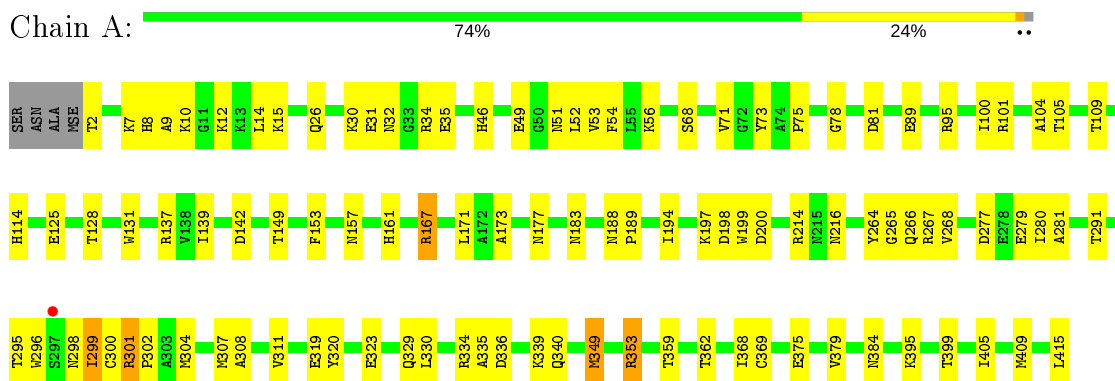
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total	O	0	0
			135	135		
6	B	82	Total	O	0	0
			82	82		
6	C	121	Total	O	0	0
			121	121		
6	D	104	Total	O	0	0
			104	104		

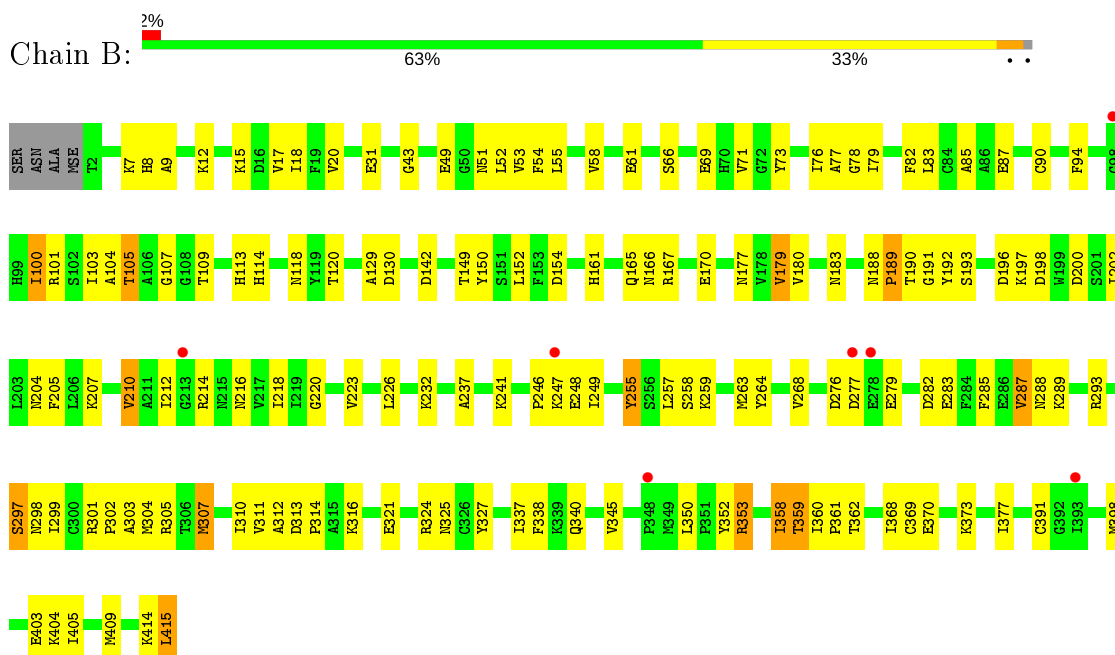
### 3 Residue-property plots [i](#)

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: Aminotransferase class I and II



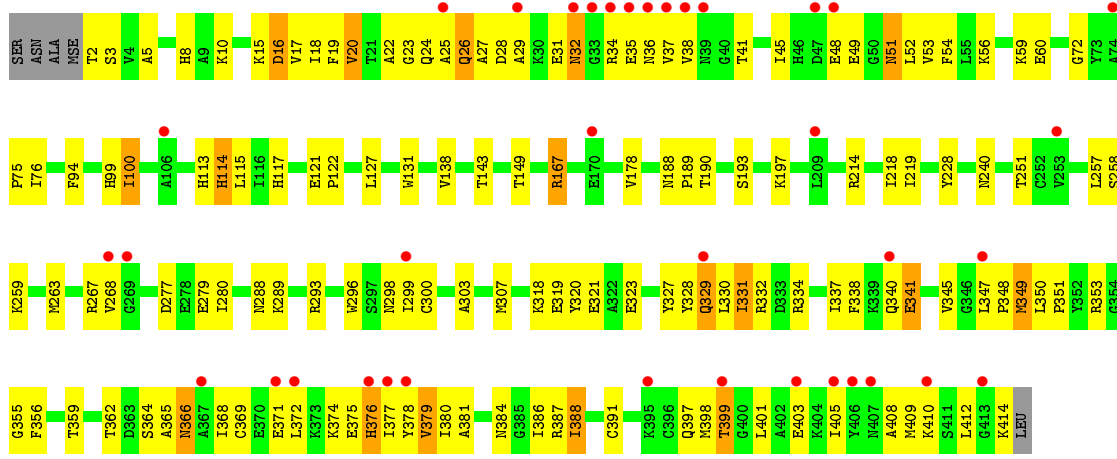
- Molecule 1: Aminotransferase class I and II



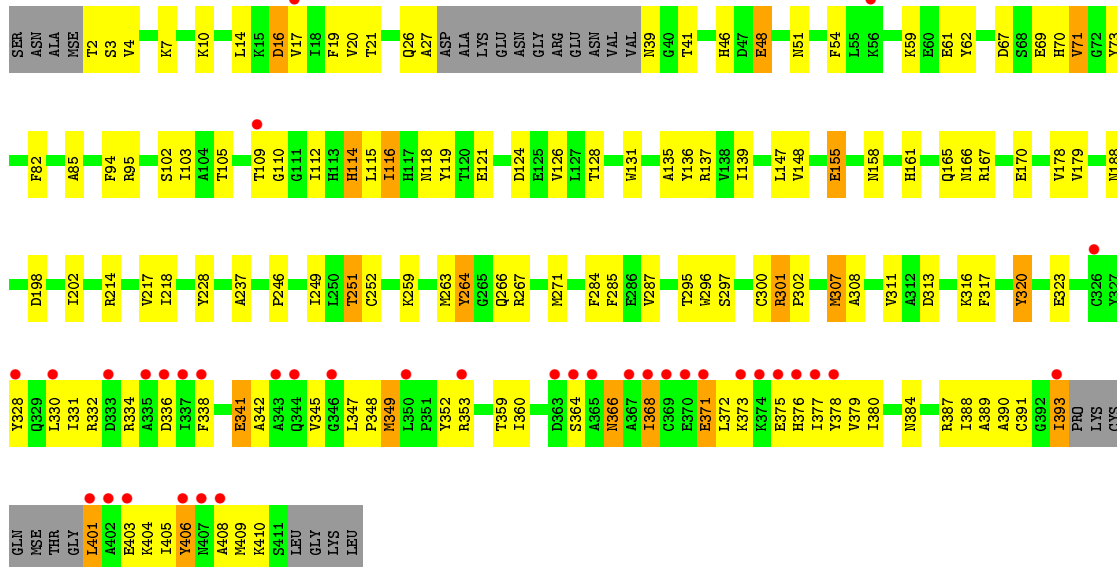
- Molecule 1: Aminotransferase class I and II







• Molecule 1: Aminotransferase class I and II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.99Å 81.06Å 106.39Å 102.40° 101.37° 102.95°	Depositor
Resolution (Å)	42.40 – 2.20 42.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (42.40-2.20) 96.5 (42.40-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.190 , 0.263 0.183 , 0.253	Depositor DCC
$R_{free}$ test set	4226 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtrriage
Anisotropy	0.553	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13495	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AKG, OAA, CL

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	0.69	0/3371	0.81	0/4548
1	B	0.63	0/3300	0.78	0/4454
1	C	0.68	0/3353	0.80	2/4527 (0.0%)
1	D	0.67	0/3169	0.82	5/4280 (0.1%)
All	All	0.67	0/13193	0.80	7/17809 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	95	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	387	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	C	188	ASN	C-N-CD	-5.48	108.55	120.60
1	D	119	TYR	N-CA-C	5.47	125.78	111.00
1	D	188	ASN	C-N-CD	-5.33	108.86	120.60
1	C	94	PHE	N-CA-C	5.26	125.21	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	228	TYR	Mainchain
1	D	228	TYR	Mainchain

## 5.2 Too-close contacts [i](#)

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	3310	0	3224	95	0
1	B	3239	0	3163	159	0
1	C	3291	0	3194	155	0
1	D	3109	0	3016	153	0
2	A	18	0	24	10	0
2	B	6	0	8	1	0
2	C	18	0	24	17	0
2	D	24	0	32	5	0
3	A	9	0	2	0	0
3	B	9	0	2	0	0
3	C	9	0	2	1	0
4	C	1	0	0	0	0
5	C	10	0	4	3	0
6	A	135	0	0	8	0
6	B	82	0	0	15	0
6	C	121	0	0	10	0
6	D	104	0	0	5	0
All	All	13495	0	12695	531	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 21.

All (531) 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:339:LYS:HG2	1:A:349:MSE:HE1	1.25	1.14
1:C:189:PRO:HB2	1:C:359[B]:THR:HG21	1.37	1.07
1:C:29:ALA:HB2	1:C:37:VAL:HG11	1.30	1.06
1:C:267:ARG:NH2	2:C:426:GOL:H31	1.72	1.03
1:D:7:LYS:HA	1:D:10:LYS:HE2	1.43	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:LYS:O	1:B:415:LEU:HB2	1.63	0.98
1:C:267:ARG:HH22	2:C:426:GOL:H31	1.29	0.96
1:C:364:SER:OG	1:C:414:LYS:HE2	1.66	0.95
1:B:263:MSE:HA	1:D:71:VAL:HG22	1.47	0.95
1:B:232:LYS:NZ	1:B:325:ASN:HD21	1.64	0.94
1:C:368:ILE:HD13	1:C:409:MSE:HG2	1.51	0.92
1:B:257:LEU:HD13	1:B:263:MSE:HE3	1.52	0.91
1:C:347:LEU:HD12	1:C:348:PRO:HD2	1.52	0.90
1:A:368:ILE:HD13	1:A:409:MSE:HG2	1.52	0.89
1:D:54:PHE:CE2	1:D:59:LYS:HB2	2.07	0.88
1:D:54:PHE:CD2	1:D:59:LYS:HB2	2.08	0.88
1:C:113:HIS:HD2	1:C:114:HIS:ND1	1.72	0.87
1:D:54:PHE:HE2	1:D:59:LYS:CB	1.87	0.87
1:B:232:LYS:HZ1	1:B:325:ASN:HD21	1.23	0.86
1:C:131:TRP:CH2	1:C:384:ASN:HB3	2.10	0.86
1:D:368:ILE:HD12	1:D:409:MSE:HG2	1.55	0.86
1:D:313:ASP:HB3	1:D:316:LYS:HB2	1.60	0.84
1:C:117:HIS:HB2	2:C:424:GOL:H2	1.58	0.83
1:B:71:VAL:HG13	1:D:54:PHE:CE1	2.13	0.83
1:D:112:ILE:O	1:D:116[A]:ILE:HG22	1.77	0.83
1:D:330:LEU:HG	1:D:334:ARG:HE	1.43	0.83
1:B:223:VAL:HG12	1:B:226:LEU:HB2	1.60	0.82
1:A:52:LEU:HD23	1:A:53:VAL:N	1.93	0.82
1:A:335:ALA:O	1:A:339:LYS:HG3	1.80	0.82
1:B:78:GLY:CA	1:B:304:MSE:HE1	2.10	0.81
1:D:54:PHE:CE2	1:D:59:LYS:CB	2.62	0.81
1:C:117:HIS:CA	2:C:424:GOL:H2	2.10	0.81
1:B:223:VAL:CG1	1:B:226:LEU:HB2	2.10	0.81
1:A:307:MSE:HE2	1:A:311:VAL:HG21	1.63	0.81
1:B:368:ILE:HD13	1:B:409:MSE:HG2	1.60	0.81
1:D:178:VAL:CG1	1:D:217:VAL:HG22	2.11	0.81
1:B:78:GLY:HA3	1:B:304:MSE:HE1	1.62	0.80
1:B:293:ARG:HA	1:B:297:SER:HA	1.64	0.80
1:C:117:HIS:CB	2:C:424:GOL:H2	2.11	0.80
1:C:258:SER:HA	1:C:263:MSE:O	1.82	0.79
1:A:9:ALA:O	1:A:12:LYS:HG3	1.83	0.79
1:C:318:LYS:HA	1:C:321:GLU:HG2	1.65	0.78
1:A:266:GLN:HA	6:A:458:HOH:O	1.83	0.78
1:C:131:TRP:CZ2	1:C:350:LEU:HD11	2.19	0.78
1:C:189:PRO:HB2	1:C:359[B]:THR:CG2	2.14	0.77
1:B:337:ILE:O	1:B:340[A]:GLN:HG2	1.85	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:CG1	1:D:54:PHE:CD1	2.68	0.76
1:C:117:HIS:HA	2:C:424:GOL:H2	1.67	0.76
1:D:375:GLU:O	1:D:376:HIS:CG	2.38	0.76
1:B:177:ASN:OD1	1:B:216:ASN:HB2	1.86	0.76
1:D:331:ILE:HA	1:D:334:ARG:HD2	1.66	0.76
1:B:71:VAL:HG13	1:D:54:PHE:CD1	2.22	0.75
1:B:352:TYR:CD1	1:B:358:ILE:HD11	2.21	0.75
1:D:347:LEU:HB2	1:D:406:TYR:CE1	2.22	0.74
1:C:318:LYS:HG2	1:C:321:GLU:OE2	1.88	0.74
1:D:16:ASP:O	1:D:20:VAL:HG23	1.87	0.74
1:D:373:LYS:HD3	1:D:378:TYR:CE1	2.21	0.74
1:D:328[B]:TYR:HA	1:D:331:ILE:HG22	1.68	0.74
1:A:101[A]:ARG:HG3	1:A:281:ALA:O	1.88	0.73
1:B:190:THR:HA	1:B:359:THR:HG22	1.70	0.73
1:D:331:ILE:HD12	1:D:334:ARG:HD2	1.71	0.73
1:B:204:ASN:HA	1:B:207:LYS:HE2	1.71	0.73
1:C:369:CYS:SG	1:C:381:ALA:HB2	2.28	0.73
1:B:113:HIS:CD2	1:D:295:THR:HG22	2.23	0.73
1:D:155:GLU:HG3	6:D:417:HOH:O	1.87	0.72
1:D:179:VAL:HG22	1:D:218:ILE:HB	1.71	0.72
1:B:166:ASN:O	1:B:170:GLU:HG3	1.88	0.72
1:D:368:ILE:O	1:D:372:LEU:HG	1.90	0.72
1:D:267:ARG:HH22	2:D:423[B]:GOL:H2	1.55	0.71
1:D:307:MSE:O	1:D:307:MSE:HE3	1.91	0.71
1:C:327:TYR:O	1:C:331:ILE:HG23	1.88	0.71
1:B:71:VAL:CG1	1:D:54:PHE:CE1	2.73	0.71
1:B:313:ASP:HB3	1:B:316:LYS:HD3	1.73	0.71
1:B:212:ILE:CG2	1:B:214:ARG:HH12	2.04	0.71
1:A:26:GLN:HE21	2:A:424:GOL:H32	1.54	0.71
1:D:328[A]:TYR:HA	1:D:331:ILE:HG22	1.71	0.70
1:D:54:PHE:HE2	1:D:59:LYS:CA	2.03	0.70
1:B:258:SER:HB2	6:B:491:HOH:O	1.91	0.70
1:A:299[A]:ILE:HG13	1:A:304:MSE:HE2	1.71	0.70
1:C:379:VAL:HG21	1:C:388:ILE:HD13	1.72	0.70
1:C:127:LEU:CD1	1:C:167:ARG:HG2	2.21	0.70
1:A:49:GLU:HG2	6:A:444:HOH:O	1.90	0.70
1:B:352:TYR:CD1	1:B:358:ILE:CD1	2.75	0.70
1:C:3:SER:OG	1:C:10:LYS:HE3	1.92	0.69
1:C:376:HIS:HA	1:C:378:TYR:HE2	1.57	0.69
1:C:127:LEU:HD13	1:C:167:ARG:HG2	1.75	0.69
1:D:131:TRP:CH2	1:D:384:ASN:HB3	2.27	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ILE:HG21	1:C:409:MSE:HG3	1.73	0.69
1:D:54:PHE:HE2	1:D:59:LYS:HA	1.58	0.68
1:C:113:HIS:CD2	1:C:114:HIS:ND1	2.60	0.68
1:A:291:THR:O	1:A:295:THR:HG23	1.92	0.68
1:A:300:CYS:HB2	6:C:526:HOH:O	1.93	0.68
1:D:328[A]:TYR:CZ	1:D:332:ARG:HD3	2.29	0.67
1:C:379:VAL:HG11	1:C:386:ILE:HG22	1.76	0.67
1:C:338:PHE:HB2	1:C:398:MSE:CE	2.24	0.67
1:A:265:GLY:HA3	1:C:72:GLY:O	1.94	0.67
1:C:20:VAL:HG23	6:C:440:HOH:O	1.95	0.67
1:C:257:LEU:HD21	1:C:307:MSE:HE3	1.77	0.67
1:C:338:PHE:CD1	1:C:398:MSE:HE3	2.30	0.67
1:B:12:LYS:CE	1:D:287:VAL:HG13	2.26	0.67
1:D:375:GLU:O	1:D:376:HIS:CD2	2.49	0.67
1:B:190:THR:HA	1:B:359:THR:CG2	2.24	0.66
1:C:193:SER:HB2	1:C:353:ARG:HD3	1.76	0.66
1:D:307:MSE:HE1	1:D:311:VAL:HG21	1.76	0.66
1:A:308:ALA:HB1	6:A:470:HOH:O	1.96	0.66
1:C:366:ASN:H	1:C:366:ASN:ND2	1.91	0.66
1:A:26:GLN:NE2	2:A:424:GOL:H32	2.10	0.66
1:C:117:HIS:HB2	2:C:424:GOL:H32	1.77	0.66
1:B:8:HIS:CE1	6:B:429:HOH:O	2.48	0.66
1:C:143:THR:CG2	2:C:424:GOL:H11	2.27	0.65
1:B:350:LEU:HD21	1:B:361:PRO:HG3	1.77	0.65
1:B:12:LYS:HE3	1:D:287:VAL:HG13	1.78	0.65
1:B:223:VAL:O	1:B:223:VAL:HG12	1.96	0.65
1:D:263:MSE:HB2	1:D:266:GLN:HG2	1.77	0.65
1:C:337:ILE:HG21	1:C:399:THR:HG22	1.78	0.65
1:C:114:HIS:HB3	1:C:288:ASN:ND2	2.12	0.65
1:B:100:ILE:HG12	1:B:101:ARG:N	2.09	0.65
1:C:114:HIS:HB3	1:C:288:ASN:HD22	1.61	0.65
1:C:368:ILE:HD13	1:C:409:MSE:CG	2.25	0.65
1:C:379:VAL:CG1	1:C:386:ILE:HG22	2.27	0.65
1:D:103:ILE:HD11	1:D:285:PHE:HA	1.78	0.65
1:D:161:HIS:O	1:D:165:GLN:HG3	1.96	0.65
1:A:319:GLU:O	1:A:323:GLU:HG3	1.97	0.65
1:D:54:PHE:CE2	1:D:59:LYS:HA	2.32	0.65
1:D:307:MSE:HG3	1:D:308:ALA:N	2.11	0.64
1:B:298:ASN:OD1	1:D:267:ARG:HD3	1.97	0.64
1:C:379:VAL:HG11	1:C:386:ILE:CG2	2.27	0.64
1:B:53:VAL:HG21	1:B:327:TYR:CE1	2.32	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:VAL:HG13	1:D:217:VAL:HG22	1.80	0.64
1:D:328[A]:TYR:OH	1:D:332:ARG:HD3	1.97	0.64
1:A:299[A]:ILE:HG13	1:A:304:MSE:CE	2.27	0.64
1:B:200:ASP:OD1	1:B:241:LYS:HE3	1.97	0.64
1:C:372:LEU:HD11	1:C:405:ILE:HG12	1.80	0.64
1:D:246:PRO:HG2	1:D:249:ILE:HD12	1.79	0.64
1:A:266:GLN:HG2	6:A:458:HOH:O	1.98	0.63
1:B:17:VAL:HG13	1:B:18:ILE:HG13	1.80	0.63
1:C:364:SER:HG	1:C:414:LYS:HE2	1.63	0.63
1:D:334:ARG:NH1	1:D:393:ILE:O	2.31	0.63
1:C:371:GLU:OE1	1:C:412:LEU:HD11	1.99	0.63
1:C:117:HIS:HB2	2:C:424:GOL:C2	2.27	0.63
1:B:90:CYS:HB2	1:B:255:TYR:CD1	2.33	0.63
1:B:113:HIS:ND1	1:B:114:HIS:HD2	1.97	0.63
1:B:71:VAL:HG11	1:D:54:PHE:CD1	2.33	0.63
1:D:264:TYR:N	1:D:264:TYR:CD2	2.67	0.62
1:A:26:GLN:HE21	2:A:424:GOL:C3	2.12	0.62
1:B:312:ALA:O	1:B:314:PRO:HD3	2.00	0.62
1:C:143:THR:HG21	2:C:424:GOL:H11	1.82	0.62
1:C:364:SER:CB	1:C:414:LYS:HE2	2.29	0.62
1:B:7:LYS:HD3	6:B:480:HOH:O	2.00	0.62
1:B:118:ASN:ND2	1:B:287:VAL:HG13	2.14	0.61
1:B:277:ASP:OD1	1:B:279:GLU:HB2	1.99	0.61
1:D:368:ILE:CD1	1:D:409:MSE:HG2	2.27	0.61
1:D:85:ALA:CB	1:D:307:MSE:HE2	2.30	0.61
1:D:85:ALA:HB1	1:D:307:MSE:CE	2.31	0.61
1:C:149:THR:O	1:C:167:ARG:HD2	2.00	0.61
1:B:82:PHE:CD2	1:B:304:MSE:HE2	2.36	0.61
1:C:331:ILE:HG13	1:C:332:ARG:N	2.16	0.61
1:B:73:TYR:HE1	2:D:423[A]:GOL:H12	1.63	0.61
1:C:338:PHE:HB2	1:C:398:MSE:HE2	1.82	0.60
1:A:26:GLN:HE22	5:C:423:AKG:H41	1.66	0.60
1:B:210:VAL:HG21	1:B:249:ILE:HG12	1.82	0.60
1:A:299[A]:ILE:HD11	1:A:304:MSE:SE	2.52	0.60
1:D:48:GLU:N	1:D:48:GLU:CD	2.48	0.60
1:A:125:GLU:OE1	1:A:171:LEU:CD2	2.50	0.60
1:A:277:ASP:HB3	1:A:280:ILE:HG12	1.82	0.60
1:B:118:ASN:CG	1:B:287:VAL:HG13	2.22	0.60
1:D:118:ASN:CG	1:D:287:VAL:HG12	2.22	0.60
1:C:15:LYS:O	1:C:15:LYS:HG3	2.02	0.60
1:C:337:ILE:O	1:C:341[A]:GLU:HG2	2.02	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:CG1	1:D:54:PHE:HD1	2.15	0.59
1:B:313:ASP:OD2	1:B:316:LYS:HD2	2.02	0.59
1:B:78:GLY:HA2	1:B:304:MSE:HE1	1.81	0.59
1:B:71:VAL:HG13	1:D:54:PHE:HE1	1.61	0.59
1:A:298:ASN:O	1:C:267:ARG:CD	2.50	0.59
1:C:299:ILE:HG22	1:C:300:CYS:N	2.18	0.59
1:B:120:THR:HG22	1:B:179:VAL:HG11	1.85	0.59
1:C:143:THR:HG21	2:C:424:GOL:H31	1.84	0.59
1:B:82:PHE:CG	1:B:304:MSE:HG2	2.38	0.59
1:B:352:TYR:CG	1:B:358:ILE:HD11	2.38	0.58
1:B:109:THR:HG21	1:D:297:SER:HB3	1.86	0.58
1:D:41:THR:HB	1:D:380:ILE:HD11	1.85	0.58
1:D:217:VAL:C	1:D:218:ILE:HD13	2.24	0.58
1:C:279:GLU:HG3	6:C:493:HOH:O	2.03	0.58
1:A:183:ASN:ND2	1:A:188:ASN:H	2.02	0.58
1:B:177:ASN:HB2	6:B:483:HOH:O	2.04	0.58
1:C:117:HIS:HB2	2:C:424:GOL:C3	2.34	0.58
1:B:165:GLN:HG2	1:B:205:PHE:CG	2.39	0.57
1:C:329:GLN:HG2	1:C:330:LEU:N	2.18	0.57
1:C:131:TRP:CZ3	1:C:384:ASN:HB3	2.38	0.57
1:D:54:PHE:CE2	1:D:59:LYS:CA	2.84	0.57
1:B:12:LYS:NZ	1:B:142:ASP:OD1	2.35	0.57
1:B:165:GLN:HG2	1:B:205:PHE:CD2	2.39	0.57
1:C:267:ARG:HH22	2:C:426:GOL:C3	2.10	0.57
1:C:29:ALA:HB2	1:C:37:VAL:CG1	2.20	0.57
1:C:27:ALA:HB2	6:C:462:HOH:O	2.03	0.57
1:D:320:TYR:O	1:D:323:GLU:HB2	2.05	0.57
1:B:154:ASP:O	6:B:486:HOH:O	2.18	0.57
1:C:328:TYR:HE1	6:C:536:HOH:O	1.88	0.57
1:B:129:ALA:HB1	1:B:152:LEU:HB2	1.87	0.56
1:C:100:ILE:N	1:C:100:ILE:HD13	2.20	0.56
2:A:421:GOL:H2	1:C:5:ALA:O	2.05	0.56
1:C:299:ILE:CG2	1:C:300:CYS:N	2.68	0.56
1:B:212:ILE:HG22	1:B:214:ARG:NH1	2.20	0.56
1:C:359[B]:THR:HG22	1:C:387:ARG:HA	1.86	0.56
1:C:350:LEU:HB3	1:C:351:PRO:HD2	1.87	0.56
1:C:45:ILE:O	1:C:52:LEU:HD12	2.05	0.56
1:C:38:VAL:CG1	1:C:377:ILE:HA	2.36	0.56
1:B:369:CYS:O	1:B:373:LYS:HG3	2.06	0.56
1:C:143:THR:HG21	2:C:424:GOL:C2	2.35	0.56
1:B:264:TYR:CD2	1:D:71:VAL:HG13	2.40	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:HIS:NE2	1:A:198:ASP:OD1	2.25	0.56
1:C:338:PHE:CD2	1:C:349:MSE:HE2	2.40	0.56
1:B:293:ARG:HD2	1:B:297:SER:HB2	1.86	0.56
1:D:330:LEU:CD2	1:D:334:ARG:HH21	2.19	0.56
1:B:58:VAL:HA	1:B:310:ILE:HD11	1.87	0.55
1:D:330:LEU:O	1:D:330:LEU:HD12	2.06	0.55
1:D:131:TRP:CZ3	1:D:384:ASN:HB3	2.40	0.55
1:B:368:ILE:CD1	1:B:409:MSE:HG2	2.36	0.55
2:A:424:GOL:H32	5:C:423:AKG:O4	2.06	0.55
1:D:331:ILE:HD11	1:D:390:ALA:C	2.27	0.55
1:C:340:GLN:HG3	1:C:341[A]:GLU:N	2.22	0.55
1:B:232:LYS:HE2	1:B:321:GLU:OE2	2.07	0.55
1:B:76:ILE:HB	1:B:289:LYS:CE	2.37	0.55
1:C:257:LEU:HD21	1:C:307:MSE:CE	2.36	0.55
1:C:338:PHE:HD2	1:C:349:MSE:HE2	1.71	0.55
1:B:197:LYS:HD2	1:B:197:LYS:O	2.07	0.55
1:A:336:ASP:HA	1:A:339:LYS:HD2	1.89	0.54
1:B:247:LYS:HG2	1:B:276:ASP:HB3	1.88	0.54
1:C:193:SER:H	1:C:353:ARG:HD2	1.73	0.54
1:B:289:LYS:NZ	6:B:495:HOH:O	2.41	0.54
1:C:143:THR:HG21	2:C:424:GOL:C3	2.38	0.54
1:C:29:ALA:CB	1:C:37:VAL:HG11	2.22	0.54
1:C:193:SER:H	1:C:353:ARG:CD	2.21	0.54
1:D:347:LEU:HB2	1:D:406:TYR:CD1	2.42	0.54
1:C:190:THR:HG22	1:C:350:LEU:HD12	1.89	0.54
1:D:116[A]:ILE:HG12	1:D:116[A]:ILE:O	2.07	0.54
1:D:371:GLU:OE1	1:D:371:GLU:N	2.41	0.53
1:B:212:ILE:HG22	1:B:214:ARG:HH12	1.74	0.53
1:C:340:GLN:HG3	1:C:341[B]:GLU:N	2.24	0.53
1:C:338:PHE:HB2	1:C:398:MSE:HE3	1.90	0.53
1:B:54:PHE:HD2	1:D:67:ASP:OD1	1.91	0.53
1:B:212:ILE:HG21	1:B:214:ARG:HH12	1.72	0.53
1:B:212:ILE:CG2	1:B:214:ARG:NH1	2.72	0.53
1:D:167:ARG:HD2	1:D:170:GLU:OE1	2.09	0.53
1:D:54:PHE:HE2	1:D:59:LYS:CG	2.22	0.53
1:D:198:ASP:O	1:D:202:ILE:HG13	2.08	0.52
1:C:143:THR:HG21	2:C:424:GOL:C1	2.39	0.52
1:B:73:TYR:CE1	2:D:423[A]:GOL:H12	2.43	0.52
1:C:379:VAL:CG1	1:C:386:ILE:CG2	2.87	0.52
1:A:298:ASN:O	1:C:267:ARG:HD2	2.09	0.52
1:A:131:TRP:CZ3	1:A:384[A]:ASN:ND2	2.77	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:MSE:O	1:B:311:VAL:HG23	2.09	0.52
1:C:27:ALA:CB	6:C:462:HOH:O	2.58	0.52
1:C:35:GLU:HG3	1:C:35:GLU:O	2.08	0.52
1:B:104:ALA:HB2	1:B:304:MSE:HE1	1.92	0.52
1:D:103:ILE:CD1	1:D:285:PHE:HA	2.39	0.52
1:A:177:ASN:OD1	1:A:216:ASN:HB2	2.10	0.52
1:B:103:ILE:HG22	1:B:104:ALA:O	2.10	0.52
1:D:338:PHE:CD1	1:D:401:LEU:HD23	2.44	0.52
1:C:22:ALA:O	1:C:25:ALA:HB3	2.09	0.51
1:A:336:ASP:OD2	1:B:204:ASN:HB3	2.10	0.51
1:B:17:VAL:HG13	1:B:18:ILE:N	2.25	0.51
1:B:232:LYS:HZ2	1:B:325:ASN:HD21	1.55	0.51
1:C:368:ILE:HG21	1:C:409:MSE:CG	2.40	0.51
1:D:85:ALA:HB1	1:D:307:MSE:HE1	1.91	0.51
1:C:375:GLU:O	1:C:376:HIS:HB2	2.09	0.51
1:B:105:THR:HG23	1:B:107:GLY:O	2.11	0.51
1:B:82:PHE:CD2	1:B:304:MSE:CE	2.93	0.51
1:B:78:GLY:HA3	1:B:304:MSE:CE	2.38	0.51
1:B:83:LEU:O	1:B:87:GLU:HG3	2.11	0.51
1:C:127:LEU:HD11	1:C:167:ARG:HG2	1.92	0.51
1:A:46:HIS:CE1	2:A:424:GOL:H12	2.46	0.51
1:B:258:SER:CB	6:B:491:HOH:O	2.54	0.51
1:D:338:PHE:CD2	1:D:349:MSE:HE1	2.45	0.51
1:A:109:THR:HG23	1:A:139:ILE:HD11	1.93	0.51
1:B:246:PRO:HD2	1:B:249:ILE:HD12	1.92	0.51
1:B:189:PRO:O	1:B:359:THR:HG22	2.11	0.51
1:C:34:ARG:O	1:C:37:VAL:HG12	2.10	0.51
1:D:115:LEU:HD13	1:D:252:CYS:SG	2.51	0.51
1:D:331:ILE:HD13	1:D:391:CYS:HA	1.92	0.51
1:A:73:TYR:O	1:A:301:ARG:NH1	2.43	0.50
1:B:76:ILE:HB	1:B:289:LYS:HE3	1.93	0.50
1:B:297:SER:HB3	1:D:109:THR:HG21	1.93	0.50
1:B:71:VAL:HB	1:D:263:MSE:HA	1.93	0.50
1:B:9:ALA:HB2	6:B:429:HOH:O	2.10	0.50
1:C:22:ALA:O	1:C:26:GLN:HG2	2.11	0.50
1:C:49:GLU:HG3	1:C:51:ASN:HD21	1.75	0.50
1:D:148:VAL:HG13	1:D:167:ARG:HH21	1.76	0.50
1:D:267:ARG:HH12	2:D:423[A]:GOL:H12	1.77	0.50
1:D:330:LEU:O	1:D:334:ARG:HG3	2.11	0.50
1:A:49:GLU:HB2	1:A:51:ASN:ND2	2.26	0.50
1:C:38:VAL:HG12	1:C:377:ILE:HA	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ALA:HB3	1:D:307:MSE:HE2	1.92	0.50
1:A:14:LEU:HD22	2:A:423:GOL:H32	1.93	0.50
1:A:71:VAL:CG1	1:C:263:MSE:HA	2.41	0.50
1:B:104:ALA:HB2	1:B:304:MSE:CE	2.41	0.50
1:C:114:HIS:CE1	1:C:296:TRP:CH2	3.00	0.50
1:C:319:GLU:O	1:C:323:GLU:HG3	2.11	0.50
1:C:379:VAL:CG1	1:C:380:ILE:N	2.74	0.50
1:D:342:ALA:HB2	1:D:349:MSE:HE1	1.94	0.50
1:D:352:TYR:C	1:D:352:TYR:CD1	2.85	0.50
1:C:32:ASN:HD21	1:C:376:HIS:CD2	2.30	0.50
1:D:21:THR:HG22	1:D:41:THR:HG21	1.94	0.50
1:D:372:LEU:O	1:D:375:GLU:HB3	2.12	0.50
1:C:121[B]:GLU:OE2	1:C:122:PRO:HD2	2.12	0.50
1:A:299[A]:ILE:HD11	1:A:304:MSE:HG3	1.93	0.49
1:A:128:THR:O	1:A:149:THR:HA	2.13	0.49
1:A:197:LYS:O	1:A:200:ASP:HB2	2.12	0.49
1:B:52:LEU:HD11	1:B:264:TYR:CE2	2.47	0.49
1:D:307:MSE:HE1	1:D:311:VAL:CG2	2.41	0.49
1:C:338:PHE:CD2	1:C:349:MSE:CE	2.96	0.49
1:A:104:ALA:HB1	1:A:299[A]:ILE:HG12	1.95	0.49
1:D:148:VAL:CG1	1:D:167:ARG:HH21	2.26	0.49
1:D:330:LEU:HD21	1:D:334:ARG:HH21	1.76	0.49
1:B:161:HIS:HE1	1:B:198:ASP:OD1	1.96	0.49
1:B:232:LYS:HZ1	1:B:325:ASN:ND2	2.03	0.49
1:B:345:VAL:HG21	1:B:403:GLU:HG3	1.95	0.49
1:C:115:LEU:HD11	1:C:218:ILE:HG21	1.94	0.49
1:C:347:LEU:HD12	1:C:348:PRO:CD	2.34	0.49
1:C:368:ILE:HD11	1:C:414:LYS:HG2	1.94	0.49
1:B:350:LEU:HG	1:B:361:PRO:HD3	1.95	0.48
1:C:197:LYS:HG3	6:C:482:HOH:O	2.13	0.48
1:B:54:PHE:O	1:B:55:LEU:C	2.51	0.48
1:C:16:ASP:OD2	1:C:19:PHE:HD2	1.97	0.48
1:D:301:ARG:N	1:D:302:PRO:HD2	2.29	0.48
1:B:283:GLU:O	1:B:287:VAL:HB	2.12	0.48
1:B:404:LYS:NZ	6:B:494:HOH:O	2.46	0.48
1:D:85:ALA:CB	1:D:307:MSE:CE	2.90	0.48
1:A:125:GLU:OE1	1:A:171:LEU:HD21	2.14	0.48
1:B:85:ALA:HB1	1:B:311:VAL:HG21	1.95	0.48
1:D:379:VAL:HG11	1:D:388:ILE:HG22	1.94	0.48
1:C:338:PHE:HD2	1:C:349:MSE:CE	2.26	0.48
1:D:263:MSE:HB2	1:D:266:GLN:CG	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:PHE:HD2	1:D:59:LYS:HB2	1.66	0.48
1:A:7:LYS:HA	1:A:10:LYS:HE3	1.94	0.48
1:A:405:ILE:O	1:A:409:MSE:HG3	2.14	0.48
1:C:299:ILE:CG2	1:C:300:CYS:H	2.26	0.48
1:B:218:ILE:HD12	1:B:218:ILE:N	2.29	0.48
1:D:54:PHE:CE2	1:D:59:LYS:CG	2.96	0.48
1:A:339:LYS:CG	1:A:349:MSE:HE1	2.17	0.48
1:C:340:GLN:HG3	1:C:341[A]:GLU:HG2	1.94	0.48
1:D:271:MSE:HG3	1:D:284:PHE:CZ	2.49	0.48
1:B:257:LEU:CD1	1:B:263:MSE:HE3	2.35	0.48
1:D:368:ILE:HG13	1:D:368:ILE:O	2.14	0.48
1:A:52:LEU:HD21	1:A:264:TYR:HE2	1.79	0.47
1:B:223:VAL:HG11	1:B:226:LEU:HD22	1.96	0.47
1:A:101[A]:ARG:HG2	1:A:281:ALA:HB1	1.97	0.47
1:A:73:TYR:OH	2:C:426:GOL:H32	2.14	0.47
1:C:18:ILE:HG21	3:C:425:OAA:H22	1.96	0.47
1:A:153:PHE:HB3	1:A:157:ASN:HA	1.97	0.47
1:B:223:VAL:O	1:B:223:VAL:CG1	2.63	0.47
1:B:77:ALA:HB2	1:B:289:LYS:HD3	1.95	0.47
1:B:338:PHE:HA	6:B:454:HOH:O	2.14	0.47
1:B:43:GLY:HA2	1:B:391:CYS:SG	2.54	0.47
1:C:345:VAL:HG11	1:C:403:GLU:HG2	1.95	0.47
1:C:45:ILE:HG22	1:C:53:VAL:CG2	2.44	0.47
1:C:259:LYS:HB2	6:C:472:HOH:O	2.13	0.47
1:C:99:HIS:C	1:C:100:ILE:HD13	2.34	0.47
1:A:81:ASP:HB3	6:A:470:HOH:O	2.14	0.47
1:B:259:LYS:NZ	1:D:73:TYR:OH	2.48	0.47
1:C:408:ALA:O	1:C:412:LEU:HD12	2.14	0.47
1:D:316:LYS:NZ	6:D:455:HOH:O	2.48	0.47
2:B:416:GOL:C3	1:D:259:LYS:HZ1	2.28	0.47
1:D:102:SER:C	1:D:103:ILE:HD12	2.35	0.47
1:A:307:MSE:HE2	1:A:311:VAL:CG2	2.39	0.47
1:A:52:LEU:C	1:A:52:LEU:HD23	2.35	0.47
1:B:130:ASP:HA	1:B:149:THR:HG21	1.97	0.47
1:C:38:VAL:O	1:C:38:VAL:HG13	2.15	0.47
1:D:251:THR:HG23	6:D:420:HOH:O	2.15	0.47
1:A:301:ARG:N	1:A:302:PRO:HD2	2.29	0.47
1:B:301:ARG:N	1:B:302:PRO:HD2	2.30	0.46
1:B:370:GLU:HA	1:B:370:GLU:OE1	2.15	0.46
1:D:349:MSE:HB3	1:D:349:MSE:HE3	1.82	0.46
1:D:4:VAL:O	1:D:4:VAL:HG12	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299[A]:ILE:HD11	1:A:304:MSE:CG	2.46	0.46
1:B:193:SER:H	1:B:353:ARG:HG3	1.81	0.46
1:C:22:ALA:HA	1:C:41:THR:HG21	1.97	0.46
1:A:368:ILE:CD1	1:A:409:MSE:HG2	2.34	0.46
1:A:137:ARG:NH2	2:A:423:GOL:O1	2.49	0.46
1:D:218:ILE:HD13	1:D:218:ILE:N	2.28	0.46
1:A:266:GLN:CA	6:A:458:HOH:O	2.54	0.46
1:B:120:THR:CG2	1:B:179:VAL:HG11	2.46	0.46
1:A:329:GLN:HA	1:A:329:GLN:NE2	2.30	0.46
1:B:150:TYR:HB3	1:B:167:ARG:HG3	1.98	0.46
1:C:49:GLU:HG3	1:C:51:ASN:ND2	2.31	0.46
1:D:352:TYR:O	1:D:352:TYR:CD1	2.68	0.46
1:B:370:GLU:OE1	1:B:373:LYS:HE2	2.16	0.46
1:B:190:THR:HG22	1:B:350:LEU:HD12	1.98	0.46
1:B:268:VAL:HG21	1:B:303:ALA:CB	2.45	0.46
1:C:75:PRO:HD3	5:C:423:AKG:O1	2.15	0.45
1:B:232:LYS:HE3	1:B:324:ARG:HH12	1.81	0.45
1:A:12:LYS:NZ	1:A:142:ASP:OD1	2.42	0.45
1:A:340:GLN:HB2	6:A:438:HOH:O	2.16	0.45
1:B:15:LYS:NZ	6:B:490:HOH:O	2.49	0.45
1:B:79:ILE:HD11	1:B:301:ARG:HG3	1.98	0.45
1:B:94:PHE:CD1	1:B:237:ALA:HA	2.52	0.45
1:A:298:ASN:O	1:C:267:ARG:HD3	2.15	0.45
1:A:95:ARG:CZ	1:A:100:ILE:HD12	2.47	0.45
1:C:131:TRP:CZ3	1:C:384:ASN:CB	2.99	0.45
1:B:191:GLY:O	1:B:353:ARG:N	2.46	0.45
1:C:355:GLY:HA3	6:C:494:HOH:O	2.16	0.45
1:B:73:TYR:OH	2:D:423[B]:GOL:H12	2.17	0.45
1:B:165:GLN:HG2	1:B:205:PHE:CD1	2.52	0.45
1:D:135:ALA:O	1:D:136:TYR:C	2.54	0.45
1:D:116[A]:ILE:HG21	1:D:139:ILE:HG22	1.99	0.45
1:D:264:TYR:HD2	1:D:264:TYR:H	1.57	0.45
1:A:46:HIS:HE1	2:A:424:GOL:C1	2.30	0.45
1:D:128:THR:HG22	1:D:147:LEU:HD11	1.99	0.45
1:A:173:ALA:O	1:A:214[A]:ARG:NH2	2.50	0.45
1:B:82:PHE:HD2	1:B:304:MSE:HE2	1.82	0.45
1:C:397:GLN:O	1:C:401:LEU:HB2	2.17	0.45
1:D:352:TYR:HD1	1:D:352:TYR:O	2.00	0.45
1:A:267:ARG:NH1	6:A:475:HOH:O	2.50	0.44
1:D:345:VAL:HG13	1:D:406:TYR:CE1	2.52	0.44
1:C:190:THR:HA	1:C:359[A]:THR:HG22	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LYS:CA	1:D:10:LYS:HE2	2.31	0.44
1:B:287:VAL:HG12	1:B:288:ASN:N	2.32	0.44
1:C:193:SER:N	1:C:353:ARG:HD2	2.31	0.44
1:C:368:ILE:CG2	1:C:409:MSE:HG3	2.42	0.44
1:D:331:ILE:CD1	1:D:391:CYS:HA	2.47	0.44
1:A:167:ARG:HD2	1:A:167:ARG:HA	1.29	0.44
1:A:71:VAL:HG12	1:C:263:MSE:HA	1.99	0.44
1:C:371:GLU:O	1:C:374:LYS:HB2	2.18	0.44
1:A:75:PRO:HG2	1:A:78:GLY:O	2.17	0.44
1:D:341:GLU:OE2	1:D:403:GLU:HG3	2.18	0.44
1:D:405:ILE:O	1:D:408:ALA:HB3	2.18	0.44
1:A:268:VAL:HG13	1:A:299[A]:ILE:HD13	1.98	0.44
1:B:66:SER:O	1:B:69:GLU:N	2.48	0.44
1:C:349:MSE:HG2	1:C:349:MSE:O	2.14	0.44
1:A:125:GLU:HB2	1:A:171:LEU:HD22	2.00	0.44
1:A:52:LEU:HD23	1:A:53:VAL:H	1.80	0.44
1:D:166:ASN:O	1:D:170:GLU:HG3	2.18	0.43
1:B:314:PRO:HG3	6:B:489:HOH:O	2.18	0.43
1:C:268:VAL:HG21	1:C:303:ALA:HB3	2.00	0.43
1:D:338:PHE:CE1	1:D:401:LEU:HD23	2.53	0.43
1:B:358:ILE:HD12	1:B:358:ILE:HA	1.62	0.43
1:B:76:ILE:HB	1:B:289:LYS:HE2	2.00	0.43
1:D:82:PHE:CD1	1:D:307:MSE:HG2	2.53	0.43
1:D:330:LEU:HG	1:D:334:ARG:NE	2.22	0.43
1:A:409:MSE:HE2	1:A:415:LEU:HD23	2.00	0.43
1:D:158:ASN:OD1	6:D:494:HOH:O	2.21	0.43
1:D:366:ASN:OD1	1:D:366:ASN:N	2.50	0.43
1:A:369:CYS:SG	1:A:379:VAL:HG23	2.58	0.43
1:B:165:GLN:HG2	1:B:205:PHE:CE2	2.54	0.43
1:B:299:ILE:HD13	1:B:299:ILE:HA	1.73	0.43
1:D:85:ALA:HB1	1:D:307:MSE:HE2	1.94	0.43
1:A:49:GLU:HB2	1:A:51:ASN:HD22	1.84	0.43
1:B:71:VAL:CG1	1:D:54:PHE:HE1	2.25	0.43
1:C:36:ASN:O	1:C:376:HIS:HB3	2.19	0.43
1:B:73:TYR:CZ	1:D:264:TYR:HB3	2.54	0.43
1:D:328[B]:TYR:HD1	1:D:331:ILE:CG2	2.32	0.43
1:C:32:ASN:HD21	1:C:376:HIS:HD2	1.65	0.43
1:D:39:ASN:OD1	1:D:39:ASN:C	2.56	0.43
1:D:82:PHE:HD1	1:D:307:MSE:HG2	1.83	0.43
1:D:328[B]:TYR:O	1:D:331:ILE:HG22	2.19	0.43
1:B:183:ASN:ND2	1:B:188:ASN:H	2.17	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105[A]:THR:OG1	1:D:110:GLY:HA3	2.20	0.42
1:D:328[B]:TYR:CA	1:D:331:ILE:HG22	2.43	0.42
1:A:8:HIS:HD1	1:C:121[B]:GLU:CD	2.21	0.42
1:B:61:GLU:OE1	1:B:316:LYS:CE	2.67	0.42
1:B:360:ILE:HD13	1:B:405:ILE:HG21	2.01	0.42
1:C:257:LEU:HD13	1:C:263:MSE:HE1	2.01	0.42
1:D:300:CYS:HA	6:D:476:HOH:O	2.19	0.42
1:B:259:LYS:N	6:B:468:HOH:O	2.46	0.42
1:D:62:TYR:O	1:D:70:HIS:HE1	2.02	0.42
1:A:56:LYS:HB3	1:A:56:LYS:HE2	1.53	0.42
1:B:268:VAL:HG21	1:B:303:ALA:HB3	2.01	0.42
1:A:395:LYS:O	1:A:399:THR:HG23	2.20	0.42
1:B:192:TYR:HA	1:B:353:ARG:HG3	2.02	0.42
1:C:277:ASP:HB3	1:C:280:ILE:HD12	2.00	0.42
1:C:331:ILE:HA	1:C:334:ARG:HD2	2.02	0.42
1:C:356:PHE:HB3	1:C:391:CYS:SG	2.60	0.42
1:C:379:VAL:CG2	1:C:388:ILE:HD13	2.45	0.42
1:A:298:ASN:OD1	1:C:267:ARG:HD2	2.19	0.42
1:A:299[B]:ILE:CG2	1:A:300:CYS:N	2.82	0.42
1:B:196:ASP:N	6:B:487:HOH:O	2.53	0.42
1:A:268:VAL:HG13	1:A:299[A]:ILE:CD1	2.50	0.42
1:A:31:GLU:HG2	1:A:32:ASN:ND2	2.35	0.42
1:D:126:VAL:O	1:D:147:LEU:HD12	2.19	0.42
1:A:100:ILE:O	1:A:101[A]:ARG:NE	2.46	0.42
1:B:79:ILE:HG21	1:B:305:ARG:NH2	2.34	0.42
1:A:189:PRO:HB2	1:A:359:THR:OG1	2.20	0.42
1:D:114:HIS:CE1	1:D:296:TRP:CH2	3.08	0.41
1:D:69:GLU:OE1	1:D:301:ARG:HD3	2.20	0.41
1:C:356:PHE:CG	1:C:391:CYS:HB3	2.55	0.41
1:A:46:HIS:HE1	2:A:424:GOL:H12	1.85	0.41
1:C:28:ASP:O	1:C:28:ASP:OD1	2.38	0.41
1:C:379:VAL:HG13	1:C:380:ILE:H	1.85	0.41
1:B:282:ASP:O	1:B:285:PHE:HB3	2.19	0.41
1:B:377:ILE:HD11	1:B:404:LYS:HD2	2.01	0.41
1:C:20:VAL:O	1:C:23:GLY:N	2.53	0.41
1:C:365:ALA:HA	1:C:386:ILE:HD11	2.02	0.41
1:D:26:GLN:O	1:D:27:ALA:C	2.58	0.41
1:A:194:ILE:HG22	1:A:199:TRP:CD1	2.55	0.41
1:A:279:GLU:HB2	1:C:2:THR:HG23	2.02	0.41
1:A:46:HIS:HA	1:A:51:ASN:O	2.20	0.41
1:A:105:THR:HA	1:A:296:TRP:CZ2	2.55	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:TRP:HD1	1:A:298:ASN:N	2.18	0.41
1:C:178:VAL:HG23	1:C:178:VAL:O	2.20	0.41
1:C:8[A]:HIS:HD2	6:C:420:HOH:O	2.03	0.41
1:A:10:LYS:HB3	1:A:10:LYS:HE2	1.76	0.41
1:B:180:VAL:O	1:B:220:GLY:N	2.48	0.41
1:D:121:GLU:O	1:D:124:ASP:HB2	2.21	0.41
1:D:69:GLU:HA	1:D:301:ARG:CD	2.50	0.41
1:B:193:SER:N	1:B:353:ARG:HG3	2.36	0.41
1:A:330:LEU:O	1:A:334:ARG:HG3	2.21	0.41
1:B:191:GLY:HA2	6:B:477:HOH:O	2.20	0.41
1:C:380:ILE:HA	1:C:380:ILE:HD13	1.85	0.41
1:B:258:SER:HA	1:B:263:MSE:O	2.21	0.41
1:C:76:ILE:CD1	1:C:293:ARG:HD2	2.50	0.41
1:A:183:ASN:HD21	1:A:188:ASN:HB3	1.86	0.40
1:B:82:PHE:CD2	1:B:304:MSE:HG2	2.55	0.40
1:C:341[A]:GLU:H	1:C:341[A]:GLU:HG2	1.76	0.40
1:D:373:LYS:HD3	1:D:378:TYR:HE1	1.78	0.40
1:D:61:GLU:OE1	1:D:316:LYS:HE2	2.22	0.40
1:B:55:LEU:HB2	1:B:58:VAL:HG23	2.03	0.40
1:A:14:LEU:HD12	1:C:289:LYS:HG2	2.04	0.40
1:D:342:ALA:CB	1:D:349:MSE:CE	2.99	0.40
1:D:347:LEU:HA	1:D:348:PRO:HD3	1.84	0.40
1:D:389:ALA:HB1	1:D:391:CYS:SG	2.61	0.40
1:D:94:PHE:CG	1:D:237:ALA:HA	2.57	0.40
1:A:353[B]:ARG:HA	1:A:353[B]:ARG:HD2	1.68	0.40
1:B:257:LEU:C	1:B:257:LEU:HD12	2.42	0.40
1:D:359:THR:HG22	1:D:360:ILE:N	2.35	0.40
1:B:210:VAL:HG13	1:B:248:GLU:HB2	2.03	0.40
1:C:219:ILE:HB	1:C:251:THR:HG23	2.02	0.40
1:B:293:ARG:NH1	1:D:19:PHE:HE2	2.19	0.40
1:D:54:PHE:CE2	1:D:59:LYS:HG3	2.57	0.40
1:B:198:ASP:O	1:B:202:ILE:HG13	2.21	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	421/418 (101%)	414 (98%)	7 (2%)	0	100	100
1	B	413/418 (99%)	404 (98%)	9 (2%)	0	100	100
1	C	419/418 (100%)	409 (98%)	10 (2%)	0	100	100
1	D	391/418 (94%)	377 (96%)	14 (4%)	0	100	100
All	All	1644/1672 (98%)	1604 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	349/335 (104%)	330 (95%)	19 (5%)	22	26
1	B	341/335 (102%)	322 (94%)	19 (6%)	21	25
1	C	347/335 (104%)	314 (90%)	33 (10%)	8	8
1	D	327/335 (98%)	291 (89%)	36 (11%)	6	5
All	All	1364/1340 (102%)	1257 (92%)	107 (8%)	13	13

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	15	LYS
1	A	30	LYS
1	A	34	ARG
1	A	35	GLU
1	A	54	PHE
1	A	68	SER
1	A	89	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	114	HIS
1	A	167	ARG
1	A	299[A]	ILE
1	A	299[B]	ILE
1	A	301	ARG
1	A	320	TYR
1	A	349	MSE
1	A	353[A]	ARG
1	A	353[B]	ARG
1	A	362	THR
1	A	375	GLU
1	B	20	VAL
1	B	31	GLU
1	B	49	GLU
1	B	51	ASN
1	B	100	ILE
1	B	105	THR
1	B	179	VAL
1	B	189	PRO
1	B	210	VAL
1	B	255	TYR
1	B	287	VAL
1	B	297	SER
1	B	307	MSE
1	B	353	ARG
1	B	358	ILE
1	B	359	THR
1	B	362	THR
1	B	398	MSE
1	B	415	LEU
1	C	16	ASP
1	C	17	VAL
1	C	20	VAL
1	C	24	GLN
1	C	26	GLN
1	C	31	GLU
1	C	32	ASN
1	C	48	GLU
1	C	51	ASN
1	C	54	PHE
1	C	56	LYS
1	C	59	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	60	GLU
1	C	100	ILE
1	C	114	HIS
1	C	138	VAL
1	C	167	ARG
1	C	214	ARG
1	C	240	ASN
1	C	298	ASN
1	C	320	TYR
1	C	329	GLN
1	C	331	ILE
1	C	341[A]	GLU
1	C	341[B]	GLU
1	C	349	MSE
1	C	362	THR
1	C	366	ASN
1	C	376	HIS
1	C	379	VAL
1	C	388	ILE
1	C	399	THR
1	C	410	LYS
1	D	2	THR
1	D	3	SER
1	D	14	LEU
1	D	16	ASP
1	D	17	VAL
1	D	46	HIS
1	D	48	GLU
1	D	51[A]	ASN
1	D	51[B]	ASN
1	D	71	VAL
1	D	114	HIS
1	D	116[A]	ILE
1	D	116[B]	ILE
1	D	137	ARG
1	D	155	GLU
1	D	214	ARG
1	D	251	THR
1	D	264	TYR
1	D	301	ARG
1	D	307	MSE
1	D	317	PHE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	320	TYR
1	D	336	ASP
1	D	341	GLU
1	D	349	MSE
1	D	353	ARG
1	D	364	SER
1	D	366	ASN
1	D	368	ILE
1	D	371	GLU
1	D	377	ILE
1	D	393	ILE
1	D	401	LEU
1	D	404	LYS
1	D	406	TYR
1	D	410	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	26	GLN
1	A	32	ASN
1	A	46	HIS
1	A	51	ASN
1	A	158	ASN
1	A	183	ASN
1	A	216	ASN
1	A	329	GLN
1	B	8	HIS
1	B	26	GLN
1	B	36	ASN
1	B	114	HIS
1	B	183	ASN
1	B	215	ASN
1	B	325	ASN
1	C	24	GLN
1	C	51	ASN
1	C	70	HIS
1	C	113	HIS
1	C	204	ASN
1	C	288	ASN
1	C	366	ASN
1	C	376	HIS

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	D	70	HIS
1	D	165	GLN
1	D	215	ASN
1	D	240	ASN
1	D	309	ASN
1	D	376	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\# Z  > 2$
2	GOL	A	423	-	5,5,5	0.36	0	5,5,5	0.41	0
3	OAA	A	422	-	2,8,8	1.30	0	2,10,10	1.53	1 (50%)
2	GOL	D	421	-	5,5,5	0.32	0	5,5,5	0.38	0
5	AKG	C	423	-	3,9,9	0.92	0	4,11,11	3.91	1 (25%)
3	OAA	B	422	-	2,8,8	2.37	1 (50%)	2,10,10	1.95	1 (50%)
3	OAA	C	425	-	2,8,8	1.97	1 (50%)	2,10,10	0.71	0
2	GOL	B	416	-	5,5,5	0.31	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	426	-	5,5,5	0.42	0	5,5,5	0.54	0
2	GOL	A	421	-	5,5,5	0.35	0	5,5,5	0.64	0
2	GOL	D	416	-	5,5,5	0.37	0	5,5,5	0.37	0
2	GOL	C	421	-	5,5,5	0.38	0	5,5,5	0.40	0
2	GOL	D	423[A]	-	5,5,5	0.38	0	5,5,5	0.37	0
2	GOL	D	423[B]	-	5,5,5	0.31	0	5,5,5	0.37	0
2	GOL	A	424	-	5,5,5	0.30	0	5,5,5	0.49	0
2	GOL	C	424	-	5,5,5	0.46	0	5,5,5	0.89	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
2	GOL	A	423	-	-	3/4/4/4	-
3	OAA	A	422	-	-	2/2/8/8	-
2	GOL	D	421	-	-	2/4/4/4	-
5	AKG	C	423	-	-	0/3/9/9	-
3	OAA	B	422	-	-	2/2/8/8	-
3	OAA	C	425	-	-	2/2/8/8	-
2	GOL	B	416	-	-	2/4/4/4	-
2	GOL	C	426	-	-	0/4/4/4	-
2	GOL	A	421	-	-	3/4/4/4	-
2	GOL	D	416	-	-	0/4/4/4	-
2	GOL	C	421	-	-	4/4/4/4	-
2	GOL	D	423[A]	-	-	3/4/4/4	-
2	GOL	D	423[B]	-	-	2/4/4/4	-
2	GOL	A	424	-	-	2/4/4/4	-
2	GOL	C	424	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	422	OAA	C2-C3	-3.35	1.48	1.51
3	C	425	OAA	C2-C3	-2.75	1.49	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	423	AKG	C3-C4-C5	7.54	125.33	112.67
3	B	422	OAA	C1-C2-C3	-2.67	110.75	115.51
3	A	422	OAA	C1-C2-C3	2.07	119.20	115.51

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	422	OAA	C1-C2-C3-O3
3	A	422	OAA	C1-C2-C3-C4
3	C	425	OAA	C1-C2-C3-O3
3	C	425	OAA	C1-C2-C3-C4
2	B	416	GOL	O1-C1-C2-C3
2	A	421	GOL	O1-C1-C2-C3
2	C	421	GOL	O1-C1-C2-O2
2	C	421	GOL	O1-C1-C2-C3
2	D	423[A]	GOL	O1-C1-C2-C3
2	A	424	GOL	C1-C2-C3-O3
2	A	423	GOL	O1-C1-C2-O2
2	A	421	GOL	O1-C1-C2-O2
2	A	423	GOL	O1-C1-C2-C3
2	D	421	GOL	O1-C1-C2-C3
2	C	421	GOL	C1-C2-C3-O3
2	D	423[B]	GOL	O1-C1-C2-C3
2	B	416	GOL	O1-C1-C2-O2
2	D	423[B]	GOL	O1-C1-C2-O2
2	A	424	GOL	O2-C2-C3-O3
3	B	422	OAA	C1-C2-C3-O3
2	D	423[A]	GOL	O1-C1-C2-O2
2	C	424	GOL	O2-C2-C3-O3
3	B	422	OAA	C1-C2-C3-C4
2	A	423	GOL	C1-C2-C3-O3
2	D	423[A]	GOL	C1-C2-C3-O3
2	D	421	GOL	O1-C1-C2-O2
2	A	421	GOL	O2-C2-C3-O3
2	C	421	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	423	GOL	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	423	AKG	3	0
3	C	425	OAA	1	0
2	B	416	GOL	1	0
2	C	426	GOL	4	0
2	A	421	GOL	1	0
2	D	423[A]	GOL	3	0
2	D	423[B]	GOL	2	0
2	A	424	GOL	7	0
2	C	424	GOL	13	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, 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	407/418 (97%)	-0.34	1 (0%) 95 94	30, 44, 63, 85	0
1	B	407/418 (97%)	-0.05	7 (1%) 70 68	36, 58, 85, 110	0
1	C	406/418 (97%)	0.33	37 (9%) 9 8	29, 48, 101, 131	0
1	D	386/418 (92%)	0.32	37 (9%) 8 6	31, 53, 115, 166	0
All	All	1606/1672 (96%)	0.06	82 (5%) 28 26	29, 51, 95, 166	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	346	GLY	7.0
1	C	371	GLU	6.2
1	D	343	ALA	6.0
1	B	213	GLY	5.9
1	D	335	ALA	5.2
1	C	25	ALA	5.2
1	C	33	GLY	5.2
1	D	377	ILE	5.1
1	C	35	GLU	5.1
1	D	402	ALA	4.9
1	C	34	ARG	4.8
1	C	413	GLY	4.5
1	C	372	LEU	4.4
1	D	370	GLU	4.3
1	C	410	LYS	4.2
1	C	405	ILE	4.2
1	C	329	GLN	4.2
1	C	32	ASN	4.0
1	C	29	ALA	3.9
1	D	407	ASN	3.9
1	C	37	VAL	3.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	368	ILE	3.7
1	D	403	GLU	3.6
1	D	378	TYR	3.5
1	C	378	TYR	3.4
1	C	39	ASN	3.4
1	D	406	TYR	3.2
1	D	364	SER	3.2
1	D	337	ILE	3.1
1	C	106	ALA	3.1
1	D	17	VAL	3.0
1	C	38	VAL	3.0
1	C	377	ILE	3.0
1	B	393	ILE	3.0
1	D	408	ALA	2.9
1	D	376	HIS	2.9
1	C	48	GLU	2.9
1	C	36	ASN	2.9
1	D	336	ASP	2.9
1	D	375	GLU	2.9
1	D	374	LYS	2.8
1	D	326	CYS	2.8
1	D	338	PHE	2.8
1	D	365	ALA	2.8
1	D	344	GLN	2.7
1	C	367	ALA	2.7
1	B	277	ASP	2.7
1	C	347	LEU	2.7
1	C	209	LEU	2.7
1	C	395	LYS	2.6
1	D	328[A]	TYR	2.5
1	C	47	ASP	2.4
1	D	367	ALA	2.4
1	D	373	LYS	2.4
1	C	406	TYR	2.4
1	C	340	GLN	2.4
1	B	247	LYS	2.4
1	B	278	GLU	2.4
1	D	56	LYS	2.3
1	C	403	GLU	2.3
1	D	109	THR	2.3
1	C	407	ASN	2.3
1	C	299	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	353	ARG	2.3
1	D	393	ILE	2.3
1	C	399	THR	2.3
1	D	330	LEU	2.3
1	D	401	LEU	2.2
1	D	369	CYS	2.2
1	B	348	PRO	2.2
1	B	98	GLY	2.2
1	A	297	SER	2.2
1	C	170	GLU	2.2
1	C	253	VAL	2.1
1	C	376	HIS	2.1
1	D	371	GLU	2.1
1	C	74	ALA	2.1
1	C	268	VAL	2.1
1	D	333	ASP	2.0
1	C	269	GLY	2.0
1	D	350	LEU	2.0
1	D	363	ASP	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	C	421	6/6	0.68	0.13	74,80,81,81	0
5	AKG	C	423	10/10	0.81	0.22	53,65,76,76	0
2	GOL	A	423	6/6	0.82	0.24	66,77,79,79	0
3	OAA	C	425	9/9	0.82	0.30	77,81,94,94	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	426	6/6	0.85	0.44	57,63,72,73	0
3	OAA	A	422	9/9	0.87	0.31	52,62,74,82	0
2	GOL	A	424	6/6	0.89	0.23	72,79,84,87	0
2	GOL	D	421	6/6	0.90	0.24	80,83,85,87	0
3	OAA	B	422	9/9	0.90	0.16	46,60,71,72	0
2	GOL	B	416	6/6	0.91	0.42	64,70,74,74	0
2	GOL	C	424	6/6	0.91	0.16	38,49,60,62	0
2	GOL	D	423[B]	6/6	0.92	0.46	61,62,64,65	6
2	GOL	D	423[A]	6/6	0.92	0.46	59,62,63,64	6
2	GOL	D	416	6/6	0.92	0.41	70,73,79,80	0
2	GOL	A	421	6/6	0.96	0.15	51,57,59,60	0
4	CL	C	422	1/1	0.97	0.07	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.