



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:55 AM UTC

PDB ID : 5GL3 / pdb_00005gl3
Title : Crystal structure of TON_0340 in complex with Mg
Authors : Lee, S.G.; Sohn, Y.S.; Oh, B.H.
Deposited on : 2016-07-07
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

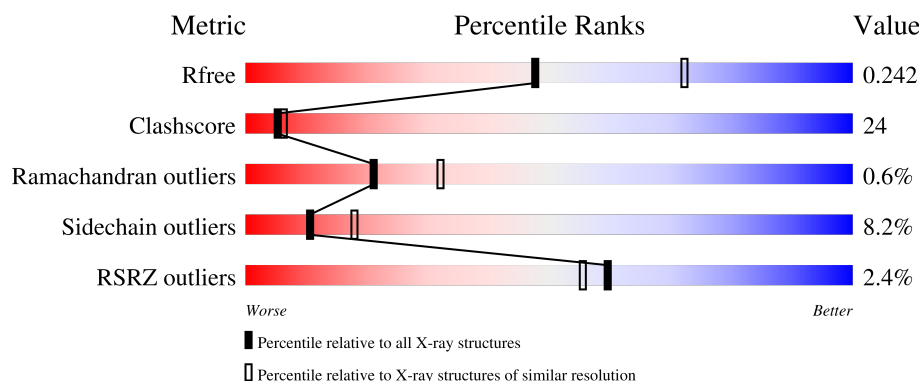
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	269	% 60% 34% 6%
1	B	269	2% 55% 36% 6%
1	C	269	4% 63% 31% 6%
1	D	269	% 62% 33%
1	E	269	5% 56% 38% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	269	% 60% 35% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12418 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2045	1303	347	387	8			
1	B	260	Total	C	N	O	S	0	0	0
			1979	1266	333	373	7			
1	C	268	Total	C	N	O	S	0	0	0
			2037	1298	346	386	7			
1	D	269	Total	C	N	O	S	0	0	0
			2045	1303	347	387	8			
1	E	269	Total	C	N	O	S	0	0	0
			2045	1303	347	387	8			
1	F	269	Total	C	N	O	S	0	0	0
			2045	1303	347	387	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	LEU	-	expression tag	UNP B6YTD8
B	269	LEU	-	expression tag	UNP B6YTD8
C	269	LEU	-	expression tag	UNP B6YTD8
D	269	LEU	-	expression tag	UNP B6YTD8
E	269	LEU	-	expression tag	UNP B6YTD8
F	269	LEU	-	expression tag	UNP B6YTD8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Mg 2	0	0
2	E	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0

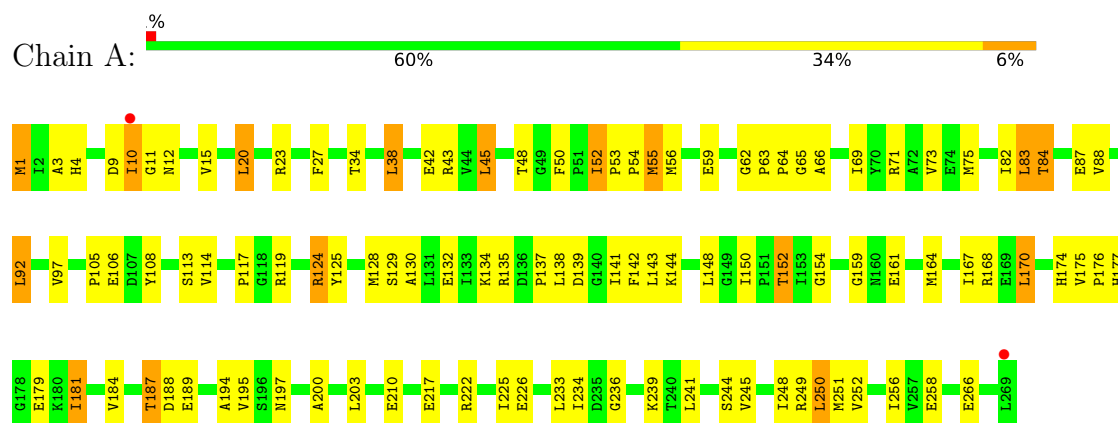
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	44	Total 44	O 44	0	0
3	C	28	Total 28	O 28	0	0
3	D	28	Total 28	O 28	0	0
3	E	26	Total 26	O 26	0	0
3	F	39	Total 39	O 39	0	0

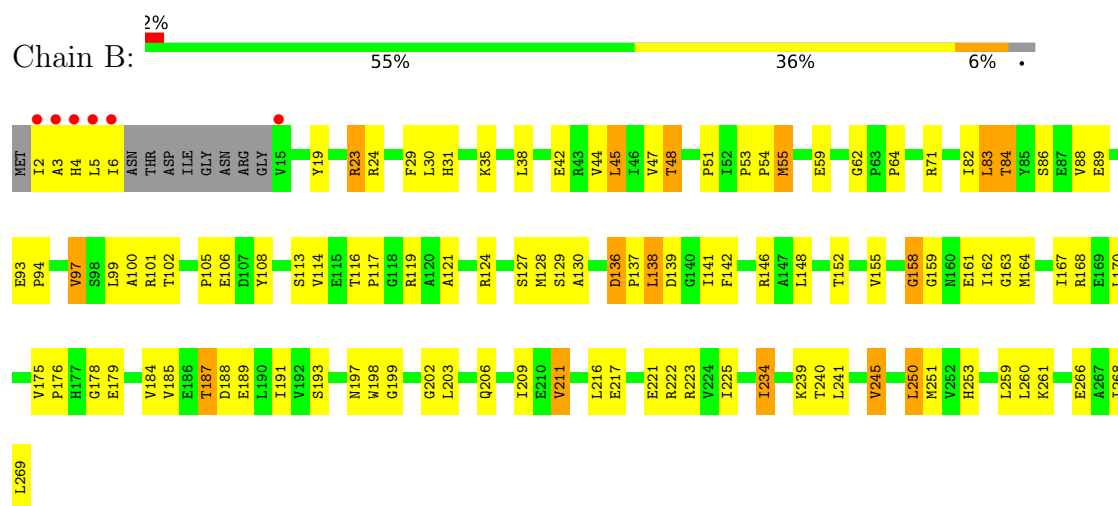
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

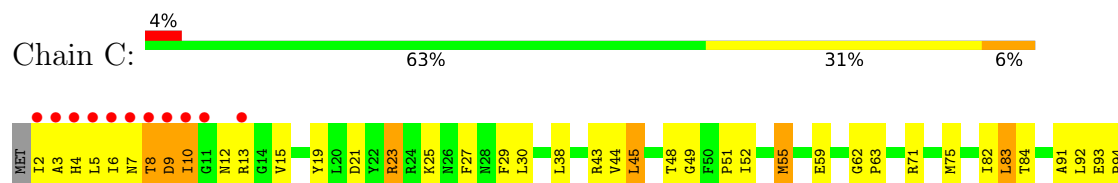
• Molecule 1: Uncharacterized protein

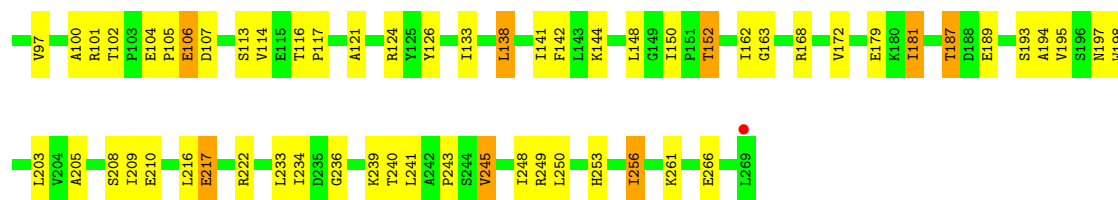


• Molecule 1: Uncharacterized protein

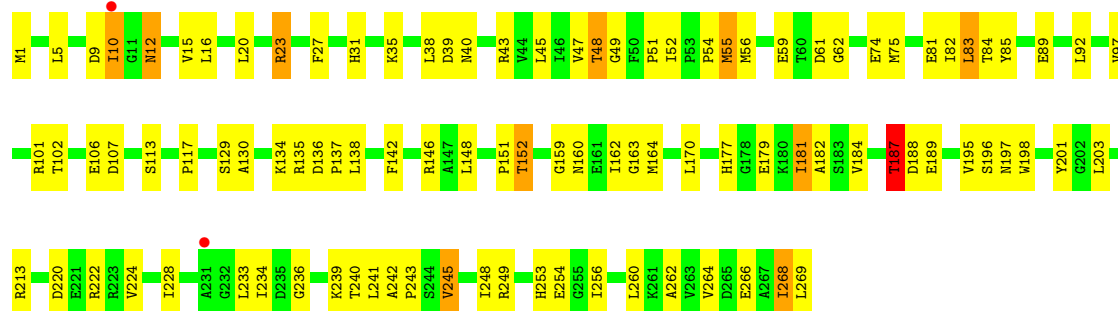


• Molecule 1: Uncharacterized protein

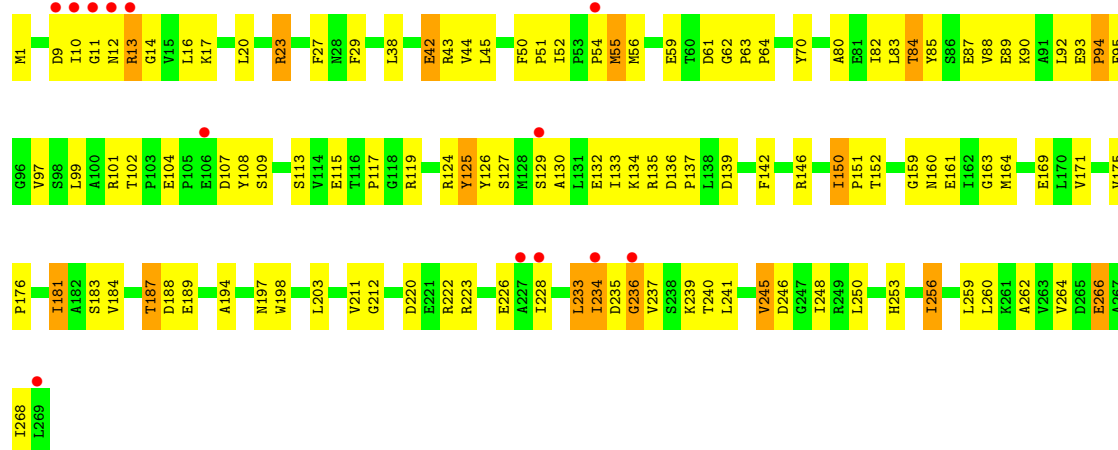




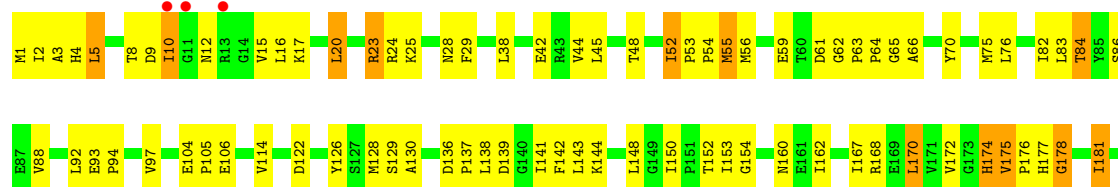
• Molecule 1: Uncharacterized protein

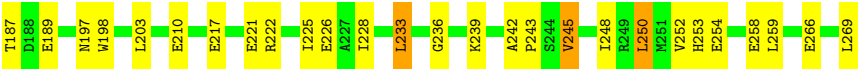


• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.98Å 106.98Å 363.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.8 (50.00-2.40) 87.9 (50.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.199 , 0.243 0.197 , 0.242	Depositor DCC
R_{free} test set	3738 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12418	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.48	0/2080	0.95	6/2819 (0.2%)
1	B	0.47	0/2013	0.99	7/2728 (0.3%)
1	C	0.44	0/2072	0.93	4/2809 (0.1%)
1	D	0.43	0/2080	0.93	2/2819 (0.1%)
1	E	0.40	0/2080	0.96	9/2819 (0.3%)
1	F	0.46	0/2080	0.98	11/2819 (0.4%)
All	All	0.45	0/12405	0.96	39/16813 (0.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	ILE	N-CA-C	7.91	118.46	110.23
1	A	11	GLY	N-CA-C	-7.67	104.50	114.85
1	A	250	LEU	N-CA-C	7.38	120.27	111.33
1	F	181	ILE	N-CA-C	7.05	119.90	111.09
1	F	175	VAL	N-CA-C	6.58	115.44	107.61
1	B	127	SER	N-CA-C	-6.51	102.13	110.53
1	D	181	ILE	N-CA-C	6.23	117.79	111.00
1	E	150	ILE	CA-C-N	6.16	126.52	119.93
1	E	150	ILE	C-N-CA	6.16	126.52	119.93
1	B	250	LEU	N-CA-C	6.10	118.71	111.33
1	F	52	ILE	CA-C-N	6.10	124.11	119.66
1	F	52	ILE	C-N-CA	6.10	124.11	119.66
1	E	11	GLY	N-CA-C	-6.04	106.70	114.85
1	A	52	ILE	CA-C-N	5.91	123.98	119.66
1	A	52	ILE	C-N-CA	5.91	123.98	119.66
1	A	181	ILE	N-CA-C	5.89	117.82	111.58
1	C	181	ILE	N-CA-C	5.89	118.45	111.09
1	B	138	LEU	N-CA-C	-5.70	105.97	114.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	234	ILE	N-CA-C	5.65	117.31	109.80
1	B	86	SER	N-CA-C	5.64	117.88	111.11
1	B	234	ILE	N-CA-C	5.58	117.20	109.45
1	B	136	ASP	N-CA-C	5.57	116.42	109.57
1	F	44	VAL	N-CA-C	5.52	116.53	108.58
1	F	86	SER	N-CA-C	5.50	117.71	111.11
1	C	104	GLU	CA-C-N	5.48	126.69	119.84
1	C	104	GLU	C-N-CA	5.48	126.69	119.84
1	E	181	ILE	N-CA-C	5.48	117.39	111.58
1	F	250	LEU	N-CA-C	5.46	117.93	111.33
1	A	174	HIS	N-CA-C	5.45	120.20	113.50
1	B	44	VAL	N-CA-C	5.33	116.25	108.58
1	F	174	HIS	CA-C-N	-5.21	118.80	123.33
1	F	174	HIS	C-N-CA	-5.21	118.80	123.33
1	E	136	ASP	CA-C-N	5.21	125.14	119.78
1	E	136	ASP	C-N-CA	5.21	125.14	119.78
1	C	44	VAL	N-CA-C	5.15	115.51	107.99
1	E	50	PHE	CA-C-N	5.13	124.89	119.76
1	E	50	PHE	C-N-CA	5.13	124.89	119.76
1	D	187	THR	N-CA-C	-5.10	101.62	109.52
1	F	143	LEU	N-CA-C	-5.05	105.85	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2045	0	2090	100	0
1	B	1979	0	2024	107	0
1	C	2037	0	2078	105	0
1	D	2045	0	2090	97	0
1	E	2045	0	2090	107	0
1	F	2045	0	2090	121	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	45	0	0	1	0
3	B	44	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	2	0
3	E	26	0	0	1	0
3	F	39	0	0	0	0
All	All	12418	0	12462	600	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 24.

All (600) 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:F:152:THR:HG22	1:F:187:THR:HG23	1.23	1.14
1:E:52:ILE:HD11	1:E:59:GLU:HB3	1.28	1.07
1:A:152:THR:HG22	1:A:188:ASP:H	1.23	1.03
1:D:159:GLY:HA2	1:D:164:MET:HG2	1.36	1.03
1:B:152:THR:HG23	1:B:188:ASP:H	1.21	1.00
1:D:55:MET:H	1:D:55:MET:HE2	1.27	0.99
1:D:62:GLY:H	1:D:197:ASN:HD21	1.13	0.97
1:E:159:GLY:HA2	1:E:164:MET:HG2	1.48	0.96
1:B:159:GLY:HA2	1:B:164:MET:HG2	1.45	0.95
1:A:105:PRO:HG3	1:A:141:ILE:HG13	1.48	0.94
1:B:31:HIS:HE1	1:B:35:LYS:HE3	1.32	0.91
1:A:159:GLY:HA2	1:A:164:MET:HG2	1.50	0.91
1:E:84:THR:HG21	1:E:88:VAL:HG11	1.53	0.91
1:E:82:ILE:HD12	1:E:97:VAL:HG11	1.53	0.91
1:C:2:ILE:N	1:F:9:ASP:HB3	1.85	0.90
1:C:48:THR:HG22	1:C:49:GLY:H	1.36	0.89
1:F:82:ILE:HD12	1:F:97:VAL:HG11	1.54	0.87
1:A:82:ILE:HD12	1:A:97:VAL:HG11	1.55	0.87
1:B:31:HIS:CE1	1:B:35:LYS:HE3	2.10	0.86
1:C:6:ILE:O	1:C:193:SER:HB2	1.76	0.86
1:F:1:MET:HE1	1:F:23:ARG:HH12	1.38	0.86
1:B:152:THR:CG2	1:B:188:ASP:H	1.88	0.85
1:F:152:THR:HG22	1:F:187:THR:CG2	2.08	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ILE:HG22	1:D:269:LEU:HD23	1.60	0.83
1:B:6:ILE:HG22	1:B:193:SER:HB2	1.60	0.83
1:E:54:PRO:HD2	1:E:55:MET:HE2	1.60	0.83
1:C:52:ILE:HD11	1:C:59:GLU:HB3	1.59	0.82
1:F:144:LYS:O	1:F:148:LEU:HD23	1.80	0.82
1:F:5:LEU:HD11	1:F:259:LEU:HG	1.62	0.81
1:C:62:GLY:H	1:C:197:ASN:HD21	1.29	0.81
1:B:6:ILE:HG22	1:B:193:SER:CB	2.11	0.80
1:B:48:THR:HG22	1:B:114:VAL:O	1.81	0.80
1:F:1:MET:HE1	1:F:23:ARG:NH1	1.96	0.80
1:B:55:MET:HE1	1:B:239:LYS:HD3	1.63	0.79
1:F:1:MET:CE	1:F:4:HIS:H	1.97	0.78
1:A:55:MET:HE1	1:A:239:LYS:HB3	1.66	0.78
1:B:159:GLY:CA	1:B:164:MET:HG2	2.13	0.77
1:A:84:THR:HG21	1:A:88:VAL:HG11	1.66	0.77
1:D:159:GLY:CA	1:D:164:MET:HG2	2.13	0.77
1:E:176:PRO:HA	1:F:106:GLU:HG2	1.66	0.77
1:A:119:ARG:HG3	1:A:139:ASP:OD1	1.85	0.77
1:D:52:ILE:HD13	1:D:236:GLY:HA2	1.66	0.77
1:C:52:ILE:CD1	1:C:236:GLY:HA2	2.16	0.76
1:D:62:GLY:H	1:D:197:ASN:ND2	1.81	0.76
1:E:63:PRO:HB2	1:E:64:PRO:HD3	1.68	0.76
1:C:52:ILE:CD1	1:C:59:GLU:HB3	2.16	0.75
1:A:159:GLY:CA	1:A:164:MET:HG2	2.17	0.75
1:F:48:THR:CG2	1:F:114:VAL:HB	2.17	0.75
1:B:152:THR:HG23	1:B:188:ASP:N	2.00	0.75
1:C:13:ARG:HH22	1:F:28:ASN:HD21	1.35	0.75
1:B:159:GLY:HA2	1:B:164:MET:CG	2.17	0.75
1:F:48:THR:HG22	1:F:114:VAL:HB	1.69	0.74
1:E:163:GLY:HA2	1:E:187:THR:HB	1.69	0.74
1:F:70:TYR:CE2	1:F:97:VAL:HG13	2.23	0.74
1:B:119:ARG:HG3	1:B:139:ASP:OD1	1.87	0.74
1:E:62:GLY:H	1:E:197:ASN:HD21	1.35	0.74
1:A:48:THR:HG22	1:A:114:VAL:O	1.87	0.74
1:D:55:MET:HE2	1:D:55:MET:N	2.01	0.74
1:A:48:THR:O	1:A:84:THR:HG22	1.88	0.73
1:B:6:ILE:HD11	1:B:202:GLY:HA3	1.70	0.73
1:D:151:PRO:HG3	1:F:25:LYS:HA	1.69	0.73
1:A:152:THR:HG22	1:A:188:ASP:N	2.02	0.73
1:F:1:MET:CE	1:F:23:ARG:HH12	2.01	0.73
1:C:82:ILE:HD12	1:C:97:VAL:HG11	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:HD11	1:F:198:TRP:CH2	2.25	0.72
1:B:187:THR:HG23	1:B:189:GLU:O	1.89	0.72
1:C:2:ILE:HD11	1:C:209:ILE:HD11	1.72	0.72
1:C:43:ARG:NH1	1:C:107:ASP:HB3	2.05	0.71
1:E:152:THR:HG23	1:E:188:ASP:H	1.56	0.71
1:B:198:TRP:HE1	1:B:253:HIS:HD2	1.35	0.71
1:C:48:THR:O	1:C:84:THR:HG22	1.91	0.71
1:A:234:ILE:HG22	1:A:241:LEU:HD12	1.73	0.71
1:D:152:THR:CG2	1:D:188:ASP:H	2.04	0.71
1:F:52:ILE:HD13	1:F:236:GLY:HA2	1.73	0.70
1:C:62:GLY:H	1:C:197:ASN:ND2	1.90	0.70
1:F:48:THR:HG22	1:F:114:VAL:O	1.92	0.70
1:E:119:ARG:HG3	1:E:139:ASP:OD1	1.92	0.69
1:E:159:GLY:CA	1:E:164:MET:HG2	2.20	0.69
1:A:48:THR:HG22	1:A:114:VAL:HB	1.73	0.69
1:A:187:THR:CG2	1:A:189:GLU:O	2.41	0.69
1:D:52:ILE:CD1	1:D:236:GLY:HA2	2.23	0.69
1:E:119:ARG:NH1	1:E:125:TYR:OH	2.26	0.69
1:B:93:GLU:HB3	1:B:94:PRO:HD3	1.75	0.69
1:A:52:ILE:HD13	1:A:236:GLY:HA2	1.75	0.69
1:F:154:GLY:N	1:F:187:THR:HG21	2.07	0.68
1:A:105:PRO:HG3	1:A:141:ILE:CG1	2.24	0.68
1:F:55:MET:HE1	1:F:239:LYS:HD3	1.75	0.68
1:C:7:ASN:OD1	1:C:193:SER:HA	1.94	0.68
1:A:9:ASP:HB3	1:B:2:ILE:N	2.08	0.68
1:D:163:GLY:HA2	1:D:187:THR:HB	1.76	0.68
1:A:52:ILE:HD12	1:A:59:GLU:HB3	1.76	0.68
1:D:23:ARG:HH11	1:D:23:ARG:HG3	1.57	0.67
1:D:12:ASN:OD1	1:D:15:VAL:HG23	1.94	0.67
1:D:159:GLY:HA2	1:D:164:MET:CG	2.18	0.67
1:C:55:MET:HE1	1:C:239:LYS:HD3	1.76	0.67
1:D:262:ALA:O	1:D:266:GLU:HB2	1.95	0.67
1:F:198:TRP:HE1	1:F:253:HIS:HD2	1.42	0.67
1:B:116:THR:HB	1:B:162:ILE:HD12	1.76	0.67
1:C:245:VAL:HG22	1:C:253:HIS:NE2	2.10	0.67
1:E:52:ILE:HD13	1:E:236:GLY:HA2	1.74	0.67
1:E:62:GLY:H	1:E:197:ASN:ND2	1.92	0.67
1:C:52:ILE:HD13	1:C:236:GLY:HA2	1.77	0.67
1:B:2:ILE:HD11	1:B:209:ILE:HD12	1.77	0.67
1:C:48:THR:HG22	1:C:49:GLY:N	2.10	0.66
1:A:52:ILE:CD1	1:A:59:GLU:HB3	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:CD1	1:D:59:GLU:HB3	2.24	0.66
1:E:160:ASN:HB3	1:E:181:ILE:HG22	1.78	0.66
1:C:8:THR:HG22	1:F:1:MET:N	2.10	0.66
1:C:124:ARG:HD3	1:C:126:TYR:OH	1.96	0.66
1:A:159:GLY:HA2	1:A:164:MET:CG	2.24	0.66
1:B:6:ILE:HG21	1:B:199:GLY:HA2	1.78	0.66
1:C:8:THR:HG22	1:F:1:MET:H2	1.61	0.66
1:E:64:PRO:HG3	1:E:228:ILE:HD12	1.77	0.65
1:F:52:ILE:CD1	1:F:59:GLU:HB3	2.26	0.65
1:E:93:GLU:HB2	1:E:94:PRO:HD3	1.78	0.65
1:F:16:LEU:O	1:F:20:LEU:HD22	1.96	0.65
1:A:251:MET:HE2	1:A:251:MET:H	1.62	0.65
1:B:55:MET:HE3	1:B:55:MET:H	1.62	0.64
1:B:245:VAL:HG22	1:B:253:HIS:CE1	2.31	0.64
1:F:88:VAL:O	1:F:92:LEU:HD13	1.97	0.64
1:E:55:MET:HE1	1:E:239:LYS:HD3	1.79	0.64
1:F:48:THR:O	1:F:84:THR:HG23	1.97	0.64
1:C:71:ARG:O	1:C:75:MET:HG3	1.97	0.64
1:B:245:VAL:HG22	1:B:253:HIS:NE2	2.13	0.64
1:C:121:ALA:HB2	1:C:168:ARG:NH2	2.13	0.64
1:A:48:THR:CG2	1:A:114:VAL:HB	2.28	0.64
1:C:198:TRP:HE1	1:C:253:HIS:HD2	1.46	0.64
1:D:52:ILE:HG22	1:D:55:MET:HE3	1.80	0.64
1:E:159:GLY:HA2	1:E:164:MET:CG	2.25	0.64
1:B:84:THR:HG21	1:B:88:VAL:HG11	1.79	0.63
1:D:113:SER:HB2	1:D:142:PHE:CZ	2.34	0.63
1:E:160:ASN:HB3	1:E:181:ILE:CG2	2.28	0.63
1:A:187:THR:HG21	1:A:189:GLU:O	1.99	0.63
1:F:1:MET:HE3	1:F:4:HIS:H	1.64	0.63
1:E:124:ARG:HD3	1:E:126:TYR:OH	1.98	0.63
1:D:152:THR:HG22	1:D:188:ASP:H	1.63	0.63
1:E:52:ILE:CD1	1:E:236:GLY:HA2	2.29	0.63
1:B:2:ILE:O	1:B:6:ILE:HG13	1.98	0.63
1:B:71:ARG:NH2	1:B:217:GLU:O	2.32	0.63
1:C:152:THR:CG2	1:C:187:THR:OG1	2.47	0.62
1:B:5:LEU:HD23	1:B:5:LEU:O	1.99	0.62
1:E:52:ILE:O	1:E:55:MET:HE3	1.99	0.62
1:F:245:VAL:HG13	1:F:253:HIS:CE1	2.33	0.62
1:E:10:ILE:HG21	1:E:248:ILE:HD11	1.81	0.62
1:E:89:GLU:OE1	1:E:99:LEU:HD13	1.99	0.62
1:F:222:ARG:O	1:F:226:GLU:HG2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	1:A:3:ALA:H	1.65	0.62
1:C:2:ILE:HD11	1:C:209:ILE:CD1	2.29	0.61
1:C:93:GLU:HB3	1:C:94:PRO:HD3	1.81	0.61
1:E:119:ARG:HH11	1:E:119:ARG:HG2	1.64	0.61
1:D:228:ILE:O	1:D:233:LEU:HB2	2.00	0.61
1:E:45:LEU:HB2	1:E:108:TYR:CD1	2.36	0.61
1:F:84:THR:HG21	1:F:88:VAL:HG11	1.82	0.61
1:C:43:ARG:HH11	1:C:107:ASP:HB3	1.65	0.61
1:D:137:PRO:O	1:D:138:LEU:HD12	2.00	0.61
1:F:105:PRO:HG3	1:F:141:ILE:HG13	1.81	0.61
1:A:244:SER:HB2	1:A:248:ILE:O	2.01	0.61
1:C:19:TYR:CE2	1:F:4:HIS:HE1	2.18	0.61
1:E:234:ILE:CG2	1:E:239:LYS:HA	2.31	0.61
1:F:52:ILE:CD1	1:F:236:GLY:HA2	2.30	0.61
1:F:177:HIS:HB2	1:F:181:ILE:HD12	1.81	0.60
1:A:132:GLU:HG2	1:A:134:LYS:HE3	1.82	0.60
1:E:54:PRO:HA	1:E:56:MET:HE2	1.83	0.60
1:C:48:THR:HG21	1:C:62:GLY:C	2.26	0.60
1:C:243:PRO:O	1:C:250:LEU:HG	2.01	0.60
1:D:82:ILE:HD12	1:D:97:VAL:HG21	1.84	0.60
1:E:87:GLU:OE2	1:E:135:ARG:NH1	2.32	0.60
1:A:177:HIS:HB2	1:A:181:ILE:HD12	1.82	0.60
1:C:113:SER:HB2	1:C:142:PHE:CZ	2.37	0.60
1:E:245:VAL:HG13	1:E:253:HIS:NE2	2.16	0.60
1:A:48:THR:HG21	1:A:66:ALA:HB2	1.82	0.60
1:A:144:LYS:O	1:A:148:LEU:HD13	2.01	0.60
1:E:127:SER:O	1:E:181:ILE:HD13	2.02	0.60
1:B:168:ARG:HH11	1:B:168:ARG:HG2	1.66	0.59
1:D:198:TRP:HE1	1:D:253:HIS:HD2	1.50	0.59
1:D:234:ILE:HG22	1:D:241:LEU:HD12	1.84	0.59
1:B:62:GLY:HA2	1:B:114:VAL:HG12	1.85	0.59
1:F:52:ILE:HD12	1:F:59:GLU:HB3	1.83	0.59
1:D:9:ASP:HB3	1:E:1:MET:HA	1.83	0.59
1:D:245:VAL:HG13	1:D:253:HIS:CE1	2.37	0.59
1:F:160:ASN:HB3	1:F:181:ILE:HG23	1.85	0.59
1:B:6:ILE:CD1	1:B:202:GLY:HA3	2.31	0.59
1:C:187:THR:HG23	1:C:189:GLU:O	2.02	0.59
1:D:160:ASN:HB3	1:D:181:ILE:HG23	1.84	0.59
1:A:152:THR:HG21	1:A:187:THR:HA	1.84	0.59
1:C:9:ASP:O	1:F:1:MET:N	2.31	0.59
1:F:55:MET:HE1	1:F:239:LYS:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:GLY:H	1:F:197:ASN:ND2	2.02	0.58
1:B:2:ILE:HD11	1:B:209:ILE:CD1	2.32	0.58
1:B:6:ILE:HG22	1:B:193:SER:HB3	1.85	0.58
1:C:266:GLU:HG3	1:F:252:VAL:HG21	1.85	0.58
1:A:62:GLY:H	1:A:197:ASN:ND2	1.99	0.58
1:B:2:ILE:CD1	1:B:209:ILE:HD12	2.33	0.58
1:D:129:SER:O	1:D:130:ALA:HB3	2.04	0.58
1:C:82:ILE:HD12	1:C:97:VAL:CG1	2.33	0.58
1:C:168:ARG:O	1:C:172:VAL:HG23	2.04	0.58
1:C:9:ASP:C	1:C:10:ILE:HD12	2.28	0.58
1:E:84:THR:HG21	1:E:88:VAL:CG1	2.30	0.58
1:B:240:THR:HG22	1:B:241:LEU:H	1.69	0.57
1:F:53:PRO:HA	1:F:56:MET:HE2	1.84	0.57
1:C:19:TYR:OH	1:C:23:ARG:HG3	2.04	0.57
1:D:48:THR:C	1:D:84:THR:HG22	2.29	0.57
1:A:152:THR:CG2	1:A:187:THR:HA	2.35	0.57
1:B:187:THR:CG2	1:B:189:GLU:O	2.50	0.57
1:F:1:MET:HE3	1:F:3:ALA:N	2.19	0.57
1:F:198:TRP:HE1	1:F:253:HIS:CD2	2.22	0.57
1:F:10:ILE:HG23	1:F:10:ILE:O	2.04	0.57
1:F:130:ALA:HA	1:F:181:ILE:HD11	1.86	0.57
1:D:177:HIS:HB2	1:D:181:ILE:HD12	1.85	0.57
1:D:48:THR:O	1:D:84:THR:HG22	2.05	0.57
1:E:115:GLU:OE1	1:E:161:GLU:HG2	2.05	0.57
1:D:27:PHE:CZ	1:E:16:LEU:HD23	2.40	0.57
1:D:52:ILE:HD12	1:D:59:GLU:HB3	1.84	0.57
1:E:241:LEU:HD12	1:E:241:LEU:N	2.20	0.57
1:C:48:THR:C	1:C:84:THR:HG22	2.29	0.57
1:A:71:ARG:CZ	1:A:75:MET:HE1	2.35	0.56
1:A:62:GLY:H	1:A:197:ASN:HD21	1.53	0.56
1:E:187:THR:HG23	1:E:189:GLU:O	2.06	0.56
1:F:12:ASN:CG	1:F:15:VAL:HG23	2.31	0.56
1:F:65:GLY:H	1:F:197:ASN:ND2	2.02	0.56
1:D:187:THR:HG23	1:D:189:GLU:O	2.05	0.56
1:F:142:PHE:CD1	1:F:162:ILE:HD13	2.40	0.56
1:F:1:MET:CE	1:F:4:HIS:N	2.67	0.56
1:F:221:GLU:OE2	1:F:225:ILE:HD11	2.06	0.56
1:A:43:ARG:HG2	1:A:108:TYR:HD1	1.71	0.56
1:D:213:ARG:HD3	3:D:425:HOH:O	2.06	0.56
1:D:1:MET:HA	1:E:9:ASP:HB2	1.88	0.56
1:D:75:MET:HE2	1:D:213:ARG:NH2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:VAL:HG13	1:E:175:VAL:HG21	1.88	0.56
1:F:10:ILE:O	1:F:10:ILE:CG2	2.54	0.56
1:C:48:THR:HG23	1:C:114:VAL:O	2.06	0.55
1:F:105:PRO:O	1:F:150:ILE:HD13	2.07	0.55
1:A:124:ARG:HH11	1:A:124:ARG:CG	2.20	0.55
1:D:52:ILE:HD11	1:D:59:GLU:HB3	1.87	0.55
1:E:134:LYS:O	1:E:135:ARG:HG3	2.05	0.55
1:F:152:THR:C	1:F:187:THR:HG23	2.30	0.55
1:A:10:ILE:HD12	1:A:194:ALA:HB1	1.87	0.55
1:A:64:PRO:HD2	1:A:197:ASN:HD21	1.72	0.55
1:C:198:TRP:HE1	1:C:253:HIS:CD2	2.25	0.55
1:F:48:THR:HG21	1:F:66:ALA:HB2	1.88	0.55
1:A:225:ILE:HD12	1:A:250:LEU:HD21	1.89	0.55
1:D:106:GLU:CD	1:D:106:GLU:H	2.13	0.55
1:C:144:LYS:O	1:C:148:LEU:HD13	2.06	0.55
1:E:113:SER:HB2	1:E:142:PHE:CZ	2.42	0.55
1:C:23:ARG:O	1:C:23:ARG:HD3	2.07	0.54
1:D:23:ARG:HD3	1:D:27:PHE:HA	1.89	0.54
1:B:162:ILE:HG23	1:B:185:VAL:HG11	1.89	0.54
1:B:225:ILE:HD12	1:B:250:LEU:HD21	1.88	0.54
1:F:62:GLY:H	1:F:197:ASN:HD21	1.55	0.54
1:E:43:ARG:HD3	1:E:107:ASP:O	2.07	0.54
1:F:187:THR:HG22	1:F:189:GLU:H	1.72	0.54
1:A:10:ILE:HD11	1:A:195:VAL:HG23	1.89	0.54
1:B:113:SER:HB2	1:B:142:PHE:CZ	2.41	0.54
1:E:220:ASP:HB3	1:E:223:ARG:HB3	1.89	0.54
1:C:105:PRO:HG3	1:C:141:ILE:HG13	1.89	0.54
1:E:10:ILE:HD11	1:E:194:ALA:HB1	1.88	0.54
1:A:12:ASN:CG	1:A:15:VAL:HG23	2.33	0.54
1:C:48:THR:H	1:C:84:THR:HG22	1.72	0.54
1:A:10:ILE:HD11	1:A:195:VAL:CG2	2.37	0.54
1:D:40:ASN:ND2	1:F:24:ARG:HH12	2.06	0.54
1:E:187:THR:CG2	1:E:189:GLU:O	2.56	0.53
1:F:130:ALA:CA	1:F:181:ILE:HD11	2.38	0.53
1:E:152:THR:HG22	1:E:188:ASP:OD2	2.09	0.53
1:A:225:ILE:HD12	1:A:250:LEU:CD2	2.39	0.53
1:E:241:LEU:HD12	1:E:241:LEU:H	1.72	0.53
1:B:23:ARG:O	1:B:23:ARG:HD3	2.09	0.53
1:A:159:GLY:C	1:A:164:MET:HG2	2.34	0.53
1:D:61:ASP:HB2	1:D:245:VAL:HG23	1.90	0.53
1:D:184:VAL:O	1:D:184:VAL:HG12	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HB2	1:B:266:GLU:OE2	2.09	0.53
1:D:101:ARG:O	1:D:102:THR:C	2.51	0.53
1:E:125:TYR:N	1:E:125:TYR:CD2	2.76	0.53
1:C:240:THR:HG22	1:C:241:LEU:H	1.73	0.53
1:A:222:ARG:O	1:A:226:GLU:HG3	2.09	0.53
1:B:251:MET:HE3	1:F:217:GLU:CD	2.35	0.52
1:C:4:HIS:HE1	1:F:4:HIS:O	1.92	0.52
1:F:128:MET:HE1	1:F:175:VAL:HG11	1.90	0.52
1:F:10:ILE:HD11	1:F:198:TRP:HH2	1.75	0.52
1:B:198:TRP:HE1	1:B:253:HIS:CD2	2.23	0.52
1:C:106:GLU:CD	1:C:106:GLU:H	2.18	0.52
1:E:234:ILE:HG23	1:E:239:LYS:HA	1.92	0.52
1:F:52:ILE:HD11	1:F:59:GLU:HB3	1.92	0.52
1:A:187:THR:HG22	1:A:189:GLU:O	2.10	0.51
1:A:48:THR:O	1:A:84:THR:CG2	2.56	0.51
1:E:146:ARG:HA	3:E:418:HOH:O	2.10	0.51
1:C:23:ARG:HG2	1:C:29:PHE:HE2	1.75	0.51
1:B:268:ILE:HG22	1:B:269:LEU:HD23	1.91	0.51
1:D:48:THR:HG21	1:D:62:GLY:C	2.36	0.51
1:D:85:TYR:O	1:D:89:GLU:HG3	2.10	0.51
1:D:170:LEU:H	1:D:170:LEU:CD1	2.24	0.51
1:B:54:PRO:N	1:B:55:MET:HE3	2.25	0.51
1:B:216:LEU:O	1:B:261:LYS:HE2	2.10	0.51
1:B:152:THR:HG22	1:B:188:ASP:OD2	2.10	0.51
1:C:7:ASN:CG	1:C:19:TYR:CD1	2.89	0.51
1:C:19:TYR:CE2	1:F:4:HIS:CE1	2.99	0.51
1:A:45:LEU:HD21	1:A:83:LEU:HB2	1.94	0.50
1:C:222:ARG:HG3	1:C:250:LEU:HD13	1.93	0.50
1:D:62:GLY:N	1:D:197:ASN:HD21	1.96	0.50
1:F:54:PRO:HA	1:F:56:MET:HE2	1.94	0.50
1:B:82:ILE:HD12	1:B:97:VAL:HG11	1.93	0.50
1:D:240:THR:HG22	1:D:241:LEU:N	2.26	0.50
1:E:9:ASP:OD2	1:E:16:LEU:HD22	2.11	0.50
1:A:12:ASN:OD1	1:A:15:VAL:HG23	2.11	0.50
1:B:62:GLY:H	1:B:197:ASN:HD21	1.59	0.50
1:C:152:THR:HG22	1:C:187:THR:OG1	2.12	0.50
1:F:5:LEU:HD21	1:F:259:LEU:HD23	1.93	0.50
1:B:5:LEU:HD13	1:B:260:LEU:HD23	1.92	0.50
1:B:128:MET:HE1	1:B:175:VAL:HG11	1.94	0.50
1:C:3:ALA:HB2	1:C:30:LEU:CB	2.42	0.50
1:D:43:ARG:NH1	1:D:107:ASP:HB3	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLY:C	1:B:164:MET:HG2	2.37	0.50
1:C:256:ILE:HD12	1:F:259:LEU:CD1	2.41	0.50
1:F:1:MET:HE2	1:F:4:HIS:HB2	1.93	0.50
1:D:146:ARG:HG3	1:D:146:ARG:HH11	1.76	0.49
1:C:12:ASN:OD1	1:C:15:VAL:HG23	2.11	0.49
1:C:21:ASP:O	1:C:25:LYS:HG3	2.12	0.49
1:D:198:TRP:HE1	1:D:253:HIS:CD2	2.30	0.49
1:B:62:GLY:H	1:B:197:ASN:ND2	2.10	0.49
1:D:52:ILE:O	1:D:55:MET:HE3	2.13	0.49
1:D:170:LEU:HD12	1:D:170:LEU:N	2.28	0.49
1:F:93:GLU:HB3	1:F:94:PRO:HD3	1.95	0.49
1:D:187:THR:CG2	1:D:189:GLU:O	2.60	0.49
1:E:70:TYR:CE2	1:E:97:VAL:HG13	2.46	0.49
1:C:152:THR:CG2	1:C:187:THR:HA	2.43	0.49
1:F:10:ILE:HD13	1:F:248:ILE:CD1	2.43	0.49
1:A:167:ILE:HB	1:A:170:LEU:HD22	1.93	0.49
1:C:121:ALA:HB2	1:C:168:ARG:HH21	1.77	0.49
1:E:115:GLU:OE1	1:E:115:GLU:HA	2.12	0.49
1:E:130:ALA:CA	1:E:181:ILE:HD11	2.42	0.49
1:A:53:PRO:HA	1:A:56:MET:HE2	1.94	0.48
1:C:266:GLU:HG3	1:F:252:VAL:CG2	2.43	0.48
1:A:106:GLU:HG3	1:A:148:LEU:HD23	1.94	0.48
1:D:47:VAL:HG22	1:D:83:LEU:HB3	1.95	0.48
1:E:198:TRP:CD2	1:E:256:ILE:HD12	2.48	0.48
1:F:168:ARG:O	1:F:172:VAL:HG23	2.13	0.48
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.78	0.48
1:E:134:LYS:O	1:E:135:ARG:CG	2.61	0.48
1:F:153:ILE:C	1:F:187:THR:HG21	2.37	0.48
1:B:2:ILE:HD12	1:B:206:GLN:OE1	2.14	0.48
1:B:5:LEU:CD1	1:B:259:LEU:HG	2.43	0.48
1:C:45:LEU:HD21	1:C:83:LEU:HB2	1.96	0.48
1:F:222:ARG:HG3	1:F:250:LEU:HD13	1.95	0.48
1:A:128:MET:HE1	1:A:175:VAL:HG11	1.95	0.48
1:A:236:GLY:HA3	3:A:431:HOH:O	2.12	0.48
1:B:155:VAL:HG22	1:B:191:ILE:HB	1.96	0.48
1:C:205:ALA:O	1:C:209:ILE:HG13	2.14	0.48
1:D:54:PRO:N	1:D:55:MET:HE2	2.29	0.48
1:D:55:MET:H	1:D:55:MET:CE	2.12	0.48
1:E:152:THR:CG2	1:E:188:ASP:H	2.24	0.48
1:B:48:THR:CG2	1:B:114:VAL:HB	2.44	0.48
1:E:52:ILE:CD1	1:E:59:GLU:HB3	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ARG:HG3	1:E:223:ARG:HH11	1.78	0.48
1:E:228:ILE:HG23	1:E:233:LEU:HD22	1.95	0.48
1:B:5:LEU:HD23	1:B:5:LEU:C	2.39	0.47
1:D:51:PRO:HD2	1:D:117:PRO:HG2	1.96	0.47
1:D:163:GLY:CA	1:D:187:THR:HB	2.43	0.47
1:E:235:ASP:O	1:E:237:VAL:N	2.47	0.47
1:A:134:LYS:O	1:A:135:ARG:HB2	2.12	0.47
1:B:161:GLU:O	1:B:164:MET:HB2	2.14	0.47
1:C:256:ILE:CD1	1:F:259:LEU:HD11	2.44	0.47
1:A:48:THR:CG2	1:A:66:ALA:HB2	2.44	0.47
1:A:130:ALA:N	1:A:181:ILE:HD11	2.29	0.47
1:D:245:VAL:HG13	1:D:253:HIS:NE2	2.30	0.47
1:E:228:ILE:HG23	1:E:233:LEU:CD2	2.44	0.47
1:C:256:ILE:HD12	1:F:259:LEU:HD11	1.95	0.47
1:E:240:THR:HG22	1:E:241:LEU:N	2.29	0.47
1:B:5:LEU:HD13	1:B:260:LEU:CD2	2.44	0.47
1:F:12:ASN:OD1	1:F:15:VAL:HG23	2.14	0.47
1:F:55:MET:CE	1:F:239:LYS:HB3	2.43	0.47
1:B:48:THR:HG23	1:B:114:VAL:HB	1.96	0.47
1:B:168:ARG:HG2	1:B:168:ARG:NH1	2.28	0.47
1:E:10:ILE:CG2	1:E:248:ILE:HD11	2.42	0.47
1:E:82:ILE:CD1	1:E:97:VAL:HG11	2.37	0.47
1:E:93:GLU:C	1:E:95:PHE:H	2.23	0.47
1:E:125:TYR:N	1:E:125:TYR:HD2	2.12	0.47
1:F:122:ASP:OD1	1:F:126:TYR:OH	2.32	0.47
1:A:69:ILE:O	1:A:73:VAL:HG23	2.15	0.47
1:D:228:ILE:HB	1:D:233:LEU:HD22	1.95	0.47
1:E:44:VAL:O	1:E:80:ALA:HA	2.15	0.47
1:A:152:THR:CG2	1:A:187:THR:HG23	2.45	0.47
1:E:212:GLY:O	1:E:268:ILE:HD13	2.15	0.47
1:F:245:VAL:HG13	1:F:253:HIS:NE2	2.30	0.47
1:D:12:ASN:CG	1:D:15:VAL:HG23	2.40	0.47
1:B:234:ILE:HD12	1:B:239:LYS:HA	1.97	0.46
1:D:49:GLY:O	1:D:117:PRO:HD3	2.15	0.46
1:B:42:GLU:CD	1:B:42:GLU:H	2.24	0.46
1:B:221:GLU:OE2	1:B:225:ILE:HD11	2.14	0.46
1:A:52:ILE:CD1	1:A:236:GLY:HA2	2.42	0.46
1:B:161:GLU:OE1	1:B:164:MET:HE3	2.15	0.46
1:D:134:LYS:O	1:D:135:ARG:HB2	2.15	0.46
1:D:260:LEU:O	1:D:264:VAL:HG23	2.15	0.46
1:E:260:LEU:O	1:E:264:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:PRO:HD2	1:B:55:MET:CE	2.45	0.46
1:C:4:HIS:HB3	1:F:9:ASP:HB2	1.98	0.46
1:C:205:ALA:O	1:C:208:SER:HB2	2.16	0.46
1:D:146:ARG:HG3	1:D:146:ARG:NH1	2.30	0.46
1:E:64:PRO:HG3	1:E:228:ILE:CD1	2.46	0.46
1:B:163:GLY:HA2	1:B:187:THR:HB	1.98	0.46
1:E:101:ARG:O	1:E:102:THR:C	2.58	0.46
1:E:130:ALA:HA	1:E:181:ILE:HD11	1.97	0.46
1:E:222:ARG:O	1:E:226:GLU:HG3	2.15	0.46
1:C:51:PRO:HB2	1:C:133:ILE:HG23	1.98	0.46
1:D:9:ASP:C	1:D:10:ILE:HG13	2.41	0.46
1:C:27:PHE:CZ	1:F:16:LEU:HD23	2.51	0.46
1:B:53:PRO:C	1:B:55:MET:HE3	2.41	0.46
1:B:89:GLU:CD	1:B:99:LEU:HD13	2.40	0.46
1:B:176:PRO:C	1:B:178:GLY:H	2.23	0.46
1:D:35:LYS:NZ	1:F:189:GLU:OE2	2.48	0.46
1:F:64:PRO:HD2	1:F:197:ASN:HD21	1.80	0.46
1:F:222:ARG:NH1	1:F:254:GLU:OE1	2.49	0.46
1:B:101:ARG:O	1:B:102:THR:C	2.59	0.46
1:C:240:THR:HG22	1:C:241:LEU:N	2.30	0.46
1:C:249:ARG:HH12	1:F:269:LEU:CD1	2.29	0.46
1:E:104:GLU:O	1:E:107:ASP:HB2	2.16	0.46
1:B:105:PRO:HG3	1:B:141:ILE:HG13	1.99	0.45
1:C:152:THR:HG21	1:C:187:THR:HA	1.97	0.45
1:A:87:GLU:HG2	1:A:88:VAL:N	2.32	0.45
1:F:129:SER:O	1:F:130:ALA:HB3	2.17	0.45
1:A:124:ARG:CG	1:A:124:ARG:NH1	2.79	0.45
1:B:54:PRO:HD2	1:B:55:MET:HE2	1.98	0.45
1:D:23:ARG:HG3	1:D:23:ARG:NH1	2.29	0.45
1:D:152:THR:CG2	1:D:187:THR:HA	2.46	0.45
1:D:152:THR:HG23	1:D:188:ASP:H	1.76	0.45
1:A:9:ASP:CB	1:B:2:ILE:N	2.76	0.45
1:B:152:THR:HG22	1:B:188:ASP:CG	2.42	0.45
1:C:5:LEU:HB2	1:F:8:THR:HG23	1.98	0.45
1:C:19:TYR:HE2	1:F:4:HIS:HE1	1.61	0.45
1:D:54:PRO:O	1:D:56:MET:HG2	2.16	0.45
1:E:262:ALA:O	1:E:266:GLU:HB2	2.16	0.45
1:D:31:HIS:CE1	1:D:35:LYS:HE3	2.52	0.45
1:D:177:HIS:O	1:D:181:ILE:HB	2.17	0.45
1:C:163:GLY:HA2	1:C:187:THR:HB	1.99	0.45
1:D:129:SER:O	1:D:130:ALA:CB	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ASP:OD1	1:E:246:ASP:OD2	2.35	0.45
1:F:62:GLY:HA2	1:F:114:VAL:HG12	1.99	0.45
1:F:228:ILE:HB	1:F:233:LEU:HD22	1.99	0.45
1:A:159:GLY:N	1:A:164:MET:HE3	2.32	0.45
1:B:64:PRO:HD2	1:B:197:ASN:HD21	1.82	0.45
1:C:9:ASP:O	1:C:10:ILE:HG13	2.17	0.45
1:E:55:MET:CE	1:E:239:LYS:HD3	2.46	0.45
1:E:129:SER:O	1:E:130:ALA:HB3	2.17	0.45
1:A:168:ARG:HG2	1:A:168:ARG:NH1	2.32	0.44
1:B:136:ASP:HA	1:B:137:PRO:HD3	1.83	0.44
1:C:23:ARG:O	1:C:27:PHE:HA	2.17	0.44
1:C:27:PHE:HZ	1:F:16:LEU:HD23	1.82	0.44
1:C:187:THR:CG2	1:C:189:GLU:O	2.64	0.44
1:E:9:ASP:CG	1:E:16:LEU:HD22	2.42	0.44
1:F:29:PHE:CD1	1:F:29:PHE:C	2.95	0.44
1:A:42:GLU:CD	1:A:42:GLU:H	2.25	0.44
1:B:121:ALA:HA	1:B:184:VAL:HG21	2.00	0.44
1:C:249:ARG:NE	1:F:266:GLU:OE2	2.51	0.44
1:E:13:ARG:HB3	1:E:17:LYS:HE2	1.99	0.44
1:B:100:ALA:O	1:B:101:ARG:HD3	2.17	0.44
1:A:65:GLY:H	1:A:197:ASN:ND2	2.15	0.44
1:D:228:ILE:HD12	1:D:233:LEU:HD23	1.99	0.44
1:F:130:ALA:N	1:F:181:ILE:HD11	2.33	0.44
1:C:248:ILE:O	1:C:253:HIS:HE1	1.99	0.44
1:D:159:GLY:O	1:D:182:ALA:HA	2.16	0.44
1:A:113:SER:HB2	1:A:142:PHE:CZ	2.53	0.44
1:C:105:PRO:HB3	1:C:150:ILE:HD12	1.99	0.44
1:F:42:GLU:H	1:F:42:GLU:CD	2.26	0.44
1:A:52:ILE:HD11	1:A:59:GLU:HB3	1.99	0.44
1:A:71:ARG:HG2	1:A:75:MET:HE3	1.99	0.44
1:B:19:TYR:CD2	1:B:19:TYR:C	2.96	0.44
1:B:211:VAL:O	1:B:211:VAL:HG13	2.17	0.44
1:D:43:ARG:NH2	1:D:81:GLU:OE1	2.48	0.44
1:E:159:GLY:HA3	1:E:171:VAL:HG11	2.00	0.44
1:F:126:TYR:CB	1:F:181:ILE:HG12	2.47	0.44
1:C:48:THR:HG21	1:C:63:PRO:N	2.33	0.44
1:A:63:PRO:HB2	1:A:64:PRO:HD3	1.99	0.44
1:B:4:HIS:O	1:B:5:LEU:C	2.61	0.44
1:D:222:ARG:NH1	1:D:254:GLU:OE2	2.51	0.44
1:F:228:ILE:HB	1:F:233:LEU:CD2	2.48	0.44
1:A:249:ARG:HH22	1:B:269:LEU:HB2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:VAL:HA	1:B:176:PRO:HD3	1.90	0.43
1:C:126:TYR:CB	1:C:181:ILE:HG22	2.48	0.43
1:F:104:GLU:HB3	1:F:106:GLU:OE1	2.17	0.43
1:A:62:GLY:HA2	1:A:114:VAL:HG12	2.00	0.43
1:B:225:ILE:HD12	1:B:250:LEU:CD2	2.48	0.43
1:C:59:GLU:HA	1:C:234:ILE:O	2.18	0.43
1:E:84:THR:HB	1:E:85:TYR:H	1.53	0.43
1:E:223:ARG:HG3	1:E:223:ARG:NH1	2.33	0.43
1:B:6:ILE:CG2	1:B:193:SER:HB3	2.47	0.43
1:A:105:PRO:CG	1:A:141:ILE:HG13	2.33	0.43
1:A:252:VAL:HG21	1:B:266:GLU:HG3	2.00	0.43
1:B:198:TRP:NE1	1:B:253:HIS:HD2	2.07	0.43
1:D:195:VAL:HB	1:D:198:TRP:CD2	2.54	0.43
1:F:105:PRO:HG3	1:F:141:ILE:CG1	2.46	0.43
1:A:161:GLU:O	1:A:164:MET:HB2	2.18	0.43
1:E:119:ARG:O	1:E:183:SER:HA	2.18	0.43
1:F:177:HIS:O	1:F:178:GLY:C	2.61	0.43
1:C:116:THR:HB	1:C:162:ILE:HD12	2.01	0.43
1:E:87:GLU:HG2	1:E:88:VAL:N	2.33	0.43
1:E:163:GLY:CA	1:E:187:THR:HB	2.44	0.43
1:F:128:MET:HE1	1:F:175:VAL:CG1	2.48	0.43
1:F:160:ASN:HB3	1:F:181:ILE:CG2	2.47	0.43
1:B:241:LEU:HD23	1:B:241:LEU:HA	1.88	0.43
1:E:55:MET:HE3	1:E:55:MET:H	1.82	0.43
1:E:259:LEU:O	1:E:262:ALA:HB3	2.19	0.43
1:D:197:ASN:HB3	1:D:201:TYR:CE2	2.53	0.43
1:F:105:PRO:HG2	1:F:144:LYS:HB2	2.01	0.43
1:F:126:TYR:HB2	1:F:181:ILE:HG12	2.01	0.43
1:F:242:ALA:HA	1:F:243:PRO:HD3	1.85	0.43
1:B:51:PRO:HD2	1:B:117:PRO:HG2	2.01	0.43
1:B:59:GLU:HA	1:B:234:ILE:O	2.18	0.43
1:C:3:ALA:CA	1:C:30:LEU:HD22	2.49	0.43
1:C:48:THR:HB	1:C:84:THR:HG21	2.00	0.43
1:F:139:ASP:HA	1:F:162:ILE:HD11	2.01	0.43
1:B:5:LEU:HD11	1:B:259:LEU:HG	1.99	0.43
1:C:7:ASN:HA	1:C:194:ALA:H	1.84	0.43
1:F:82:ILE:CD1	1:F:97:VAL:HG11	2.37	0.43
1:A:105:PRO:O	1:A:150:ILE:HD13	2.19	0.42
1:A:124:ARG:HH11	1:A:124:ARG:HG3	1.83	0.42
1:E:29:PHE:CD1	1:E:29:PHE:C	2.97	0.42
1:A:154:GLY:N	1:A:187:THR:HG21	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:CZ	1:A:137:PRO:HB3	2.54	0.42
1:D:196:SER:O	1:D:197:ASN:C	2.62	0.42
1:A:54:PRO:HA	1:A:56:MET:HE2	2.01	0.42
1:B:170:LEU:HD12	1:B:170:LEU:N	2.35	0.42
1:C:43:ARG:HD3	1:C:107:ASP:O	2.18	0.42
1:F:167:ILE:HB	1:F:170:LEU:HD22	2.00	0.42
1:A:4:HIS:O	1:B:4:HIS:HE1	2.03	0.42
1:A:23:ARG:HG3	1:A:27:PHE:HA	2.02	0.42
1:A:43:ARG:HG2	1:A:108:TYR:CD1	2.53	0.42
1:B:128:MET:HE1	1:B:158:GLY:O	2.19	0.42
1:D:62:GLY:N	1:D:197:ASN:ND2	2.59	0.42
1:A:197:ASN:O	1:A:200:ALA:HB3	2.19	0.42
1:F:84:THR:HG21	1:F:88:VAL:CG1	2.49	0.42
1:A:119:ARG:HH21	1:A:143:LEU:HD22	1.84	0.42
1:B:4:HIS:C	1:B:6:ILE:N	2.77	0.42
1:B:48:THR:O	1:B:84:THR:HG23	2.19	0.42
1:C:23:ARG:HG3	1:C:23:ARG:HH11	1.85	0.42
1:E:12:ASN:O	1:E:14:GLY:N	2.53	0.42
1:E:23:ARG:HD3	1:E:27:PHE:HA	2.02	0.42
1:A:34:THR:HG22	1:A:38:LEU:HD22	2.01	0.42
1:B:240:THR:HG22	1:B:241:LEU:N	2.33	0.42
1:C:126:TYR:HB3	1:C:181:ILE:HG22	2.02	0.42
1:D:136:ASP:HA	1:D:137:PRO:HD3	1.93	0.42
1:D:170:LEU:CD1	1:D:170:LEU:N	2.82	0.42
1:E:51:PRO:HD2	1:E:117:PRO:HG2	2.02	0.42
1:F:17:LYS:HB3	1:F:174:HIS:CG	2.55	0.42
1:F:63:PRO:HB2	1:F:64:PRO:HD3	2.01	0.42
1:A:234:ILE:HG22	1:A:241:LEU:CD1	2.47	0.41
1:E:132:GLU:HG2	1:E:134:LYS:HE3	2.02	0.41
1:E:234:ILE:CG2	1:E:235:ASP:N	2.83	0.41
1:F:1:MET:HE2	1:F:1:MET:HB3	1.83	0.41
1:F:61:ASP:HB2	1:F:245:VAL:HG23	2.01	0.41
1:B:47:VAL:HG22	1:B:83:LEU:HB3	2.01	0.41
1:F:136:ASP:HA	1:F:137:PRO:HD3	1.84	0.41
1:A:55:MET:O	1:A:56:MET:HB2	2.20	0.41
1:A:88:VAL:HG22	1:A:233:LEU:HD21	2.02	0.41
1:C:216:LEU:O	1:C:261:LYS:HE2	2.20	0.41
1:D:249:ARG:HG2	1:D:249:ARG:HH11	1.85	0.41
1:E:150:ILE:HA	1:E:151:PRO:HD3	1.87	0.41
1:A:175:VAL:HA	1:A:176:PRO:HD3	1.96	0.41
1:C:168:ARG:HH11	1:C:168:ARG:HG2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:VAL:CG1	1:C:179:GLU:HG2	2.50	0.41
1:D:220:ASP:O	1:D:224:VAL:HG23	2.21	0.41
1:D:236:GLY:HA3	3:D:418:HOH:O	2.20	0.41
1:A:20:LEU:HB3	1:B:24:ARG:HG2	2.01	0.41
1:C:91:ALA:HB2	1:C:233:LEU:HD13	2.03	0.41
1:E:125:TYR:OH	1:E:137:PRO:HB3	2.21	0.41
1:E:184:VAL:O	1:E:184:VAL:HG12	2.20	0.41
1:A:137:PRO:O	1:A:138:LEU:HD12	2.20	0.41
1:B:29:PHE:CD1	1:B:29:PHE:C	2.97	0.41
1:C:249:ARG:HH12	1:F:269:LEU:HD13	1.85	0.41
1:D:16:LEU:O	1:D:20:LEU:HD13	2.20	0.41
1:E:51:PRO:HB2	1:E:133:ILE:CG2	2.51	0.41
1:E:234:ILE:HG21	1:E:239:LYS:HA	2.03	0.41
1:B:129:SER:O	1:B:130:ALA:HB3	2.21	0.41
1:B:222:ARG:HD3	1:F:75:MET:HE1	2.01	0.41
1:A:88:VAL:O	1:A:92:LEU:HD22	2.21	0.41
1:A:129:SER:O	1:A:130:ALA:HB3	2.20	0.41
1:C:195:VAL:HB	1:C:198:TRP:CD2	2.56	0.41
1:C:217:GLU:OE2	1:C:217:GLU:HA	2.20	0.41
1:C:248:ILE:HB	1:C:253:HIS:CE1	2.56	0.41
1:D:198:TRP:NE1	1:D:253:HIS:HD2	2.17	0.41
1:D:242:ALA:HA	1:D:243:PRO:HD3	1.96	0.41
1:E:42:GLU:HG2	1:E:109:SER:CB	2.50	0.41
1:E:222:ARG:HA	1:E:250:LEU:HD22	2.03	0.41
1:F:76:LEU:HD23	1:F:76:LEU:HA	1.92	0.41
1:F:176:PRO:O	1:F:177:HIS:HB2	2.21	0.41
1:B:45:LEU:HB2	1:B:108:TYR:CD1	2.56	0.41
1:D:113:SER:OG	1:D:162:ILE:HB	2.21	0.41
1:D:234:ILE:HD12	1:D:239:LYS:HA	2.02	0.41
1:A:50:PHE:CE1	1:A:117:PRO:HG3	2.56	0.40
1:A:184:VAL:O	1:A:184:VAL:HG12	2.21	0.40
1:C:84:THR:HA	1:C:138:LEU:HD21	2.02	0.40
1:A:48:THR:C	1:A:84:THR:HG22	2.46	0.40
1:C:51:PRO:HD2	1:C:117:PRO:HG2	2.04	0.40
1:C:100:ALA:O	1:C:101:ARG:HD3	2.21	0.40
1:D:248:ILE:HB	1:D:253:HIS:CE1	2.56	0.40
1:E:88:VAL:O	1:E:92:LEU:HD13	2.20	0.40
1:E:90:LYS:HA	1:E:93:GLU:HG3	2.03	0.40
1:C:3:ALA:HA	1:C:30:LEU:HD22	2.04	0.40
1:B:3:ALA:HA	1:B:30:LEU:HD22	2.03	0.40
1:B:167:ILE:O	1:B:167:ILE:HG13	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:THR:CG2	1:C:49:GLY:H	2.18	0.40
1:D:159:GLY:C	1:D:164:MET:HG2	2.45	0.40
1:E:246:ASP:O	1:E:248: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	267/269 (99%)	256 (96%)	11 (4%)	0	100	100
1	B	256/269 (95%)	243 (95%)	12 (5%)	1 (0%)	30	43
1	C	266/269 (99%)	244 (92%)	20 (8%)	2 (1%)	16	25
1	D	267/269 (99%)	244 (91%)	21 (8%)	2 (1%)	18	28
1	E	267/269 (99%)	247 (92%)	17 (6%)	3 (1%)	11	18
1	F	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	43
All	All	1590/1614 (98%)	1484 (93%)	97 (6%)	9 (1%)	21	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	8	THR
1	E	13	ARG
1	E	236	GLY
1	D	12	ASN
1	C	10	ILE
1	D	10	ILE
1	F	178	GLY
1	B	158	GLY
1	E	94	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	218/218 (100%)	197 (90%)	21 (10%)	8	12
1	B	211/218 (97%)	192 (91%)	19 (9%)	9	15
1	C	217/218 (100%)	200 (92%)	17 (8%)	11	20
1	D	218/218 (100%)	200 (92%)	18 (8%)	10	17
1	E	218/218 (100%)	202 (93%)	16 (7%)	13	22
1	F	218/218 (100%)	202 (93%)	16 (7%)	13	22
All	All	1300/1308 (99%)	1193 (92%)	107 (8%)	10	18

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ILE
1	A	20	LEU
1	A	38	LEU
1	A	45	LEU
1	A	55	MET
1	A	83	LEU
1	A	84	THR
1	A	92	LEU
1	A	124	ARG
1	A	152	THR
1	A	170	LEU
1	A	179	GLU
1	A	187	THR
1	A	203	LEU
1	A	210	GLU
1	A	217	GLU
1	A	245	VAL
1	A	256	ILE
1	A	258	GLU
1	A	266	GLU
1	B	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	38	LEU
1	B	45	LEU
1	B	48	THR
1	B	55	MET
1	B	83	LEU
1	B	84	THR
1	B	97	VAL
1	B	106	GLU
1	B	124	ARG
1	B	138	LEU
1	B	146	ARG
1	B	148	LEU
1	B	179	GLU
1	B	187	THR
1	B	203	LEU
1	B	211	VAL
1	B	223	ARG
1	B	245	VAL
1	C	9	ASP
1	C	23	ARG
1	C	38	LEU
1	C	45	LEU
1	C	55	MET
1	C	83	LEU
1	C	92	LEU
1	C	102	THR
1	C	106	GLU
1	C	138	LEU
1	C	152	THR
1	C	187	THR
1	C	203	LEU
1	C	210	GLU
1	C	217	GLU
1	C	245	VAL
1	C	256	ILE
1	D	5	LEU
1	D	23	ARG
1	D	38	LEU
1	D	39	ASP
1	D	45	LEU
1	D	48	THR
1	D	55	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	74	GLU
1	D	83	LEU
1	D	92	LEU
1	D	148	LEU
1	D	152	THR
1	D	179	GLU
1	D	187	THR
1	D	203	LEU
1	D	245	VAL
1	D	256	ILE
1	D	268	ILE
1	E	20	LEU
1	E	23	ARG
1	E	38	LEU
1	E	42	GLU
1	E	55	MET
1	E	83	LEU
1	E	84	THR
1	E	125	TYR
1	E	169	GLU
1	E	187	THR
1	E	203	LEU
1	E	211	VAL
1	E	233	LEU
1	E	245	VAL
1	E	256	ILE
1	E	266	GLU
1	F	5	LEU
1	F	10	ILE
1	F	20	LEU
1	F	23	ARG
1	F	38	LEU
1	F	45	LEU
1	F	55	MET
1	F	83	LEU
1	F	84	THR
1	F	138	LEU
1	F	170	LEU
1	F	203	LEU
1	F	210	GLU
1	F	233	LEU
1	F	245	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	197	ASN
1	B	31	HIS
1	B	40	ASN
1	B	197	ASN
1	B	253	HIS
1	C	7	ASN
1	C	197	ASN
1	C	253	HIS
1	D	26	ASN
1	D	31	HIS
1	D	40	ASN
1	D	177	HIS
1	D	197	ASN
1	D	206	GLN
1	D	253	HIS
1	E	4	HIS
1	E	28	ASN
1	E	40	ASN
1	E	197	ASN
1	F	4	HIS
1	F	28	ASN
1	F	197	ASN
1	F	253	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	269/269 (100%)	-0.41	2 (0%) 84 81	23, 35, 51, 67	0
1	B	260/269 (96%)	-0.31	6 (2%) 61 57	23, 36, 55, 100	0
1	C	268/269 (99%)	-0.05	12 (4%) 38 34	22, 44, 67, 100	0
1	D	269/269 (100%)	0.02	2 (0%) 84 81	31, 46, 61, 85	0
1	E	269/269 (100%)	0.39	13 (4%) 35 32	30, 54, 79, 91	0
1	F	269/269 (100%)	-0.42	3 (1%) 78 74	22, 36, 49, 75	0
All	All	1604/1614 (99%)	-0.13	38 (2%) 59 55	22, 41, 70, 100	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ALA	5.6
1	B	4	HIS	5.1
1	C	8	THR	4.8
1	C	10	ILE	4.7
1	B	6	ILE	4.6
1	B	5	LEU	4.5
1	B	2	ILE	4.2
1	C	6	ILE	4.0
1	C	9	ASP	4.0
1	C	4	HIS	3.8
1	C	7	ASN	3.5
1	C	5	LEU	3.5
1	C	3	ALA	3.1
1	C	2	ILE	3.0
1	F	10	ILE	3.0
1	E	234	ILE	2.8
1	F	13	ARG	2.8
1	B	15	VAL	2.7
1	F	11	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	10	ILE	2.6
1	E	236	GLY	2.6
1	C	269	LEU	2.5
1	A	269	LEU	2.5
1	E	13	ARG	2.5
1	E	10	ILE	2.4
1	E	227	ALA	2.4
1	D	10	ILE	2.3
1	E	106	GLU	2.3
1	E	9	ASP	2.3
1	E	269	LEU	2.3
1	E	54	PRO	2.2
1	C	13	ARG	2.2
1	E	228	ILE	2.2
1	E	12	ASN	2.1
1	C	11	GLY	2.1
1	E	11	GLY	2.1
1	D	231	ALA	2.0
1	E	129	SER	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	302	1/1	0.85	0.14	57,57,57,57	0
2	MG	E	302	1/1	0.89	0.10	55,55,55,55	0
2	MG	A	302	1/1	0.90	0.22	55,55,55,55	0
2	MG	B	302	1/1	0.92	0.21	54,54,54,54	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	MG	C	302	1/1	0.93	0.17	64,64,64,64	0
2	MG	E	301	1/1	0.95	0.13	46,46,46,46	0
2	MG	F	302	1/1	0.95	0.22	55,55,55,55	0
2	MG	A	301	1/1	0.96	0.16	48,48,48,48	0
2	MG	D	301	1/1	0.97	0.06	37,37,37,37	0
2	MG	B	301	1/1	0.99	0.05	22,22,22,22	0
2	MG	F	301	1/1	0.99	0.04	24,24,24,24	0
2	MG	C	301	1/1	0.99	0.08	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.