



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:49 PM GMT

PDB ID : 2CW6
Title : Crystal Structure of Human HMG-CoA Lyase: Insights into Catalysis and the Molecular Basis for HydroxymethylglutaricAciduria
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

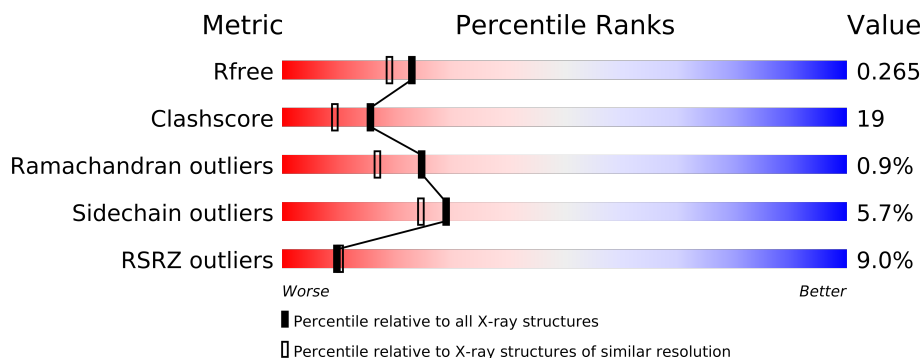
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	298	
1	B	298	
1	C	298	
1	D	298	
1	E	298	
1	F	298	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	401	-	X
2	MG	F	406	-	X
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 hydrogen and 0 are deuterium.

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.

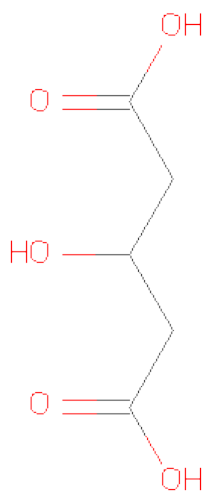
- Molecule 1 is a protein called Hydroxymethylglutaryl-CoAlyase, mitochondrial.

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-HYDROXPENTANEDIOICACID (three-letter code: 3HG) (formula: C₅H₈O₅).



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

- Molecule 4 is water.

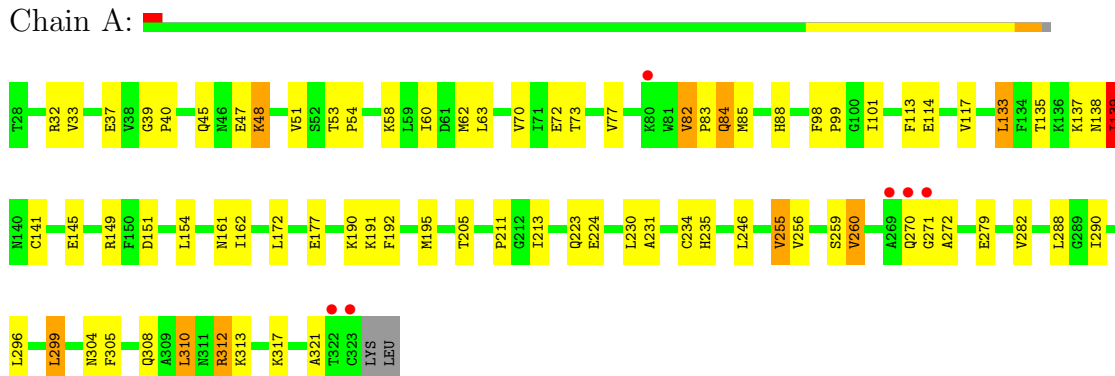
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	95	Total	O	0	0
			95	95		
4	C	96	Total	O	0	0
			96	96		
4	D	56	Total	O	0	0
			56	56		
4	E	104	Total	O	0	0
			104	104		
4	F	53	Total	O	0	0
			53	53		

3 Residue-property plots

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

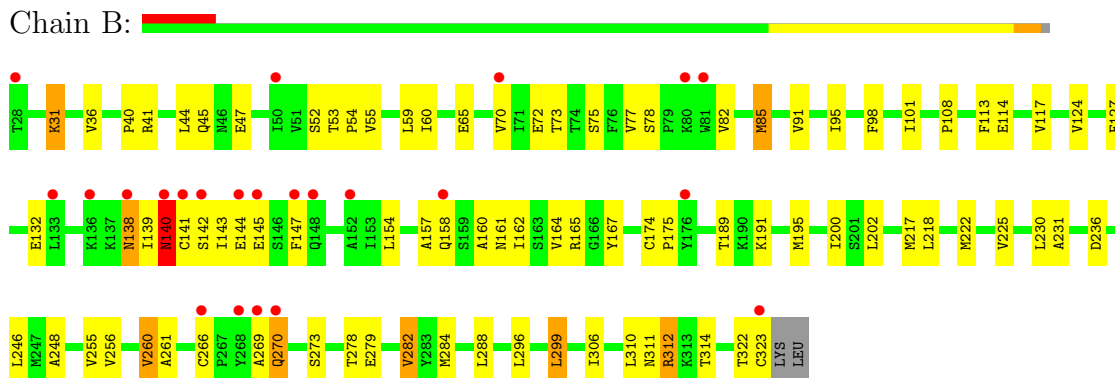
- Molecule 1: Hydroxymethylglutaryl-CoAlyase, mitochondrial

Chain A:



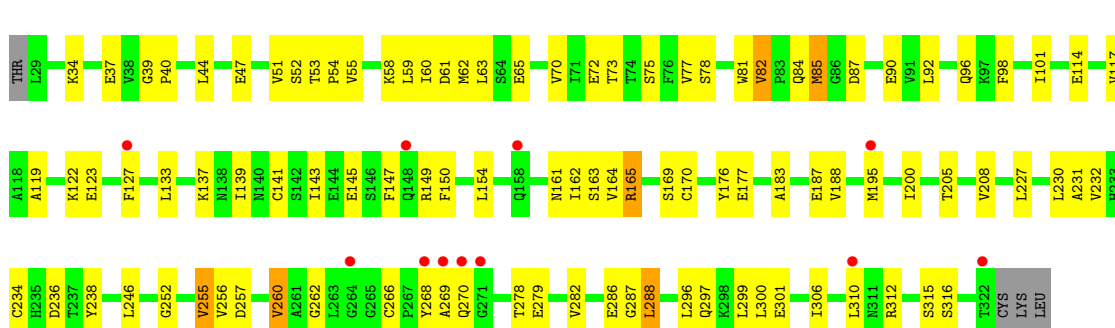
- Molecule 1: Hydroxymethylglutaryl-CoAlyase, mitochondrial

Chain B:



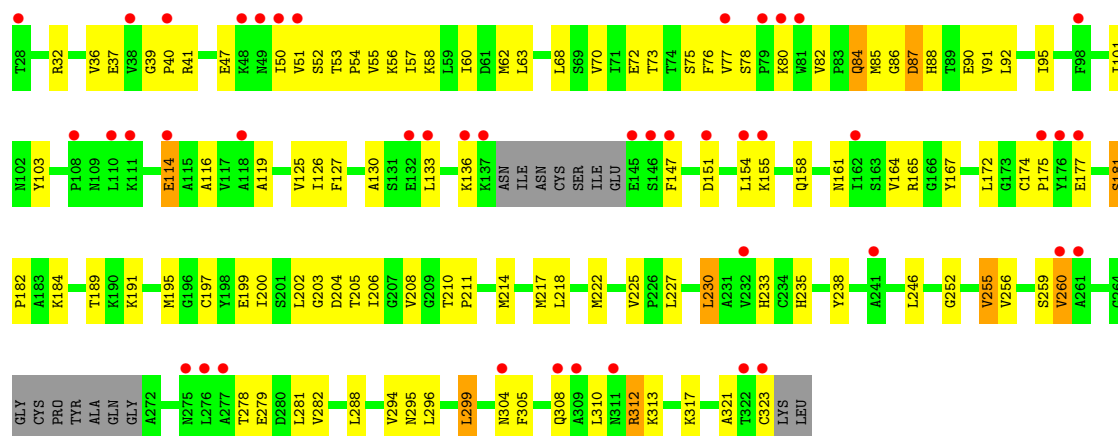
- Molecule 1: Hydroxymethylglutaryl-CoAlyase, mitochondrial

Chain C:



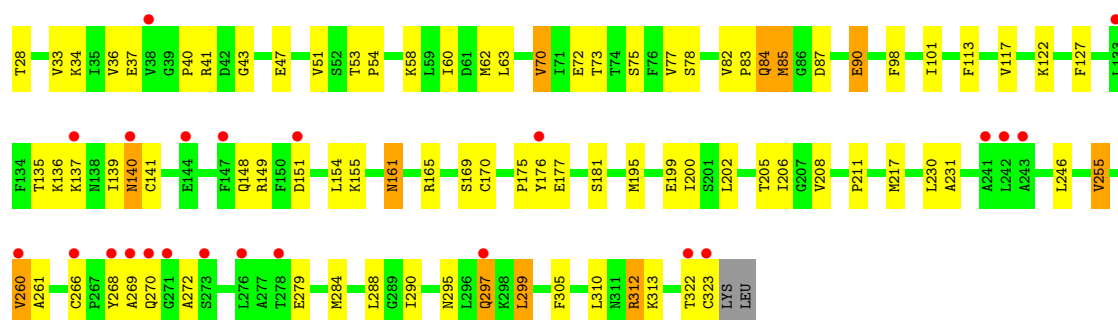
• Molecule 1: Hydroxymethylglutaryl-CoAlyase, mitochondrial

Chain D: 



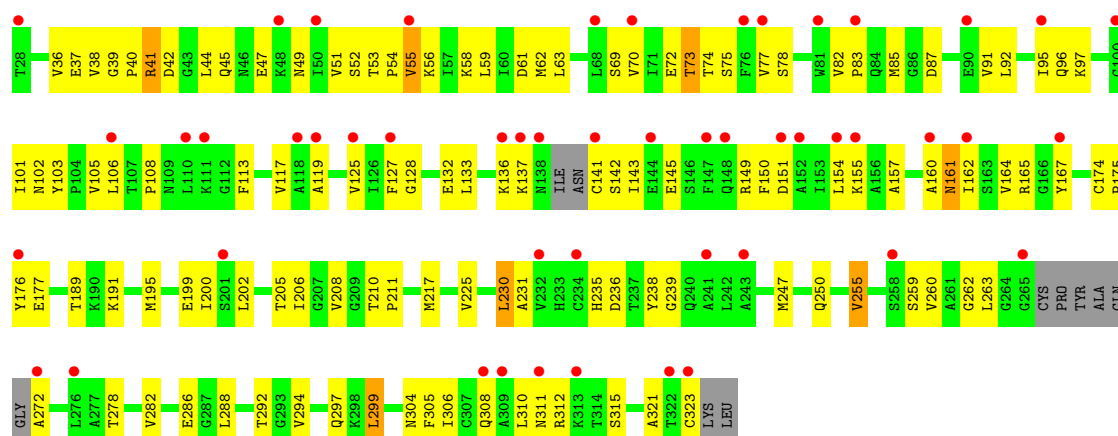
• Molecule 1: Hydroxymethylglutaryl-CoAlyase, mitochondrial

Chain E: 



• Molecule 1: Hydroxymethylglutaryl-CoAlyase, mitochondrial

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.99Å 117.08Å 86.83Å 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
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.265 0.227 , 0.265	Depositor DCC
R_{free} test set	10457 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 103975 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13543	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (489) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:270:GLN:HB2	1:F:321:ALA:HA	1.66	0.76
1:C:279:GLU:HG3	1:C:299:LEU:HD12	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:F:59:LEU:HD13	1:F:306:ILE:HB	1.72	0.72
1:A:260:VAL:O	1:A:279:GLU:OE1	2.07	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:B:31:LYS:HB2	1:B:31:LYS:NZ	2.08	0.68
1:A:154:LEU:HD13	1:A:195:MET:HG2	1.75	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:E:297:GLN:H	1:E:297:GLN:NE2	1.91	0.67
1:B:113:PHE:O	1:B:117:VAL:HG23	1.94	0.67
1:F:262:GLY:HA3	1:F:315:SER:HB2	1.77	0.67
1:E:151:ASP:O	1:E:155:LYS:HD3	1.95	0.67
1:B:139:ILE:O	1:B:140:ASN:HB2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:36:VAL:HA	1:D:70:VAL:HG13	1.76	0.66
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:C:282:VAL:CG2	1:C:296:LEU:HD13	2.25	0.66
1:C:123:GLU:HG3	1:C:163:SER:OG	1.95	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:F:87:ASP:O	1:F:91:VAL:HG23	1.95	0.66
1:A:270:GLN:O	1:A:272:ALA:N	2.27	0.66
1:C:133:LEU:O	1:C:137:LYS:HB2	1.94	0.66
1:C:279:GLU:HG2	1:C:300:LEU:HD23	1.79	0.65
1:A:60:ILE:HD13	1:A:73:THR:HG23	1.78	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:C:260:VAL:O	1:C:279:GLU:OE1	2.16	0.63
1:B:322:THR:O	1:B:323:CYS:HB2	1.96	0.63
1:F:154:LEU:HD23	1:F:164:VAL:HG21	1.80	0.63
1:E:40:PRO:HG2	1:E:72:GLU:O	1.99	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:40:PRO:HG2	1:A:72:GLU:O	1.99	0.63
1:A:137:LYS:HE2	4:A:536:HOH:O	1.98	0.63
1:E:60:ILE:HD13	1:E:73:THR:HG23	1.81	0.62
1:B:231:ALA:CB	1:B:255:VAL:HG22	2.29	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:A:45:GLN:HE22	3:A:399:3HG:H42	1.64	0.62
1:E:62:MET:HE3	1:E:305:PHE:CD2	2.34	0.62
1:C:297:GLN:O	1:C:301:GLU:HG3	1.99	0.62
1:F:36:VAL:HG22	1:F:70:VAL:HG11	1.82	0.62
1:E:83:PRO:HG2	1:E:84:GLN:HE21	1.64	0.62
1:C:75:SER:HB3	1:C:85:MET:HG2	1.80	0.62
1:B:144:GLU:HB2	4:B:770:HOH:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:84:GLN:H	1:D:84:GLN:NE2	1.98	0.61
1:B:113:PHE:CZ	1:B:162:ILE:HD12	2.35	0.61
1:F:55:VAL:CG1	1:F:56:LYS:N	2.64	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:C:231:ALA:CB	1:C:255:VAL:HG22	2.30	0.61
1:B:202:LEU:HD13	1:B:217:MET:SD	2.41	0.61
1:D:230:LEU:O	1:D:255:VAL:HG13	2.01	0.61
1:D:53:THR:N	1:D:54:PRO:HD2	2.16	0.61
1:D:167:TYR:HE1	1:D:233:HIS:HD1	1.49	0.61
1:B:36:VAL:HG22	1:B:70:VAL:HG11	1.83	0.60
1:E:75:SER:HB3	1:E:85:MET:HG2	1.81	0.60
1:B:47:GLU:HG2	1:B:310:LEU:HD21	1.83	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:F:47:GLU:CG	1:F:310:LEU:HD21	2.32	0.58
1:E:36:VAL:HG22	1:E:70:VAL:HG11	1.86	0.58
1:D:165:ARG:NH2	1:D:199:GLU:OE2	2.37	0.58
1:F:102:ASN:HD22	1:F:102:ASN:N	2.01	0.58
1:D:202:LEU:HD13	1:D:217:MET:SD	2.43	0.58
1:F:53:THR:N	1:F:54:PRO:HD2	2.19	0.58
1:F:133:LEU:HD13	1:F:136:LYS:HE2	1.86	0.58
1:C:279:GLU:N	1:C:279:GLU:OE1	2.36	0.58
1:A:51:VAL:HG13	1:A:310:LEU:HD13	1.86	0.58
1:E:63:LEU:HD21	1:E:260:VAL:CG1	2.33	0.58
1:C:98:PHE:HB2	1:C:101:ILE:HD12	1.86	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:75:SER:HB3	1:F:85:MET:HG2	1.84	0.57
1:F:157:ALA:HB1	1:F:162:ILE:O	2.04	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:C:279:GLU:HG2	1:C:300:LEU:CD2	2.35	0.57
1:A:279:GLU:HG3	1:A:299:LEU:HD13	1.87	0.57
1:C:77:VAL:HG11	1:C:82:VAL:HG11	1.86	0.57
1:E:155:LYS:HD2	1:E:155:LYS:N	2.20	0.56
1:B:260:VAL:O	1:B:279:GLU:OE1	2.24	0.56
1:C:154:LEU:CD1	1:C:195:MET:HB3	2.35	0.56
1:A:231:ALA:CB	1:A:255:VAL:HG22	2.35	0.56
1:D:37:GLU:HG2	1:D:63:LEU:HD13	1.86	0.56
1:B:282:VAL:CG2	1:B:296:LEU:HD13	2.35	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:E:137:LYS:HG2	1:E:176:TYR:OH	2.05	0.56
1:D:151:ASP:O	1:D:155:LYS:HD3	2.06	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:E:231:ALA:HB2	1:E:255:VAL:HG22	1.88	0.54
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: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:A:190:LYS:HD3	1:A:224:GLU:HB3	1.88	0.54
1:B:59:LEU:HD13	1:B:306:ILE:HB	1.89	0.54
1:E:288:LEU:HD11	1:F:211:PRO:CG	2.26	0.54
1:C:39:GLY:HA3	1:C:260:VAL:HG23	1.88	0.54
1:D:260:VAL:O	1:D:279:GLU:OE1	2.25	0.54
1:E:51:VAL:CG1	1:E:310:LEU:HD13	2.37	0.54
1:D:82:VAL:HG13	1:D:82:VAL:O	2.08	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:278:THR:HG22	1:F:299:LEU:HD11	1.90	0.53
1:C:266:CYS:SG	1:C:269:ALA:CB	2.96	0.53
1:B:147:PHE:CE1	1:B:191:LYS:HG2	2.42	0.53
1:D:256:VAL:CG2	1:D:281:LEU:HD21	2.38	0.53
1:D:50:ILE:CG2	1:D:84:GLN:HG3	2.37	0.53
1:B:174:CYS:SG	1:B:175:PRO:HD2	2.47	0.53
1:B:117:VAL:HG22	1:B:162:ILE:CD1	2.38	0.53
1:E:279:GLU:HG3	1:E:299:LEU:HD13	1.91	0.53
1:C:147:PHE:HD2	1:C:195:MET:SD	2.31	0.53
1:A:98:PHE:HB2	1:A:101:ILE:HD12	1.89	0.53
1:F:37:GLU:HG2	1:F:63:LEU:HD13	1.90	0.53
1:C:200:ILE:HD12	1:C:200:ILE:N	2.24	0.53
1:B:124:VAL:CG2	1:B:164:VAL:HG22	2.39	0.53
1:F:41:ARG:HB2	1:F:72:GLU:O	2.09	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: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:C:87:ASP:O	1:C:90:GLU:HG2	2.09	0.52
1:B:77:VAL:HG23	4:B:944:HOH:O	2.09	0.52
1:F:77:VAL:HG23	1:F:108:PRO:HG3	1.91	0.52
1:E:135:THR:HG23	1:E:139:ILE:HD11	1.91	0.52
1:C:266:CYS:SG	1:C:269:ALA:HB3	2.49	0.52
1:A:304:ASN:O	1:A:308:GLN:HG3	2.08	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:F:154:LEU:CD1	1:F:195:MET:HB3	2.39	0.52
1:A:82:VAL:O	1:A:82:VAL:HG22	2.08	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
1:F:133:LEU:O	1:F:137:LYS:HB2	2.11	0.51
1:F:51:VAL:HB	1:F:55:VAL:CG1	2.29	0.51
1:C:139:ILE:HB	1:C:149:ARG:NH2	2.15	0.51
1:E:63:LEU:HD21	1:E:260:VAL:HG11	1.93	0.51
1:E:148:GLN:HA	1:E:151:ASP:OD2	2.10	0.51
1:C:58:LYS:HD3	1:C:62:MET:HE1	1.92	0.51
1:D:133:LEU:HD23	1:D:177:GLU:HG2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:77:VAL:CG2	1:F:78:SER:H	2.24	0.50
1:D:147:PHE:CE1	1:D:191:LYS:HG2	2.47	0.50
1:B:142:SER:HB3	1:B:145:GLU:CG	2.33	0.50
1:B:138:ASN:ND2	1:B:138:ASN:C	2.65	0.50
1:B:200:ILE:HD12	1:B:200:ILE:N	2.27	0.50
1:D:172:LEU:HD11	1:D:214:MET:CE	2.41	0.50
1:A:317:LYS:NZ	1:B:236:ASP:OD2	2.45	0.50
1:F:82:VAL:HG13	1:F:82:VAL:O	2.12	0.49
1:F:154:LEU:HD13	1:F:195:MET:HB3	1.95	0.49
1:F:101:ILE:C	1:F:102:ASN:HD22	2.15	0.49
1:B:189:THR:HG22	1:B:225:VAL:HG21	1.93	0.49
1:E:58:LYS:HD3	1:E:305:PHE:CZ	2.47	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: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:E:266:CYS:HB3	1:E:269:ALA:CB	2.42	0.49
1:C:117:VAL:HG22	1:C:162:ILE:CD1	2.43	0.49
1:F:39:GLY:N	1:F:40:PRO:HD2	2.28	0.49
1:E:51:VAL:HG13	1:E:310:LEU:CD1	2.41	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: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
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:E:202:LEU:HD13	1:E:217:MET:SD	2.53	0.48
1:A:85:MET:O	1:A:88:HIS:HD2	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:282:VAL:CG2	1:D:296:LEU:HD13	2.44	0.48
1:C:262:GLY:HA3	1:C:315:SER:HB2	1.96	0.48
1:A:58:LYS:HD3	1:A:305:PHE:CZ	2.49	0.48
1:E:260:VAL:HG23	1:E:261:ALA:N	2.26	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:F:52:SER:C	1:F:54:PRO:HD2	2.33	0.48
1:E:78:SER:HB2	4:E:852:HOH:O	2.14	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:C:143:ILE:O	1:C:147:PHE:HD1	1.98	0.47
1:B:282:VAL:HG22	1:B:296:LEU:HD13	1.96	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:F:74:THR:OG1	1:F:75:SER:N	2.48	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:136:LYS:HG3	1:F:137:LYS:N	2.29	0.47
1:A:117:VAL:HG22	1:A:162:ILE:HD12	1.96	0.47
1:F:259:SER:OG	1:F:263:LEU:HB2	2.14	0.47
1:D:114:GLU:HA	1:D:114:GLU:OE1	2.15	0.47
1:A:133:LEU:HB2	1:A:177:GLU:HG3	1.96	0.47
1:F:175:PRO:HG2	1:F:176:TYR:CD1	2.50	0.47
1:F:133:LEU:HD23	1:F:177:GLU:CG	2.45	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:236:ASP:OD1	1:F:239:GLY:HA2	2.14	0.47
1:C:208:VAL:HG12	1:C:238:TYR:CE2	2.49	0.47
1:D:167:TYR:HE1	1:D:233:HIS:ND1	2.11	0.47
1:E:90:GLU:CD	1:E:90:GLU:H	2.16	0.47
1:F:297:GLN:HA	1:F:297:GLN:NE2	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:C:51:VAL:HG13	1:C:310:LEU:HD13	1.97	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:A:53:THR:N	1:A:54:PRO:HD2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:51:VAL:CG2	1:F:55:VAL:HG11	2.45	0.46
1:D:279:GLU:O	1:D:282:VAL:HG22	2.15	0.46
1:F:58:LYS:HD3	1:F:305:PHE:CZ	2.50	0.46
1:D:227:LEU:HD21	1:D:252:GLY:HA3	1.98	0.46
1:F:125:VAL:HG22	1:F:165:ARG:HB3	1.96	0.46
1:D:51:VAL:O	1:D:56:LYS:NZ	2.48	0.46
1:D:191:LYS:O	1:D:195:MET:HB2	2.16	0.46
1:E:85:MET:HE2	1:E:85:MET:HA	1.98	0.46
1:C:82:VAL:O	1:C:82:VAL:HG22	2.16	0.46
1:D:73:THR:OG1	1:D:103:TYR:HB3	2.15	0.46
1:A:234:CYS:HB3	4:A:503:HOH:O	2.16	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:F:55:VAL:HG12	1:F:56:LYS:H	1.80	0.46
1:C:77:VAL:HG11	1:C:82:VAL:CG1	2.45	0.46
1:C:53:THR:N	1:C:54:PRO:HD2	2.30	0.46
1:E:77:VAL:HG11	1:E:82:VAL:HG11	1.97	0.46
1:C:127:PHE:O	1:C:150:PHE:HZ	1.99	0.46
1:F:77:VAL:CG2	1:F:78:SER:N	2.77	0.46
1:E:37:GLU:OE2	1:E:260:VAL:HG13	2.16	0.46
1:D:278:THR:CG2	1:D:299:LEU:HD11	2.45	0.46
1:B:261:ALA:HB1	1:B:314:THR:OG1	2.16	0.46
1:D:41:ARG:C	1:D:41:ARG:HD2	2.36	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:F:52:SER:HB2	1:F:54:PRO:HD2	1.97	0.45
1:F:205:THR:O	1:F:235:HIS:ND1	2.49	0.45
1:D:80:LYS:HE2	4:D:1049:HOH:O	2.16	0.45
1:D:127:PHE:N	1:D:127:PHE:CD1	2.85	0.45
1:F:127:PHE:O	1:F:150:PHE:CZ	2.70	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:D:154:LEU:O	1:D:158:GLN:HG3	2.17	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:B:82:VAL:HG13	1:B:82:VAL:O	2.16	0.45
1:B:127:PHE:CD1	1:B:127:PHE:N	2.84	0.45
1:A:58:LYS:HZ2	1:A:62:MET:HE1	1.82	0.45
1:A:135:THR:HG22	1:A:141:CYS:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:F:206:ILE:HG13	1:F:208:VAL:HG22	1.98	0.45
1:E:136:LYS:O	1:E:140:ASN:HA	2.16	0.45
1:D:205:THR:O	1:D:235:HIS:ND1	2.43	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: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:39:GLY:HA2	1:A:259:SER:OG	2.17	0.44
1:C:52:SER:O	1:C:55:VAL:HB	2.17	0.44
1:A:60:ILE:CD1	1:A:73:THR:HG23	2.47	0.44
1:F:208:VAL:HG12	1:F:238:TYR:CE2	2.52	0.44
1:C:141:CYS:HB2	1:C:145:GLU:OE1	2.16	0.44
1:F:128:GLY:N	1:F:167:TYR:O	2.49	0.44
1:F:91:VAL:O	1:F:95:ILE:HG23	2.17	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: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: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:C:270:GLN:HG3	1:D:321:ALA:O	2.17	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:62:MET:CE	1:A:305:PHE:CD2	3.00	0.44
1:A:138:ASN:O	1:A:139:ILE:HD13	2.18	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
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:D:53:THR:O	1:D:57:ILE:HG13	2.18	0.43
1:B:77:VAL:HG22	1:B:78:SER:N	2.33	0.43
1:D:86:GLY:C	1:D:88:HIS:H	2.21	0.43
1:F:77:VAL:HG11	1:F:82:VAL:CG1	2.48	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:282:VAL:O	1:F:286:GLU:HB2	2.19	0.43
1:A:45:GLN:NE2	3:A:399:3HG:H21	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:ASN:CG	1:B:161:ASN:O	2.56	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:E:169:SER:HB2	1:E:205:THR:OG1	2.18	0.43
1:B:41:ARG:HD2	1:B:41:ARG:C	2.39	0.43
1:A:33:VAL:HG23	1:A:290:ILE:HG21	2.00	0.43
1:C:266:CYS:CB	1:C:269:ALA:HB3	2.48	0.43
1:A:98:PHE:HA	1:A:99:PRO:HD3	1.90	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:D:60:ILE:CD1	1:D:73:THR:HG23	2.48	0.42
1:C:232:VAL:CG2	1:C:234:CYS:SG	3.07	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: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: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:E:312:ARG:HD3	1:E:313:LYS:O	2.19	0.42
1:A:312:ARG:HD3	1:A:313:LYS:O	2.19	0.42
1:F:151:ASP:OD1	1:F:155:LYS:HD3	2.19	0.42
1:E:43:GLY:O	1:E:47:GLU:HG2	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:A:113:PHE:O	1:A:117:VAL:HG23	2.19	0.42
1:F:304:ASN:O	1:F:308:GLN:HG3	2.20	0.42
1:B:91:VAL:O	1:B:95:ILE:HG23	2.19	0.42
1:B:31:LYS:HB2	1:B:31:LYS:HZ3	1.82	0.42
1:F:231:ALA:HB1	1:F:255:VAL:HG22	2.01	0.42
1:F:175:PRO:HG2	1:F:176:TYR:CE1	2.55	0.42
1:E:122:LYS:NZ	4:E:739:HOH:O	2.51	0.42
1:B:218:LEU:CD1	1:B:248:ALA:HA	2.49	0.42
1:F:306:ILE:O	1:F:310:LEU:HB2	2.20	0.42
1:C:77:VAL:HG22	1:C:78:SER:N	2.35	0.42
1:B:147:PHE:CD1	1:B:191:LYS:HG2	2.55	0.42
1:D:181:SER:HA	1:D:182:PRO:HD3	1.95	0.42
1:E:137:LYS:HG2	1:E:176:TYR:CZ	2.55	0.41
1:F:247:MET:HE3	1:F:250:GLN:HE21	1.84	0.41
1:E:87:ASP:HA	1:E:90:GLU:OE1	2.20	0.41
1:A:321:ALA:O	1:B:270:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:C:117:VAL:HG22	1:C:162:ILE:HD11	2.02	0.41
1:A:37:GLU:HG2	1:A:63:LEU:HD13	2.02	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:B:85:MET:HE2	1:B:85:MET:HA	2.02	0.41
1:A:45:GLN:HE22	3:A:399:3HG:H21	1.85	0.41
1:F:132:GLU:OE2	1:F:132:GLU:HA	2.20	0.41
1:B:132:GLU:N	1:B:143:ILE:HD11	2.35	0.41
1:D:51:VAL:HG13	1:D:310:LEU:HD13	2.02	0.41
1:B:47:GLU:HG2	1:B:310:LEU:CD2	2.51	0.41
1:F:206:ILE:H	1:F:206:ILE:HG12	1.68	0.41
1:C:227:LEU:HD21	1:C:252:GLY:HA3	2.03	0.41
1:E:279:GLU:OE1	1:E:279:GLU:N	2.46	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:F:174:CYS:SG	1:F:175:PRO:HD2	2.61	0.41
1:F:132:GLU:OE2	1:F:143:ILE:HG13	2.21	0.41
1:C:122:LYS:HE2	1:C:122:LYS:HB3	1.93	0.41
1:B:98:PHE:CB	1:B:101:ILE:HD12	2.46	0.41
1:D:51:VAL:HB	1:D:55:VAL:CG1	2.49	0.41
1:F:41:ARG:HD3	1:F:75:SER:HB2	2.02	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:F:63:LEU:HD21	1:F:260:VAL:HG22	2.03	0.41
1:C:81:TRP:CG	1:E:122:LYS:HE3	2.56	0.41
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: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:C:53:THR:HG21	1:C:90:GLU:HG3	2.03	0.40
1:C:306:ILE:O	1:C:310:LEU:HB2	2.21	0.40
1:F:82:VAL:HA	1:F:83:PRO:HD2	1.96	0.40
1:A:139:ILE:HB	1:A:141:CYS:SG	2.62	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:A:77:VAL:HG11	1:A:82:VAL:CG1	2.51	0.40
1:A:205:THR:O	1:A:235:HIS:ND1	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:260:VAL:HB	1:B:261:ALA:H	1.72	0.40
1:B:191:LYS:HA	1:B:191:LYS:HD2	1.85	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:D:278:THR:O	1:D:282:VAL:HG13	2.21	0.40
1:E:34:LYS:HD3	1:E:70:VAL:HG11	2.03	0.40
1:C:165:ARG:NH1	1:C:257:ASP:OD1	2.55	0.40
1:E:322:THR:HG22	1:E:323:CYS:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	22	14
1	B	294/298 (99%)	281 (96%)	8 (3%)	5 (2%)	14	6
1	C	292/298 (98%)	279 (96%)	12 (4%)	1 (0%)	50	49
1	D	276/298 (93%)	261 (95%)	12 (4%)	3 (1%)	21	13
1	E	294/298 (99%)	281 (96%)	11 (4%)	2 (1%)	30	23
1	F	282/298 (95%)	265 (94%)	15 (5%)	2 (1%)	30	23
All	All	1732/1788 (97%)	1654 (96%)	62 (4%)	16 (1%)	25	17

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	19	14
1	B	238/240 (99%)	221 (93%)	17 (7%)	21	16
1	C	236/240 (98%)	225 (95%)	11 (5%)	36	33
1	D	227/240 (95%)	215 (95%)	12 (5%)	32	28
1	E	238/240 (99%)	225 (94%)	13 (6%)	30	26
1	F	232/240 (97%)	223 (96%)	9 (4%)	43	43
All	All	1409/1440 (98%)	1329 (94%)	80 (6%)	29	24

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	297	GLN
1	F	311	ASN
1	F	320	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	-	9,9,9	1.79	3 (33%)	11,11,11	1.84	2 (18%)

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	-	-	0/8/8/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	399	3HG	O4-C5	3.40	1.34	1.22
3	A	399	3HG	O2-C3	-3.08	1.33	1.43
3	A	399	3HG	C4-C5	-2.06	1.45	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	399	3HG	C4-C3-C2	-4.23	106.47	112.29
3	A	399	3HG	O5-C5-C4	2.76	123.72	114.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/298 (99%)	0.10	6 (2%) 62 67	19, 28, 56, 72	0
1	B	296/298 (99%)	0.59	23 (7%) 13 14	22, 39, 75, 95	0
1	C	294/298 (98%)	0.26	11 (3%) 39 44	22, 38, 62, 74	0
1	D	282/298 (94%)	0.90	44 (15%) 3 3	30, 56, 85, 95	0
1	E	296/298 (99%)	0.36	23 (7%) 13 14	23, 36, 72, 84	0
1	F	288/298 (96%)	0.99	50 (17%) 2 2	20, 60, 87, 95	0
All	All	1752/1788 (97%)	0.53	157 (8%) 10 10	19, 40, 79, 95	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	TRP	8.2
1	B	138	ASN	6.5
1	B	141	CYS	5.7
1	B	140	ASN	5.5
1	D	146	SER	4.9
1	D	176	TYR	4.9
1	B	176	TYR	4.7
1	F	141	CYS	4.7
1	D	110	LEU	4.5
1	B	81	TRP	4.5
1	D	133	LEU	4.3
1	F	127	PHE	4.1
1	F	147	PHE	4.1
1	C	322	THR	4.1
1	C	270	GLN	4.1
1	F	50	ILE	4.1
1	F	176	TYR	3.9
1	F	144	GLU	3.8
1	B	268	TYR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	137	LYS	3.8
1	E	323	CYS	3.7
1	D	114	GLU	3.6
1	E	269	ALA	3.6
1	E	268	TYR	3.6
1	F	265	GLY	3.5
1	C	148	GLN	3.5
1	F	152	ALA	3.5
1	D	147	PHE	3.5
1	E	243	ALA	3.4
1	F	311	ASN	3.4
1	F	272	ALA	3.4
1	D	80	LYS	3.4
1	D	151	ASP	3.4
1	B	136	LYS	3.4
1	F	151	ASP	3.3
1	B	145	GLU	3.3
1	B	323	CYS	3.2
1	B	269	ALA	3.2
1	F	160	ALA	3.2
1	D	154	LEU	3.2
1	B	142	SER	3.2
1	F	111	LYS	3.2
1	F	81	TRP	3.2
1	E	266	CYS	3.2
1	B	147	PHE	3.2
1	D	162	ILE	3.1
1	F	76	PHE	3.1
1	E	322	THR	3.1
1	B	50	ILE	3.1
1	B	133	LEU	3.0
1	F	110	LEU	3.0
1	F	28	THR	3.0
1	B	270	GLN	3.0
1	C	269	ALA	3.0
1	F	137	LYS	2.9
1	C	271	GLY	2.9
1	F	155	LYS	2.9
1	B	28	THR	2.9
1	C	127	PHE	2.9
1	B	266	CYS	2.8
1	E	271	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	148	GLN	2.8
1	D	28	THR	2.8
1	D	145	GLU	2.8
1	A	271	GLY	2.8
1	E	137	LYS	2.8
1	F	90	GLU	2.7
1	D	322	THR	2.6
1	E	273	SER	2.6
1	D	275	ASN	2.6
1	F	70	VAL	2.6
1	E	140	ASN	2.6
1	C	268	TYR	2.6
1	D	175	PRO	2.6
1	E	144	GLU	2.6
1	F	313	LYS	2.6
1	D	132	GLU	2.5
1	E	133	LEU	2.5
1	F	309	ALA	2.5
1	A	323	CYS	2.5
1	F	276	LEU	2.5
1	D	155	LYS	2.5
1	D	276	LEU	2.5
1	F	106	LEU	2.5
1	E	297	GLN	2.5
1	F	95	ILE	2.5
1	F	136	LYS	2.5
1	F	162	ILE	2.5
1	A	322	THR	2.5
1	E	147	PHE	2.5
1	E	270	GLN	2.5
1	D	77	VAL	2.5
1	F	48	LYS	2.4
1	F	118	ALA	2.4
1	A	270	GLN	2.4
1	B	148	GLN	2.4
1	F	83	PRO	2.4
1	A	80	LYS	2.4
1	F	138	ASN	2.4
1	D	136	LYS	2.4
1	F	100	GLY	2.4
1	F	258	SER	2.4
1	D	50	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	260	VAL	2.4
1	C	158	GLN	2.4
1	F	154	LEU	2.4
1	B	70	VAL	2.4
1	B	152	ALA	2.4
1	D	277	ALA	2.4
1	D	308	GLN	2.3
1	E	241	ALA	2.3
1	D	48	LYS	2.3
1	F	125	VAL	2.3
1	F	232	VAL	2.3
1	E	176	TYR	2.3
1	A	269	ALA	2.3
1	D	98	PHE	2.3
1	E	242	LEU	2.3
1	D	323	CYS	2.3
1	D	241	ALA	2.3
1	D	51	VAL	2.2
1	D	177	GLU	2.2
1	F	234	CYS	2.2
1	F	243	ALA	2.2
1	F	323	CYS	2.2
1	D	261	ALA	2.2
1	F	167	TYR	2.2
1	C	264	GLY	2.2
1	F	308	GLN	2.2
1	D	118	ALA	2.2
1	F	241	ALA	2.2
1	D	304	ASN	2.2
1	F	322	THR	2.2
1	F	68	LEU	2.1
1	D	40	PRO	2.1
1	D	38	VAL	2.1
1	D	108	PRO	2.1
1	B	80	LYS	2.1
1	F	201	SER	2.1
1	D	232	VAL	2.1
1	D	79	PRO	2.1
1	D	49	ASN	2.1
1	D	311	ASN	2.1
1	E	276	LEU	2.1
1	F	119	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	158	GLN	2.0
1	D	309	ALA	2.0
1	E	278	THR	2.0
1	D	111	LYS	2.0
1	E	38	VAL	2.0
1	E	151	ASP	2.0
1	E	260	VAL	2.0
1	F	55	VAL	2.0
1	C	310	LEU	2.0
1	C	195	MET	2.0
1	F	77	VAL	2.0
1	B	144	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	F	406	1/1	0.32	6.91	64,64,64,64	0
2	MG	A	401	1/1	0.21	3.46	35,35,35,35	0
3	3HG	A	399	10/10	0.22	2.69	66,66,67,67	0
2	MG	E	402	1/1	0.22	1.58	44,44,44,44	0
2	MG	C	403	1/1	0.18	1.26	37,37,37,37	0
2	MG	B	404	1/1	0.20	0.70	48,48,48,48	0
2	MG	D	405	1/1	0.22	0.02	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.