



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:12 pm BST

PDB ID : 2CW6  
Title : Crystal Structure of Human HMG-CoA Lyase: Insights into Catalysis and the Molecular Basis for Hydroxymethylglutaric Aciduria  
Authors : Fu, Z.; Runquist, J.A.; Hunt, J.F.; Mizioro, H.M.; Kim, J.-J.P.  
Deposited on : 2005-06-17  
Resolution : 2.10 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

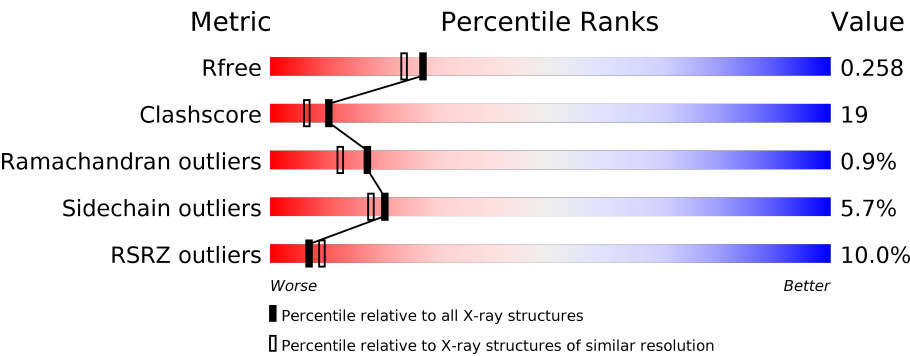
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	298	<div><div>3%</div><div><div></div><div>73%</div><div>23%</div><div>• •</div></div></div>
1	B	298	<div><div>9%</div><div><div></div><div>69%</div><div>27%</div><div>• •</div></div></div>
1	C	298	<div><div>4%</div><div><div></div><div>65%</div><div>32%</div><div>• •</div></div></div>
1	D	298	<div><div>17%</div><div><div></div><div>57%</div><div>35%</div><div>• 5%</div></div></div>
1	E	298	<div><div>9%</div><div><div></div><div>70%</div><div>25%</div><div>• •</div></div></div>
1	F	298	<div><div>17%</div><div><div></div><div>56%</div><div>38%</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	3HG	A	399	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13543 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.

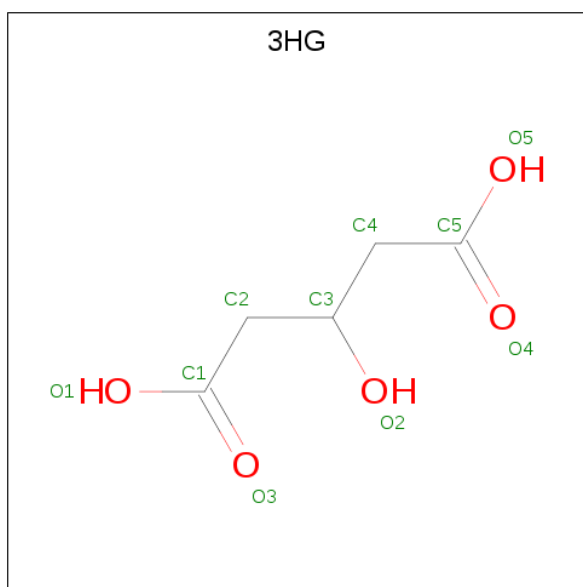
- Molecule 1 is a protein called Hydroxymethylglutaryl-CoA lyase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	B	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	C	294	Total	C	N	O	S	0	0	0
			2176	1383	363	414	16			
1	D	282	Total	C	N	O	S	0	0	0
			2089	1330	348	396	15			
1	E	296	Total	C	N	O	S	0	0	0
			2189	1390	365	417	17			
1	F	288	Total	C	N	O	S	0	0	0
			2130	1353	355	406	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 3-HYDROXPENTANEDIOIC ACID (three-letter code: 3HG) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>5</sub>).



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

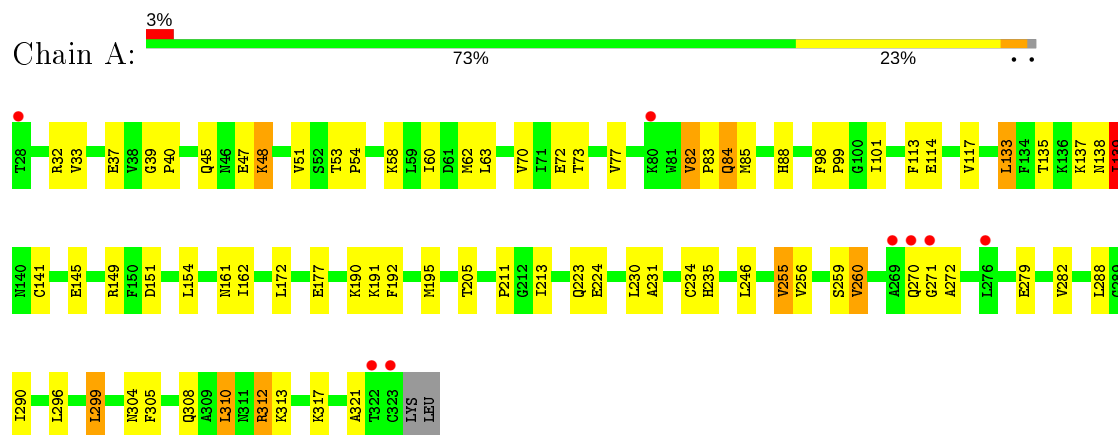
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	95	Total	O	0	0
			95	95		
4	C	96	Total	O	0	0
			96	96		
4	D	56	Total	O	0	0
			56	56		
4	E	104	Total	O	0	0
			104	104		
4	F	53	Total	O	0	0
			53	53		

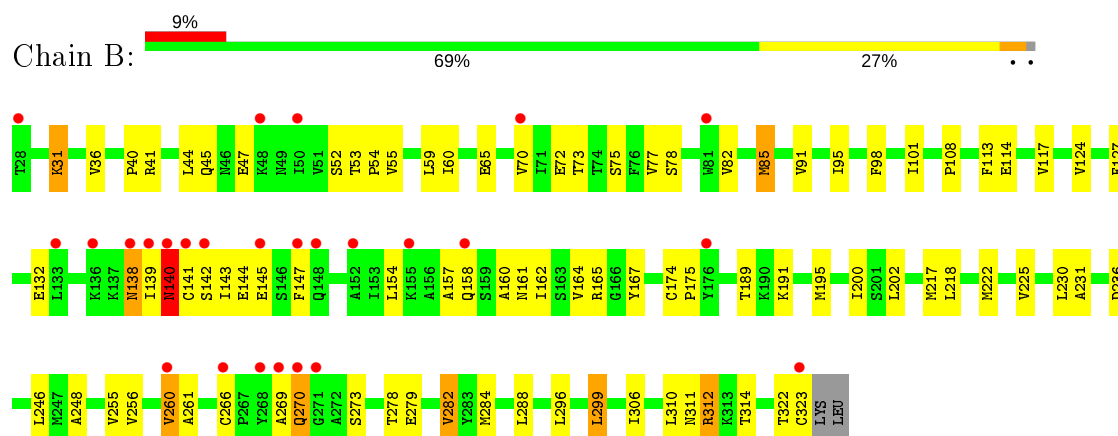
### 3 Residue-property plots [i](#)

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.

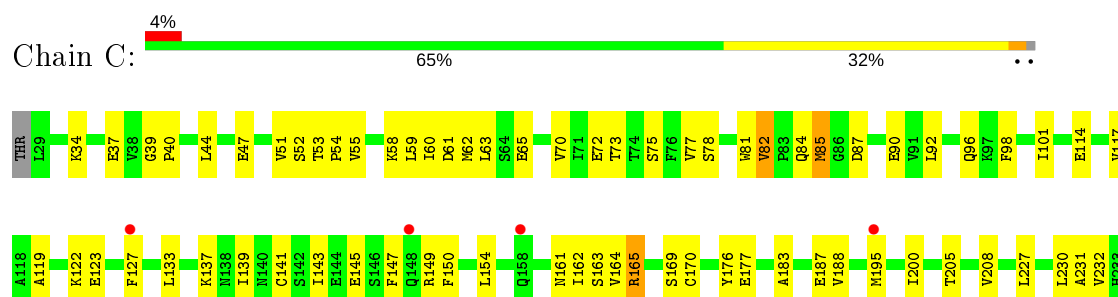
- Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial



- Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial

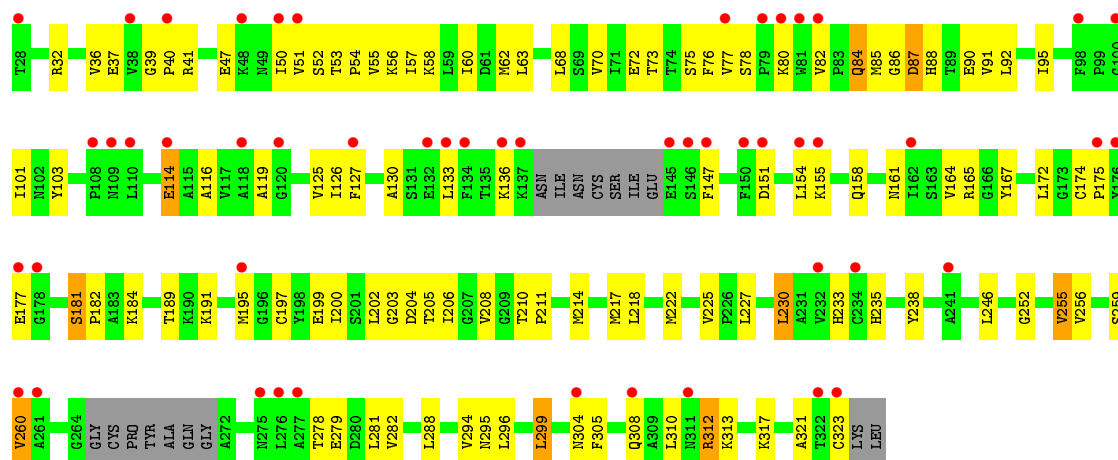


- Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial

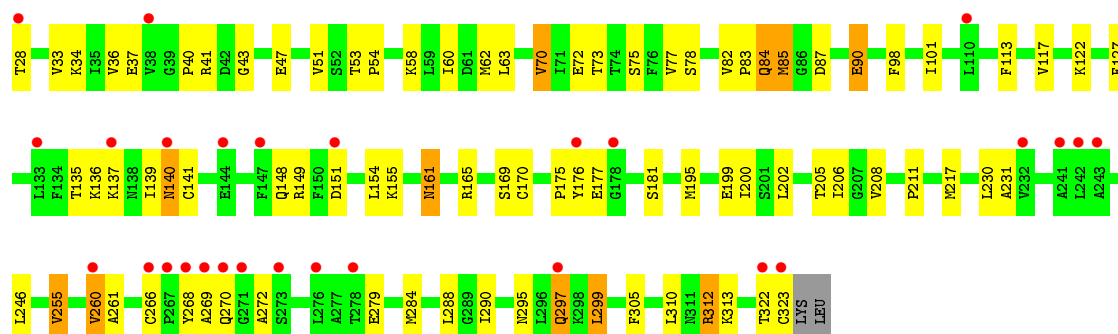




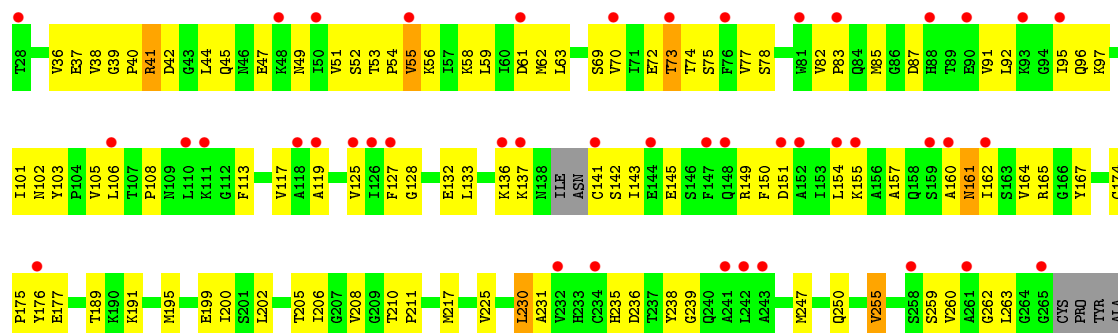
• Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial

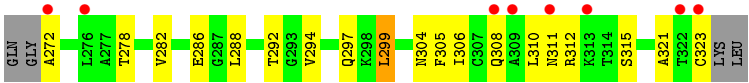


• Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial



• Molecule 1: Hydroxymethylglutaryl-CoA lyase, mitochondrial







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.99 Å   117.08 Å   86.83 Å 90.00°   112.50°   90.00°	Depositor
Resolution (Å)	30.44 – 2.10 30.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.44-2.10) 98.4 (30.44-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.10 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226   ,   0.265 0.221   ,   0.258	Depositor DCC
$R_{free}$ test set	10457 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: MG, 3HG

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	0.42	0/2224	0.65	0/3011
1	B	0.36	0/2224	0.61	0/3011
1	C	0.36	0/2211	0.59	0/2993
1	D	0.30	0/2120	0.53	0/2866
1	E	0.35	0/2224	0.59	0/3011
1	F	0.49	2/2161 (0.1%)	0.57	1/2921 (0.0%)
All	All	0.38	2/13164 (0.0%)	0.59	1/17813 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	272	ALA	C-O	-13.42	0.97	1.23
1	F	272	ALA	C-N	5.51	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	272	ALA	O-C-N	7.60	134.86	122.70

There are no chirality outliers.

There are no planarity outliers.

### 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	2189	0	2244	72	0
1	B	2189	0	2244	74	0
1	C	2176	0	2232	82	0
1	D	2089	0	2152	92	0
1	E	2189	0	2244	77	0
1	F	2130	0	2188	110	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	10	0	5	4	0
4	A	161	0	0	4	0
4	B	95	0	0	4	0
4	C	96	0	0	0	0
4	D	56	0	0	3	0
4	E	104	0	0	2	0
4	F	53	0	0	0	0
All	All	13543	0	13309	489	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 19.

All (489) 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:E:288:LEU:HD11	1:F:211:PRO:HG2	1.39	0.99
1:A:48:LYS:HD2	1:A:48:LYS:H	1.28	0.98
1:A:58:LYS:HG2	1:A:62:MET:HE2	1.47	0.97
1:F:51:VAL:HB	1:F:55:VAL:HG11	1.45	0.96
1:C:288:LEU:HD11	1:D:211:PRO:HG2	1.47	0.95
1:B:142:SER:HB3	1:B:145:GLU:HG3	1.49	0.93
1:C:139:ILE:HB	1:C:149:ARG:HH22	1.33	0.91
1:A:84:GLN:NE2	1:A:84:GLN:H	1.68	0.90
1:C:47:GLU:HG2	1:C:310:LEU:HD21	1.53	0.88
1:D:75:SER:HB3	1:D:85:MET:HG2	1.58	0.86
1:C:40:PRO:HA	1:C:44:LEU:HD23	1.56	0.86
1:D:125:VAL:HG22	1:D:165:ARG:HB3	1.60	0.84
1:A:211:PRO:HG2	1:B:288:LEU:HD21	1.59	0.84
1:B:75:SER:HB3	1:B:85:MET:HG2	1.57	0.84
1:D:58:LYS:HG2	1:D:62:MET:HE2	1.60	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:THR:HG23	1:F:294:VAL:H	1.42	0.83
1:E:58:LYS:HG2	1:E:62:MET:HE2	1.60	0.83
1:F:47:GLU:HG2	1:F:310:LEU:HD21	1.63	0.79
1:F:142:SER:HB3	1:F:145:GLU:HG3	1.66	0.78
1:B:98:PHE:HB2	1:B:101:ILE:HD12	1.66	0.78
1:F:51:VAL:CB	1:F:55:VAL:HG11	2.13	0.78
1:B:60:ILE:HD13	1:B:73:THR:HG23	1.66	0.77
1:A:84:GLN:H	1:A:84:GLN:HE21	1.30	0.77
1:A:48:LYS:HD2	1:A:48:LYS:N	1.98	0.77
1:B:266:CYS:SG	1:B:269:ALA:HB3	2.24	0.77
1:C:279:GLU:HG3	1:C:299:LEU:HD12	1.66	0.76
1:E:270:GLN:HB2	1:F:321:ALA:HA	1.66	0.76
1:E:297:GLN:H	1:E:297:GLN:CD	1.88	0.76
1:F:77:VAL:HG22	1:F:78:SER:H	1.51	0.76
1:D:50:ILE:HG22	1:D:84:GLN:HG3	1.68	0.74
1:A:138:ASN:O	1:A:139:ILE:HG23	1.87	0.74
1:D:36:VAL:HG22	1:D:70:VAL:HG11	1.68	0.74
1:A:58:LYS:HG2	1:A:62:MET:CE	2.18	0.74
1:E:260:VAL:HG23	1:E:261:ALA:H	1.52	0.74
1:E:260:VAL:O	1:E:279:GLU:OE1	2.06	0.74
1:F:113:PHE:O	1:F:117:VAL:HG23	1.89	0.73
1:E:295:ASN:OD1	1:E:297:GLN:HG2	1.89	0.73
1:C:154:LEU:HD23	1:C:164:VAL:HG21	1.71	0.72
1:A:260:VAL:O	1:A:279:GLU:OE1	2.07	0.72
1:F:59:LEU:HD13	1:F:306:ILE:HB	1.72	0.72
1:D:39:GLY:HA3	1:D:260:VAL:HG23	1.71	0.72
1:D:91:VAL:O	1:D:95:ILE:HG23	1.90	0.71
1:A:172:LEU:HD22	1:A:213:ILE:HG22	1.71	0.70
1:E:36:VAL:HA	1:E:70:VAL:HG13	1.72	0.70
1:C:52:SER:OG	1:C:55:VAL:HG23	1.90	0.70
1:C:282:VAL:HG21	1:C:296:LEU:HD13	1.73	0.69
1:F:278:THR:O	1:F:282:VAL:HG13	1.92	0.69
1:F:36:VAL:HA	1:F:70:VAL:HG13	1.75	0.69
1:F:77:VAL:HG22	1:F:78:SER:N	2.08	0.68
1:A:154:LEU:HD13	1:A:195:MET:HG2	1.75	0.68
1:B:31:LYS:HB2	1:B:31:LYS:NZ	2.08	0.68
1:D:47:GLU:HG2	1:D:310:LEU:HD21	1.74	0.68
1:E:51:VAL:HG13	1:E:310:LEU:HD13	1.76	0.68
1:A:161:ASN:ND2	1:F:149:ARG:HH12	1.92	0.67
1:B:113:PHE:O	1:B:117:VAL:HG23	1.94	0.67
1:E:297:GLN:H	1:E:297:GLN:NE2	1.91	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:O	1:B:140:ASN:HB2	1.94	0.67
1:E:151:ASP:O	1:E:155:LYS:HD3	1.95	0.67
1:F:262:GLY:HA3	1:F:315:SER:HB2	1.77	0.67
1:C:96:GLN:HB2	1:C:98:PHE:HE1	1.59	0.66
1:D:172:LEU:HD12	1:D:204:ASP:HB2	1.76	0.66
1:D:36:VAL:HA	1:D:70:VAL:HG13	1.76	0.66
1:C:123:GLU:HG3	1:C:163:SER:OG	1.95	0.66
1:C:282:VAL:CG2	1:C:296:LEU:HD13	2.25	0.66
1:F:55:VAL:HG12	1:F:56:LYS:N	2.09	0.66
1:C:96:GLN:HB2	1:C:98:PHE:CE1	2.31	0.66
1:A:270:GLN:O	1:A:272:ALA:N	2.27	0.66
1:F:87:ASP:O	1:F:91:VAL:HG23	1.95	0.66
1:C:133:LEU:O	1:C:137:LYS:HB2	1.94	0.66
1:A:60:ILE:HD13	1:A:73:THR:HG23	1.78	0.65
1:C:279:GLU:HG2	1:C:300:LEU:HD23	1.79	0.65
1:D:76:PHE:CE2	1:D:116:ALA:HA	2.30	0.65
1:B:45:GLN:HG3	1:B:82:VAL:HG21	1.76	0.65
1:A:282:VAL:CG2	1:A:296:LEU:HD13	2.26	0.65
1:E:284:MET:O	1:E:288:LEU:HD13	1.97	0.65
1:D:60:ILE:HD13	1:D:73:THR:HG23	1.79	0.64
1:E:154:LEU:CD1	1:E:195:MET:HB3	2.28	0.64
1:C:154:LEU:HD13	1:C:195:MET:HB3	1.78	0.64
1:D:154:LEU:HD13	1:D:195:MET:O	1.98	0.64
1:D:154:LEU:HD23	1:D:164:VAL:HG21	1.78	0.64
1:B:36:VAL:HA	1:B:70:VAL:HG13	1.79	0.64
1:C:278:THR:O	1:C:282:VAL:HG13	1.97	0.64
1:B:322:THR:O	1:B:323:CYS:HB2	1.96	0.63
1:C:260:VAL:O	1:C:279:GLU:OE1	2.16	0.63
1:E:40:PRO:HG2	1:E:72:GLU:O	1.99	0.63
1:F:154:LEU:HD23	1:F:164:VAL:HG21	1.80	0.63
1:B:278:THR:HG22	1:B:299:LEU:HD11	1.80	0.63
1:A:139:ILE:HG13	1:A:141:CYS:SG	2.39	0.63
1:A:137:LYS:HE2	4:A:536:HOH:O	1.98	0.63
1:A:40:PRO:HG2	1:A:72:GLU:O	1.99	0.63
1:B:231:ALA:CB	1:B:255:VAL:HG22	2.29	0.62
1:E:60:ILE:HD13	1:E:73:THR:HG23	1.81	0.62
1:A:45:GLN:HE22	3:A:399:3HG:H42	1.64	0.62
1:D:40:PRO:HG2	1:D:72:GLU:O	1.98	0.62
1:E:84:GLN:NE2	1:E:84:GLN:H	1.96	0.62
1:C:297:GLN:O	1:C:301:GLU:HG3	1.99	0.62
1:E:62:MET:HE3	1:E:305:PHE:CD2	2.34	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:HB2	4:B:770:HOH:O	1.99	0.62
1:C:75:SER:HB3	1:C:85:MET:HG2	1.80	0.62
1:E:83:PRO:HG2	1:E:84:GLN:HE21	1.64	0.62
1:F:36:VAL:HG22	1:F:70:VAL:HG11	1.82	0.62
1:A:161:ASN:CG	1:F:149:ARG:HH12	2.02	0.62
1:E:231:ALA:CB	1:E:255:VAL:HG22	2.29	0.62
1:C:139:ILE:HD12	1:C:149:ARG:NH2	2.15	0.62
1:B:31:LYS:HD3	4:B:1030:HOH:O	2.00	0.62
1:F:74:THR:H	1:F:105:VAL:HG12	1.65	0.61
1:B:113:PHE:CZ	1:B:162:ILE:HD12	2.35	0.61
1:D:84:GLN:H	1:D:84:GLN:NE2	1.98	0.61
1:E:98:PHE:HB2	1:E:101:ILE:HD12	1.82	0.61
1:E:33:VAL:HG23	1:E:290:ILE:HG21	1.82	0.61
1:F:55:VAL:CG1	1:F:56:LYS:N	2.64	0.61
1:B:202:LEU:HD13	1:B:217:MET:SD	2.41	0.61
1:C:231:ALA:CB	1:C:255:VAL:HG22	2.30	0.61
1:D:230:LEU:O	1:D:255:VAL:HG13	2.01	0.61
1:D:167:TYR:HE1	1:D:233:HIS:HD1	1.49	0.61
1:D:53:THR:N	1:D:54:PRO:HD2	2.16	0.61
1:B:36:VAL:HG22	1:B:70:VAL:HG11	1.83	0.60
1:B:47:GLU:HG2	1:B:310:LEU:HD21	1.83	0.60
1:E:75:SER:HB3	1:E:85:MET:HG2	1.81	0.60
1:E:139:ILE:HG21	1:E:149:ARG:HH12	1.65	0.60
1:D:130:ALA:O	1:D:184:LYS:HD2	2.02	0.60
1:F:202:LEU:HD13	1:F:217:MET:SD	2.41	0.60
1:D:87:ASP:O	1:D:91:VAL:HG23	2.01	0.59
1:D:278:THR:HG22	1:D:299:LEU:HD11	1.83	0.59
1:C:266:CYS:HB3	1:C:269:ALA:HB3	1.85	0.59
1:E:266:CYS:HB3	1:E:269:ALA:HB3	1.85	0.59
1:B:53:THR:N	1:B:54:PRO:HD2	2.18	0.59
1:B:278:THR:O	1:B:282:VAL:HG13	2.03	0.59
1:D:304:ASN:O	1:D:308:GLN:HG3	2.03	0.59
1:D:52:SER:HB2	1:D:54:PRO:HD2	1.84	0.58
1:E:36:VAL:HG22	1:E:70:VAL:HG11	1.86	0.58
1:F:47:GLU:CG	1:F:310:LEU:HD21	2.32	0.58
1:D:165:ARG:NH2	1:D:199:GLU:OE2	2.37	0.58
1:D:202:LEU:HD13	1:D:217:MET:SD	2.43	0.58
1:F:102:ASN:HD22	1:F:102:ASN:N	2.01	0.58
1:F:133:LEU:HD13	1:F:136:LYS:HE2	1.86	0.58
1:F:53:THR:N	1:F:54:PRO:HD2	2.19	0.58
1:A:51:VAL:HG13	1:A:310:LEU:HD13	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLU:N	1:C:279:GLU:OE1	2.36	0.58
1:C:98:PHE:HB2	1:C:101:ILE:HD12	1.86	0.58
1:E:63:LEU:HD21	1:E:260:VAL:CG1	2.33	0.58
1:E:154:LEU:HD13	1:E:195:MET:HB3	1.86	0.58
1:E:60:ILE:CD1	1:E:73:THR:HG23	2.33	0.58
1:F:157:ALA:HB1	1:F:162:ILE:O	2.04	0.57
1:F:75:SER:HB3	1:F:85:MET:HG2	1.84	0.57
1:A:135:THR:O	1:A:139:ILE:HG12	2.05	0.57
1:D:172:LEU:HD11	1:D:214:MET:HE2	1.86	0.57
1:F:40:PRO:HA	1:F:44:LEU:HD23	1.87	0.57
1:A:47:GLU:HG3	4:A:641:HOH:O	2.05	0.57
1:B:52:SER:OG	1:B:55:VAL:HG23	2.05	0.57
1:A:279:GLU:HG3	1:A:299:LEU:HD13	1.87	0.57
1:C:279:GLU:HG2	1:C:300:LEU:CD2	2.35	0.57
1:C:77:VAL:HG11	1:C:82:VAL:HG11	1.86	0.57
1:B:260:VAL:O	1:B:279:GLU:OE1	2.24	0.56
1:E:155:LYS:HD2	1:E:155:LYS:N	2.20	0.56
1:A:231:ALA:CB	1:A:255:VAL:HG22	2.35	0.56
1:C:154:LEU:CD1	1:C:195:MET:HB3	2.35	0.56
1:B:282:VAL:CG2	1:B:296:LEU:HD13	2.35	0.56
1:D:37:GLU:HG2	1:D:63:LEU:HD13	1.86	0.56
1:A:84:GLN:N	1:A:84:GLN:HE21	2.01	0.56
1:C:92:LEU:HD23	1:C:119:ALA:HB3	1.87	0.56
1:D:206:ILE:HG13	1:D:208:VAL:HG22	1.88	0.56
1:D:174:CYS:SG	1:D:175:PRO:HD2	2.46	0.56
1:D:151:ASP:O	1:D:155:LYS:HD3	2.06	0.56
1:E:137:LYS:HG2	1:E:176:TYR:OH	2.05	0.56
1:C:231:ALA:HB2	1:C:255:VAL:HG22	1.88	0.55
1:A:139:ILE:HB	1:A:149:ARG:HH22	1.72	0.55
1:D:51:VAL:HB	1:D:55:VAL:HG11	1.88	0.55
1:C:47:GLU:HG2	1:C:310:LEU:CD2	2.33	0.55
1:C:60:ILE:CD1	1:C:73:THR:HG23	2.37	0.55
1:D:282:VAL:HG21	1:D:296:LEU:HD13	1.89	0.55
1:C:176:TYR:OH	1:C:268:TYR:HE2	1.89	0.54
1:E:165:ARG:HD2	1:E:199:GLU:OE2	2.07	0.54
1:E:231:ALA:HB2	1:E:255:VAL:HG22	1.88	0.54
1:A:190:LYS:HD3	1:A:224:GLU:HB3	1.88	0.54
1:A:83:PRO:HG2	1:A:84:GLN:HE21	1.71	0.54
1:D:58:LYS:HG2	1:D:62:MET:CE	2.34	0.54
1:B:59:LEU:HD13	1:B:306:ILE:HB	1.89	0.54
1:C:39:GLY:HA3	1:C:260:VAL:HG23	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:LEU:HD11	1:F:211:PRO:CG	2.26	0.54
1:D:260:VAL:O	1:D:279:GLU:OE1	2.25	0.54
1:D:82:VAL:HG13	1:D:82:VAL:O	2.08	0.54
1:E:51:VAL:CG1	1:E:310:LEU:HD13	2.37	0.54
1:F:231:ALA:CB	1:F:255:VAL:HG22	2.38	0.54
1:C:183:ALA:O	1:C:187:GLU:HG3	2.08	0.54
1:E:127:PHE:HE1	1:E:169:SER:HG	1.54	0.54
1:C:40:PRO:HG2	1:C:72:GLU:O	2.08	0.54
1:B:160:ALA:O	1:B:161:ASN:HB3	2.08	0.54
1:B:147:PHE:CE1	1:B:191:LYS:HG2	2.42	0.53
1:C:266:CYS:SG	1:C:269:ALA:CB	2.96	0.53
1:D:256:VAL:CG2	1:D:281:LEU:HD21	2.38	0.53
1:F:278:THR:HG22	1:F:299:LEU:HD11	1.90	0.53
1:B:174:CYS:SG	1:B:175:PRO:HD2	2.47	0.53
1:D:50:ILE:CG2	1:D:84:GLN:HG3	2.37	0.53
1:B:117:VAL:HG22	1:B:162:ILE:CD1	2.38	0.53
1:A:98:PHE:HB2	1:A:101:ILE:HD12	1.89	0.53
1:C:147:PHE:HD2	1:C:195:MET:SD	2.31	0.53
1:E:279:GLU:HG3	1:E:299:LEU:HD13	1.91	0.53
1:F:37:GLU:HG2	1:F:63:LEU:HD13	1.90	0.53
1:B:124:VAL:CG2	1:B:164:VAL:HG22	2.39	0.53
1:C:200:ILE:HD12	1:C:200:ILE:N	2.24	0.53
1:C:60:ILE:HD13	1:C:73:THR:HG23	1.90	0.53
1:F:73:THR:OG1	1:F:103:TYR:HB3	2.09	0.53
1:F:41:ARG:HB2	1:F:72:GLU:O	2.09	0.53
1:D:39:GLY:N	1:D:40:PRO:HD2	2.24	0.53
1:D:126:ILE:HD11	1:D:197:CYS:SG	2.49	0.53
1:D:92:LEU:HD23	1:D:119:ALA:HB3	1.90	0.53
1:B:77:VAL:HG23	4:B:944:HOH:O	2.09	0.52
1:C:87:ASP:O	1:C:90:GLU:HG2	2.09	0.52
1:A:304:ASN:O	1:A:308:GLN:HG3	2.08	0.52
1:C:266:CYS:SG	1:C:269:ALA:HB3	2.49	0.52
1:E:135:THR:HG23	1:E:139:ILE:HD11	1.91	0.52
1:F:77:VAL:HG23	1:F:108:PRO:HG3	1.91	0.52
1:B:154:LEU:HD13	1:B:195:MET:HG2	1.91	0.52
1:B:231:ALA:HB2	1:B:255:VAL:HG22	1.90	0.52
1:F:58:LYS:O	1:F:61:ASP:HB2	2.10	0.52
1:A:82:VAL:O	1:A:82:VAL:HG22	2.08	0.52
1:F:154:LEU:CD1	1:F:195:MET:HB3	2.39	0.52
1:F:199:GLU:C	1:F:200:ILE:HD12	2.30	0.51
1:B:138:ASN:HD22	1:B:138:ASN:C	2.13	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:LEU:O	1:F:137:LYS:HB2	2.11	0.51
1:C:139:ILE:HB	1:C:149:ARG:NH2	2.15	0.51
1:F:51:VAL:HB	1:F:55:VAL:CG1	2.29	0.51
1:C:58:LYS:HD3	1:C:62:MET:HE1	1.92	0.51
1:E:148:GLN:HA	1:E:151:ASP:OD2	2.10	0.51
1:E:63:LEU:HD21	1:E:260:VAL:HG11	1.93	0.51
1:D:133:LEU:HD23	1:D:177:GLU:HG2	1.92	0.51
1:E:175:PRO:HG2	1:E:176:TYR:CD1	2.46	0.51
1:B:310:LEU:HB3	1:B:312:ARG:HG2	1.93	0.50
1:A:161:ASN:ND2	1:F:149:ARG:NH1	2.57	0.50
1:D:256:VAL:HG21	1:D:281:LEU:HD21	1.92	0.50
1:F:38:VAL:O	1:F:42:ASP:HB3	2.12	0.50
1:D:312:ARG:HD3	1:D:312:ARG:O	2.11	0.50
1:B:279:GLU:HG3	1:B:299:LEU:HD13	1.94	0.50
1:C:287:GLY:HA3	1:D:210:THR:HG21	1.94	0.50
1:D:147:PHE:CE1	1:D:191:LYS:HG2	2.47	0.50
1:F:77:VAL:CG2	1:F:78:SER:H	2.24	0.50
1:B:138:ASN:ND2	1:B:138:ASN:C	2.65	0.50
1:B:142:SER:HB3	1:B:145:GLU:CG	2.33	0.50
1:B:200:ILE:HD12	1:B:200:ILE:N	2.27	0.50
1:A:317:LYS:NZ	1:B:236:ASP:OD2	2.45	0.50
1:D:172:LEU:HD11	1:D:214:MET:CE	2.41	0.50
1:B:189:THR:HG22	1:B:225:VAL:HG21	1.93	0.49
1:F:101:ILE:C	1:F:102:ASN:HD22	2.15	0.49
1:F:154:LEU:HD13	1:F:195:MET:HB3	1.95	0.49
1:F:82:VAL:HG13	1:F:82:VAL:O	2.12	0.49
1:C:169:SER:HB2	1:C:205:THR:OG1	2.12	0.49
1:C:37:GLU:HG2	1:C:63:LEU:HD13	1.95	0.49
1:D:36:VAL:HG22	1:D:70:VAL:CG1	2.41	0.49
1:E:113:PHE:O	1:E:117:VAL:HG23	2.12	0.49
1:E:58:LYS:HD3	1:E:305:PHE:CZ	2.47	0.49
1:C:117:VAL:HG22	1:C:162:ILE:CD1	2.43	0.49
1:E:266:CYS:HB3	1:E:269:ALA:CB	2.42	0.49
1:F:39:GLY:N	1:F:40:PRO:HD2	2.28	0.49
1:B:139:ILE:O	1:B:140:ASN:CB	2.60	0.49
1:C:133:LEU:HD12	1:C:177:GLU:HG2	1.94	0.49
1:E:51:VAL:HG13	1:E:310:LEU:CD1	2.41	0.49
1:F:247:MET:HE3	1:F:250:GLN:HB2	1.94	0.49
1:F:92:LEU:HD23	1:F:119:ALA:HB3	1.94	0.49
1:A:62:MET:HE1	1:A:305:PHE:CG	2.48	0.49
1:B:40:PRO:HG2	1:B:72:GLU:O	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MET:O	1:B:288:LEU:HD23	2.13	0.48
1:F:102:ASN:ND2	1:F:102:ASN:N	2.61	0.48
1:A:85:MET:O	1:A:88:HIS:HD2	1.96	0.48
1:E:202:LEU:HD13	1:E:217:MET:SD	2.53	0.48
1:F:191:LYS:HG3	1:F:195:MET:CE	2.44	0.48
1:E:139:ILE:HG13	1:E:141:CYS:SG	2.53	0.48
1:E:297:GLN:N	1:E:297:GLN:NE2	2.58	0.48
1:F:69:SER:HA	1:F:101:ILE:HD12	1.96	0.48
1:C:262:GLY:HA3	1:C:315:SER:HB2	1.96	0.48
1:D:282:VAL:CG2	1:D:296:LEU:HD13	2.44	0.48
1:A:58:LYS:HD3	1:A:305:PHE:CZ	2.49	0.48
1:C:282:VAL:O	1:C:286:GLU:HG3	2.13	0.48
1:E:154:LEU:HD13	1:E:195:MET:O	2.14	0.48
1:E:260:VAL:HG23	1:E:261:ALA:N	2.26	0.48
1:E:78:SER:HB2	4:E:852:HOH:O	2.14	0.48
1:F:52:SER:C	1:F:54:PRO:HD2	2.33	0.48
1:C:279:GLU:HB2	1:C:316:SER:OG	2.14	0.48
1:F:200:ILE:N	1:F:200:ILE:HD12	2.29	0.48
1:B:191:LYS:O	1:B:195:MET:HB2	2.14	0.47
1:C:61:ASP:O	1:C:65:GLU:HG3	2.13	0.47
1:E:53:THR:N	1:E:54:PRO:HD2	2.29	0.47
1:B:282:VAL:HG22	1:B:296:LEU:HD13	1.96	0.47
1:C:143:ILE:O	1:C:147:PHE:HD1	1.98	0.47
1:D:218:LEU:O	1:D:222:MET:HG3	2.15	0.47
1:A:270:GLN:OE1	1:B:323:CYS:HA	2.15	0.47
1:A:51:VAL:CG1	1:A:310:LEU:HD13	2.43	0.47
1:D:92:LEU:HD23	1:D:119:ALA:CB	2.45	0.47
1:D:77:VAL:HG22	1:D:78:SER:N	2.28	0.47
1:F:74:THR:OG1	1:F:75:SER:N	2.48	0.47
1:A:117:VAL:HG22	1:A:162:ILE:HD12	1.96	0.47
1:F:136:LYS:HG3	1:F:137:LYS:N	2.29	0.47
1:F:259:SER:OG	1:F:263:LEU:HB2	2.14	0.47
1:A:133:LEU:HB2	1:A:177:GLU:HG3	1.96	0.47
1:D:114:GLU:HA	1:D:114:GLU:OE1	2.15	0.47
1:F:175:PRO:HG2	1:F:176:TYR:CD1	2.50	0.47
1:C:176:TYR:HH	1:C:268:TYR:HE2	1.55	0.47
1:F:230:LEU:O	1:F:255:VAL:HG13	2.14	0.47
1:F:133:LEU:HD23	1:F:177:GLU:CG	2.45	0.47
1:C:208:VAL:HG12	1:C:238:TYR:CE2	2.49	0.47
1:F:236:ASP:OD1	1:F:239:GLY:HA2	2.14	0.47
1:D:167:TYR:HE1	1:D:233:HIS:ND1	2.11	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:GLU:CD	1:E:90:GLU:H	2.16	0.47
1:F:297:GLN:NE2	1:F:297:GLN:HA	2.29	0.47
1:D:189:THR:HG22	1:D:225:VAL:HG21	1.97	0.47
1:F:133:LEU:N	1:F:133:LEU:HD22	2.30	0.46
1:F:92:LEU:HD23	1:F:119:ALA:CB	2.45	0.46
1:B:113:PHE:CZ	1:B:157:ALA:HA	2.50	0.46
1:C:270:GLN:CG	1:D:321:ALA:O	2.63	0.46
1:C:51:VAL:HG13	1:C:310:LEU:HD13	1.97	0.46
1:A:53:THR:N	1:A:54:PRO:HD2	2.30	0.46
1:D:227:LEU:HD21	1:D:252:GLY:HA3	1.98	0.46
1:D:279:GLU:O	1:D:282:VAL:HG22	2.15	0.46
1:F:51:VAL:CG2	1:F:55:VAL:HG11	2.45	0.46
1:F:58:LYS:HD3	1:F:305:PHE:CZ	2.50	0.46
1:F:125:VAL:HG22	1:F:165:ARG:HB3	1.96	0.46
1:C:82:VAL:O	1:C:82:VAL:HG22	2.16	0.46
1:D:191:LYS:O	1:D:195:MET:HB2	2.16	0.46
1:D:51:VAL:O	1:D:56:LYS:NZ	2.48	0.46
1:E:85:MET:HE2	1:E:85:MET:HA	1.98	0.46
1:A:234:CYS:HB3	4:A:503:HOH:O	2.16	0.46
1:D:73:THR:OG1	1:D:103:TYR:HB3	2.15	0.46
1:A:83:PRO:CD	1:A:84:GLN:NE2	2.79	0.46
1:E:211:PRO:HG2	1:F:288:LEU:HD21	1.97	0.46
1:C:127:PHE:O	1:C:150:PHE:HZ	1.99	0.46
1:C:53:THR:N	1:C:54:PRO:HD2	2.30	0.46
1:C:77:VAL:HG11	1:C:82:VAL:CG1	2.45	0.46
1:E:77:VAL:HG11	1:E:82:VAL:HG11	1.97	0.46
1:F:55:VAL:HG12	1:F:56:LYS:H	1.80	0.46
1:B:261:ALA:HB1	1:B:314:THR:OG1	2.16	0.46
1:D:278:THR:CG2	1:D:299:LEU:HD11	2.45	0.46
1:D:41:ARG:C	1:D:41:ARG:HD2	2.36	0.46
1:E:37:GLU:OE2	1:E:260:VAL:HG13	2.16	0.46
1:F:77:VAL:CG2	1:F:78:SER:N	2.77	0.46
1:D:133:LEU:HD23	1:D:177:GLU:CG	2.47	0.45
1:F:160:ALA:O	1:F:161:ASN:HB3	2.16	0.45
1:A:83:PRO:HD2	1:A:84:GLN:HE22	1.82	0.45
1:E:41:ARG:C	1:E:41:ARG:HD2	2.37	0.45
1:D:90:GLU:OE1	1:D:90:GLU:N	2.44	0.45
1:D:127:PHE:N	1:D:127:PHE:CD1	2.85	0.45
1:D:80:LYS:HE2	4:D:1049:HOH:O	2.16	0.45
1:F:127:PHE:O	1:F:150:PHE:CZ	2.70	0.45
1:F:205:THR:O	1:F:235:HIS:ND1	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:SER:HB2	1:F:54:PRO:HD2	1.97	0.45
1:D:154:LEU:O	1:D:158:GLN:HG3	2.17	0.45
1:C:149:ARG:NH1	1:E:161:ASN:HD21	2.14	0.45
1:E:37:GLU:HG2	1:E:63:LEU:HD13	1.98	0.45
1:B:127:PHE:N	1:B:127:PHE:CD1	2.84	0.45
1:B:82:VAL:O	1:B:82:VAL:HG13	2.16	0.45
1:F:210:THR:HB	1:F:211:PRO:HD2	1.99	0.45
1:F:45:GLN:HG3	1:F:82:VAL:HG21	1.98	0.45
1:A:135:THR:HG22	1:A:141:CYS:O	2.17	0.45
1:A:58:LYS:HZ2	1:A:62:MET:HE1	1.82	0.45
1:D:208:VAL:HG12	1:D:238:TYR:CE2	2.52	0.45
1:F:189:THR:HG22	1:F:225:VAL:HG21	1.97	0.45
1:D:205:THR:O	1:D:235:HIS:ND1	2.43	0.45
1:E:136:LYS:O	1:E:140:ASN:HA	2.16	0.45
1:F:206:ILE:HG13	1:F:208:VAL:HG22	1.98	0.45
1:A:282:VAL:HG21	1:A:296:LEU:HD13	1.98	0.45
1:A:45:GLN:NE2	3:A:399:3HG:H42	2.28	0.45
1:A:39:GLY:HA2	1:A:259:SER:OG	2.17	0.44
1:C:147:PHE:HZ	1:C:188:VAL:HG13	1.81	0.44
1:C:236:ASP:OD2	1:D:317:LYS:NZ	2.51	0.44
1:D:313:LYS:HE3	4:D:908:HOH:O	2.17	0.44
1:E:200:ILE:HD12	1:E:200:ILE:N	2.31	0.44
1:A:60:ILE:CD1	1:A:73:THR:HG23	2.47	0.44
1:C:141:CYS:HB2	1:C:145:GLU:OE1	2.16	0.44
1:C:52:SER:O	1:C:55:VAL:HB	2.17	0.44
1:F:128:GLY:N	1:F:167:TYR:O	2.49	0.44
1:F:208:VAL:HG12	1:F:238:TYR:CE2	2.52	0.44
1:A:223:GLN:NE2	4:A:759:HOH:O	2.50	0.44
1:B:222:MET:HE1	4:B:685:HOH:O	2.16	0.44
1:D:203:GLY:HA2	1:D:233:HIS:O	2.17	0.44
1:E:206:ILE:HG13	1:E:208:VAL:HG22	1.99	0.44
1:F:91:VAL:O	1:F:95:ILE:HG23	2.17	0.44
1:C:270:GLN:HG3	1:D:321:ALA:O	2.17	0.44
1:D:210:THR:HB	1:D:211:PRO:HD2	1.98	0.44
1:F:133:LEU:H	1:F:133:LEU:CD2	2.29	0.44
1:D:37:GLU:OE2	1:D:260:VAL:N	2.46	0.44
1:B:53:THR:N	1:B:54:PRO:CD	2.80	0.44
1:A:138:ASN:O	1:A:139:ILE:HD13	2.18	0.44
1:A:62:MET:CE	1:A:305:PHE:CD2	3.00	0.44
1:F:165:ARG:NH2	1:F:199:GLU:OE2	2.51	0.44
1:A:141:CYS:HB2	1:A:145:GLU:HB2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ALA:HB1	1:A:255:VAL:HG22	1.99	0.44
1:E:28:THR:O	1:E:28:THR:HG23	2.17	0.44
1:B:77:VAL:HG22	1:B:78:SER:N	2.33	0.43
1:D:53:THR:O	1:D:57:ILE:HG13	2.18	0.43
1:D:86:GLY:C	1:D:88:HIS:H	2.21	0.43
1:D:51:VAL:HG23	1:D:56:LYS:HG3	2.01	0.43
1:E:84:GLN:HE21	1:E:84:GLN:H	1.64	0.43
1:F:53:THR:N	1:F:54:PRO:CD	2.81	0.43
1:F:77:VAL:HG11	1:F:82:VAL:CG1	2.48	0.43
1:A:45:GLN:NE2	3:A:399:3HG:H21	2.33	0.43
1:B:161:ASN:CG	1:B:161:ASN:O	2.56	0.43
1:F:282:VAL:O	1:F:286:GLU:HB2	2.19	0.43
1:F:96:GLN:O	1:F:97:LYS:HD3	2.18	0.43
1:D:182:PRO:HD2	4:D:671:HOH:O	2.18	0.43
1:B:41:ARG:C	1:B:41:ARG:HD2	2.39	0.43
1:E:169:SER:HB2	1:E:205:THR:OG1	2.18	0.43
1:A:33:VAL:HG23	1:A:290:ILE:HG21	2.00	0.43
1:A:98:PHE:HA	1:A:99:PRO:HD3	1.90	0.43
1:C:266:CYS:CB	1:C:269:ALA:HB3	2.48	0.43
1:B:144:GLU:HA	1:B:144:GLU:OE1	2.19	0.43
1:F:106:LEU:HD12	1:F:106:LEU:N	2.33	0.43
1:B:31:LYS:HB2	1:B:31:LYS:HZ2	1.83	0.43
1:F:41:ARG:CZ	1:F:106:LEU:HD21	2.49	0.43
1:C:232:VAL:CG2	1:C:234:CYS:SG	3.07	0.42
1:D:60:ILE:CD1	1:D:73:THR:HG23	2.48	0.42
1:A:77:VAL:CG1	1:A:82:VAL:HG13	2.49	0.42
1:C:58:LYS:HD3	1:C:62:MET:CE	2.49	0.42
1:D:53:THR:N	1:D:54:PRO:CD	2.82	0.42
1:E:176:TYR:OH	1:E:268:TYR:HE2	2.02	0.42
1:F:161:ASN:O	1:F:161:ASN:ND2	2.53	0.42
1:A:231:ALA:HB2	1:A:255:VAL:HG22	2.01	0.42
1:A:312:ARG:HD3	1:A:313:LYS:O	2.19	0.42
1:E:312:ARG:HD3	1:E:313:LYS:O	2.19	0.42
1:E:43:GLY:O	1:E:47:GLU:HG2	2.19	0.42
1:F:151:ASP:OD1	1:F:155:LYS:HD3	2.19	0.42
1:A:113:PHE:O	1:A:117:VAL:HG23	2.19	0.42
1:A:191:LYS:HG3	1:A:195:MET:HE3	2.02	0.42
1:A:85:MET:O	1:A:88:HIS:CD2	2.71	0.42
1:B:91:VAL:O	1:B:95:ILE:HG23	2.19	0.42
1:F:304:ASN:O	1:F:308:GLN:HG3	2.20	0.42
1:B:31:LYS:HB2	1:B:31:LYS:HZ3	1.82	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LYS:NZ	4:E:739:HOH:O	2.51	0.42
1:F:175:PRO:HG2	1:F:176:TYR:CE1	2.55	0.42
1:F:231:ALA:HB1	1:F:255:VAL:HG22	2.01	0.42
1:B:218:LEU:CD1	1:B:248:ALA:HA	2.49	0.42
1:B:147:PHE:CD1	1:B:191:LYS:HG2	2.55	0.42
1:C:77:VAL:HG22	1:C:78:SER:N	2.35	0.42
1:F:306:ILE:O	1:F:310:LEU:HB2	2.20	0.42
1:D:181:SER:HA	1:D:182:PRO:HD3	1.95	0.42
1:A:321:ALA:O	1:B:270:GLN:HG2	2.20	0.41
1:E:137:LYS:HG2	1:E:176:TYR:CZ	2.55	0.41
1:E:87:ASP:HA	1:E:90:GLU:OE1	2.20	0.41
1:F:247:MET:HE3	1:F:250:GLN:HE21	1.84	0.41
1:B:36:VAL:HG22	1:B:70:VAL:CG1	2.50	0.41
1:E:169:SER:O	1:E:170:CYS:HB2	2.20	0.41
1:A:37:GLU:HG2	1:A:63:LEU:HD13	2.02	0.41
1:C:117:VAL:HG22	1:C:162:ILE:HD11	2.02	0.41
1:D:62:MET:HE1	1:D:305:PHE:CG	2.56	0.41
1:F:52:SER:CB	1:F:54:PRO:HD2	2.51	0.41
1:F:141:CYS:SG	1:F:145:GLU:HB2	2.60	0.41
1:E:270:GLN:C	1:E:272:ALA:H	2.24	0.41
1:A:45:GLN:HE22	3:A:399:3HG:H21	1.85	0.41
1:B:132:GLU:N	1:B:143:ILE:HD11	2.35	0.41
1:B:85:MET:HE2	1:B:85:MET:HA	2.02	0.41
1:F:132:GLU:OE2	1:F:132:GLU:HA	2.20	0.41
1:B:47:GLU:HG2	1:B:310:LEU:CD2	2.51	0.41
1:C:227:LEU:HD21	1:C:252:GLY:HA3	2.03	0.41
1:D:51:VAL:HG13	1:D:310:LEU:HD13	2.02	0.41
1:F:206:ILE:H	1:F:206:ILE:HG12	1.68	0.41
1:B:218:LEU:HD11	1:B:248:ALA:HA	2.03	0.41
1:C:161:ASN:HA	1:C:161:ASN:HD22	1.65	0.41
1:E:279:GLU:OE1	1:E:279:GLU:N	2.46	0.41
1:F:174:CYS:SG	1:F:175:PRO:HD2	2.61	0.41
1:C:122:LYS:HE2	1:C:122:LYS:HB3	1.93	0.41
1:F:132:GLU:OE2	1:F:143:ILE:HG13	2.21	0.41
1:B:98:PHE:CB	1:B:101:ILE:HD12	2.46	0.41
1:B:154:LEU:O	1:B:158:GLN:HG3	2.21	0.41
1:B:154:LEU:HD13	1:B:195:MET:O	2.21	0.41
1:D:51:VAL:HB	1:D:55:VAL:CG1	2.49	0.41
1:C:81:TRP:CG	1:E:122:LYS:HE3	2.56	0.41
1:F:63:LEU:HD21	1:F:260:VAL:HG22	2.03	0.41
1:F:41:ARG:HD3	1:F:75:SER:HB2	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HD22	1:C:306:ILE:HD13	2.02	0.40
1:C:34:LYS:HD3	1:C:70:VAL:HG21	2.03	0.40
1:D:294:VAL:HG12	1:D:295:ASN:N	2.36	0.40
1:C:53:THR:HG21	1:C:90:GLU:HG3	2.03	0.40
1:D:259:SER:O	1:D:260:VAL:C	2.58	0.40
1:F:36:VAL:HG22	1:F:70:VAL:CG1	2.50	0.40
1:A:139:ILE:HB	1:A:141:CYS:SG	2.62	0.40
1:A:205:THR:O	1:A:235:HIS:ND1	2.53	0.40
1:A:77:VAL:HG11	1:A:82:VAL:CG1	2.51	0.40
1:C:306:ILE:O	1:C:310:LEU:HB2	2.21	0.40
1:D:200:ILE:N	1:D:200:ILE:HD12	2.36	0.40
1:D:68:LEU:O	1:D:101:ILE:HD12	2.21	0.40
1:F:191:LYS:HG3	1:F:195:MET:HE3	2.02	0.40
1:F:62:MET:HE3	1:F:305:PHE:CD2	2.57	0.40
1:F:82:VAL:HA	1:F:83:PRO:HD2	1.96	0.40
1:B:191:LYS:HA	1:B:191:LYS:HD2	1.85	0.40
1:B:260:VAL:HB	1:B:261:ALA:H	1.72	0.40
1:C:169:SER:O	1:C:170:CYS:HB2	2.21	0.40
1:A:48:LYS:CD	1:A:48:LYS:N	2.76	0.40
1:C:165:ARG:NH1	1:C:257:ASP:OD1	2.55	0.40
1:D:278:THR:O	1:D:282:VAL:HG13	2.21	0.40
1:E:322:THR:HG22	1:E:323:CYS:N	2.36	0.40
1:E:34:LYS:HD3	1:E:70: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	294/298 (99%)	287 (98%)	4 (1%)	3 (1%)	15 11
1	B	294/298 (99%)	281 (96%)	8 (3%)	5 (2%)	9 4

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	292/298 (98%)	279 (96%)	12 (4%)	1 (0%)	41	41
1	D	276/298 (93%)	261 (95%)	12 (4%)	3 (1%)	14	9
1	E	294/298 (99%)	281 (96%)	11 (4%)	2 (1%)	22	18
1	F	282/298 (95%)	265 (94%)	15 (5%)	2 (1%)	22	18
All	All	1732/1788 (97%)	1654 (96%)	62 (4%)	16 (1%)	17	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	260	VAL
1	A	271	GLY
1	B	260	VAL
1	B	270	GLN
1	C	260	VAL
1	D	260	VAL
1	E	260	VAL
1	B	140	ASN
1	D	87	ASP
1	F	41	ARG
1	B	273	SER
1	D	136	LYS
1	E	177	GLU
1	F	73	THR
1	B	108	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/240 (99%)	220 (92%)	18 (8%)	13	10
1	B	238/240 (99%)	221 (93%)	17 (7%)	14	11
1	C	236/240 (98%)	225 (95%)	11 (5%)	26	25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	227/240 (95%)	215 (95%)	12 (5%)	22	20
1	E	238/240 (99%)	225 (94%)	13 (6%)	21	19
1	F	232/240 (97%)	223 (96%)	9 (4%)	32	33
All	All	1409/1440 (98%)	1329 (94%)	80 (6%)	20	18

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

Mol	Chain	Res	Type
1	A	32	ARG
1	A	48	LYS
1	A	70	VAL
1	A	82	VAL
1	A	84	GLN
1	A	114	GLU
1	A	133	LEU
1	A	139	ILE
1	A	151	ASP
1	A	192	PHE
1	A	230	LEU
1	A	246	LEU
1	A	255	VAL
1	A	256	VAL
1	A	288	LEU
1	A	299	LEU
1	A	310	LEU
1	A	312	ARG
1	B	31	LYS
1	B	44	LEU
1	B	65	GLU
1	B	85	MET
1	B	114	GLU
1	B	138	ASN
1	B	140	ASN
1	B	141	CYS
1	B	165	ARG
1	B	167	TYR
1	B	230	LEU
1	B	246	LEU
1	B	256	VAL
1	B	282	VAL
1	B	299	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	311	ASN
1	B	312	ARG
1	C	82	VAL
1	C	84	GLN
1	C	85	MET
1	C	114	GLU
1	C	165	ARG
1	C	230	LEU
1	C	246	LEU
1	C	255	VAL
1	C	256	VAL
1	C	288	LEU
1	C	312	ARG
1	D	32	ARG
1	D	84	GLN
1	D	114	GLU
1	D	161	ASN
1	D	181	SER
1	D	230	LEU
1	D	246	LEU
1	D	255	VAL
1	D	288	LEU
1	D	299	LEU
1	D	312	ARG
1	D	323	CYS
1	E	70	VAL
1	E	84	GLN
1	E	85	MET
1	E	90	GLU
1	E	140	ASN
1	E	161	ASN
1	E	181	SER
1	E	230	LEU
1	E	246	LEU
1	E	255	VAL
1	E	297	GLN
1	E	299	LEU
1	E	312	ARG
1	F	49	ASN
1	F	55	VAL
1	F	161	ASN
1	F	230	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	255	VAL
1	F	299	LEU
1	F	311	ASN
1	F	312	ARG
1	F	323	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	84	GLN
1	A	88	HIS
1	A	96	GLN
1	A	140	ASN
1	A	161	ASN
1	A	223	GLN
1	A	244	ASN
1	A	250	GLN
1	A	291	HIS
1	A	297	GLN
1	A	311	ASN
1	B	138	ASN
1	B	161	ASN
1	B	223	GLN
1	B	244	ASN
1	B	250	GLN
1	B	297	GLN
1	B	311	ASN
1	C	109	ASN
1	C	161	ASN
1	C	223	GLN
1	C	244	ASN
1	C	250	GLN
1	C	297	GLN
1	C	304	ASN
1	C	311	ASN
1	D	84	GLN
1	D	148	GLN
1	D	158	GLN
1	D	161	ASN
1	D	244	ASN
1	D	250	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	311	ASN
1	E	84	GLN
1	E	88	HIS
1	E	102	ASN
1	E	140	ASN
1	E	161	ASN
1	E	244	ASN
1	E	250	GLN
1	E	291	HIS
1	E	297	GLN
1	E	308	GLN
1	E	311	ASN
1	F	102	ASN
1	F	161	ASN
1	F	223	GLN
1	F	244	ASN
1	F	250	GLN
1	F	297	GLN
1	F	311	ASN
1	F	320	GLN

### 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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	3HG	A	399	-	3,9,9	1.86	1 (33%)	2,11,11	1.39	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
3	3HG	A	399	-	-	2/4/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	399	3HG	O2-C3	-3.17	1.33	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	399	3HG	C1-C2-C3-O2
3	A	399	3HG	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	399	3HG	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	296/298 (99%)	0.08	8 (2%) 54 60	19, 28, 56, 72	0
1	B	296/298 (99%)	0.61	26 (8%) 10 12	22, 39, 75, 95	0
1	C	294/298 (98%)	0.24	11 (3%) 41 48	22, 38, 62, 74	0
1	D	282/298 (94%)	0.95	51 (18%) 1 1	30, 56, 85, 95	0
1	E	296/298 (99%)	0.37	28 (9%) 8 10	23, 36, 72, 84	0
1	F	288/298 (96%)	1.02	52 (18%) 1 1	20, 60, 87, 95	0
All	All	1752/1788 (97%)	0.54	176 (10%) 7 9	19, 40, 79, 95	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	TRP	8.7
1	B	138	ASN	7.0
1	B	141	CYS	6.9
1	B	140	ASN	5.5
1	D	146	SER	5.3
1	D	176	TYR	5.3
1	D	110	LEU	5.1
1	F	147	PHE	4.8
1	C	270	GLN	4.7
1	B	176	TYR	4.6
1	D	133	LEU	4.5
1	E	323	CYS	4.5
1	F	141	CYS	4.4
1	C	322	THR	4.3
1	F	144	GLU	4.3
1	B	268	TYR	4.3
1	D	147	PHE	4.2
1	F	50	ILE	4.2
1	F	127	PHE	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	269	ALA	4.1
1	B	81	TRP	4.1
1	F	111	LYS	4.1
1	F	176	TYR	4.0
1	D	114	GLU	3.9
1	E	268	TYR	3.9
1	B	142	SER	3.8
1	F	152	ALA	3.8
1	B	147	PHE	3.8
1	F	272	ALA	3.7
1	F	81	TRP	3.7
1	E	243	ALA	3.6
1	B	136	LYS	3.6
1	B	323	CYS	3.6
1	E	271	GLY	3.6
1	B	266	CYS	3.5
1	D	151	ASP	3.5
1	B	145	GLU	3.5
1	E	266	CYS	3.4
1	F	311	ASN	3.4
1	D	28	THR	3.4
1	D	137	LYS	3.3
1	F	137	LYS	3.3
1	F	28	THR	3.3
1	C	269	ALA	3.3
1	E	269	ALA	3.3
1	F	155	LYS	3.3
1	F	151	ASP	3.3
1	F	76	PHE	3.2
1	F	276	LEU	3.2
1	E	322	THR	3.2
1	F	265	GLY	3.2
1	C	148	GLN	3.1
1	C	271	GLY	3.1
1	B	28	THR	3.1
1	D	154	LEU	3.1
1	F	110	LEU	3.1
1	F	106	LEU	3.1
1	B	133	LEU	3.0
1	E	147	PHE	3.0
1	A	271	GLY	3.0
1	D	175	PRO	3.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	323	CYS	3.0
1	D	77	VAL	2.9
1	F	160	ALA	2.9
1	F	90	GLU	2.9
1	F	95	ILE	2.9
1	A	323	CYS	2.9
1	F	313	LYS	2.9
1	D	162	ILE	2.9
1	F	48	LYS	2.9
1	F	136	LYS	2.9
1	D	80	LYS	2.9
1	F	309	ALA	2.9
1	F	154	LEU	2.9
1	D	145	GLU	2.9
1	E	176	TYR	2.8
1	D	322	THR	2.8
1	D	132	GLU	2.8
1	A	322	THR	2.8
1	D	276	LEU	2.8
1	F	162	ILE	2.8
1	C	127	PHE	2.8
1	F	83	PRO	2.8
1	E	137	LYS	2.8
1	B	270	GLN	2.8
1	E	140	ASN	2.7
1	D	48	LYS	2.7
1	F	118	ALA	2.7
1	E	276	LEU	2.7
1	B	50	ILE	2.7
1	E	273	SER	2.7
1	B	152	ALA	2.7
1	E	242	LEU	2.7
1	B	70	VAL	2.6
1	B	148	GLN	2.6
1	E	270	GLN	2.6
1	F	70	VAL	2.6
1	D	308	GLN	2.6
1	A	270	GLN	2.6
1	F	258	SER	2.5
1	F	61	ASP	2.5
1	B	271	GLY	2.5
1	F	242	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	119	ALA	2.5
1	E	144	GLU	2.5
1	D	277	ALA	2.5
1	F	55	VAL	2.4
1	C	268	TYR	2.4
1	D	50	ILE	2.4
1	D	118	ALA	2.4
1	D	275	ASN	2.4
1	D	232	VAL	2.4
1	D	120	GLY	2.4
1	F	148	GLN	2.4
1	D	38	VAL	2.4
1	C	158	GLN	2.4
1	D	311	ASN	2.4
1	A	28	THR	2.4
1	D	98	PHE	2.4
1	E	297	GLN	2.4
1	D	136	LYS	2.4
1	F	125	VAL	2.4
1	F	234	CYS	2.4
1	E	133	LEU	2.4
1	B	155	LYS	2.4
1	D	260	VAL	2.3
1	D	150	PHE	2.3
1	D	100	GLY	2.3
1	A	80	LYS	2.3
1	B	158	GLN	2.3
1	C	310	LEU	2.3
1	D	155	LYS	2.3
1	E	241	ALA	2.3
1	F	243	ALA	2.3
1	D	40	PRO	2.3
1	D	109	ASN	2.3
1	F	232	VAL	2.3
1	C	264	GLY	2.3
1	F	308	GLN	2.3
1	D	261	ALA	2.2
1	F	241	ALA	2.2
1	D	177	GLU	2.2
1	D	241	ALA	2.2
1	F	323	CYS	2.2
1	D	82	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	108	PRO	2.2
1	A	276	LEU	2.2
1	D	127	PHE	2.2
1	E	232	VAL	2.2
1	C	195	MET	2.2
1	D	304	ASN	2.2
1	F	73	THR	2.2
1	E	151	ASP	2.2
1	D	234	CYS	2.1
1	D	79	PRO	2.1
1	F	93	LYS	2.1
1	D	195	MET	2.1
1	F	159	SER	2.1
1	A	269	ALA	2.1
1	E	28	THR	2.1
1	E	278	THR	2.1
1	F	261	ALA	2.1
1	F	322	THR	2.1
1	B	260	VAL	2.0
1	E	260	VAL	2.0
1	E	178	GLY	2.0
1	E	267	PRO	2.0
1	E	110	LEU	2.0
1	D	51	VAL	2.0
1	D	134	PHE	2.0
1	D	178	GLY	2.0
1	F	88	HIS	2.0
1	B	139	ILE	2.0
1	F	126	ILE	2.0
1	B	48	LYS	2.0
1	E	38	VAL	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( $\text{\AA}^2$ )	Q<0.9
2	MG	A	401	1/1	0.63	0.22	35,35,35,35	0
2	MG	F	406	1/1	0.65	0.28	64,64,64,64	0
2	MG	E	402	1/1	0.70	0.22	44,44,44,44	0
3	3HG	A	399	10/10	0.81	0.23	66,66,67,67	0
2	MG	B	404	1/1	0.82	0.20	48,48,48,48	0
2	MG	C	403	1/1	0.82	0.20	37,37,37,37	0
2	MG	D	405	1/1	0.91	0.25	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.