Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 09:21 AM EDT

PDB ID	:	3ELP
Title	:	Structure of cystationine gamma lyase
Authors	:	Sun, Q.; Sivaraman, J.
Deposited on	:	2008-09-23
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 (i) 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 (1)) were used in the production of this report:

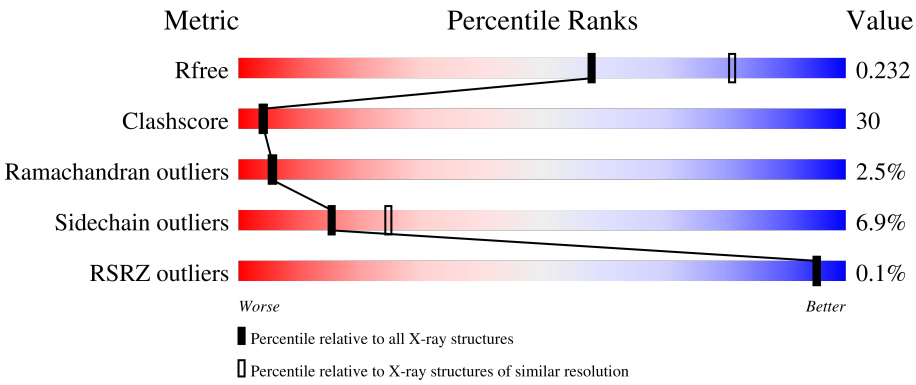
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	410	44% 34% 5% 16%
1	B	410	48% 31% • 16%
1	C	410	47% 33% • 16%
1	D	410	43% 35% 5% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11083 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 Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	343	2654	1697	451	487	19	0	0	0
1	A	343	2654	1697	451	487	19	0	0	0
1	C	343	2654	1697	451	487	19	0	0	0
1	D	343	2654	1697	451	487	19	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P32929
B	-3	SER	-	expression tag	UNP P32929
B	-2	PRO	-	expression tag	UNP P32929
B	-1	ASN	-	expression tag	UNP P32929
B	0	SER	-	expression tag	UNP P32929
A	-4	GLY	-	expression tag	UNP P32929
A	-3	SER	-	expression tag	UNP P32929
A	-2	PRO	-	expression tag	UNP P32929
A	-1	ASN	-	expression tag	UNP P32929
A	0	SER	-	expression tag	UNP P32929
C	-4	GLY	-	expression tag	UNP P32929
C	-3	SER	-	expression tag	UNP P32929
C	-2	PRO	-	expression tag	UNP P32929
C	-1	ASN	-	expression tag	UNP P32929
C	0	SER	-	expression tag	UNP P32929
D	-4	GLY	-	expression tag	UNP P32929
D	-3	SER	-	expression tag	UNP P32929
D	-2	PRO	-	expression tag	UNP P32929
D	-1	ASN	-	expression tag	UNP P32929
D	0	SER	-	expression tag	UNP P32929

- Molecule 2 is water.

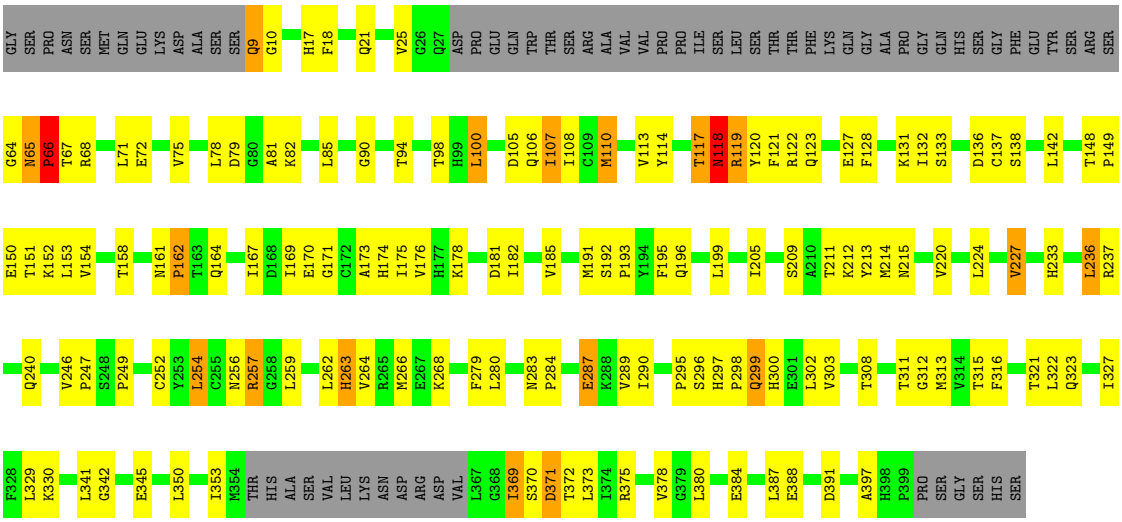
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	126	126	126	0	0
			Total	O		
2	A	120	120	120	0	0
			Total	O		
2	C	116	116	116	0	0
			Total	O		
2	D	105	105	105	0	0

3 Residue-property plots (i)

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.

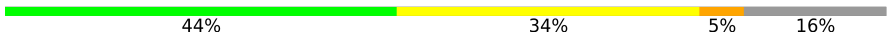
• Molecule 1: Cystathionine gamma-lyase

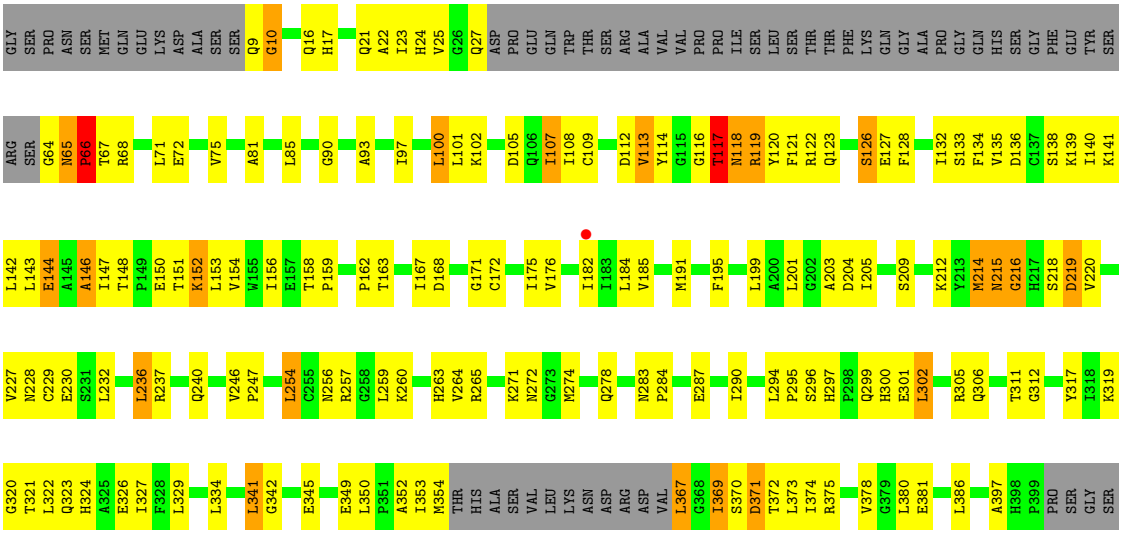
Chain B:



• Molecule 1: Cystathionine gamma-lyase

Chain A:

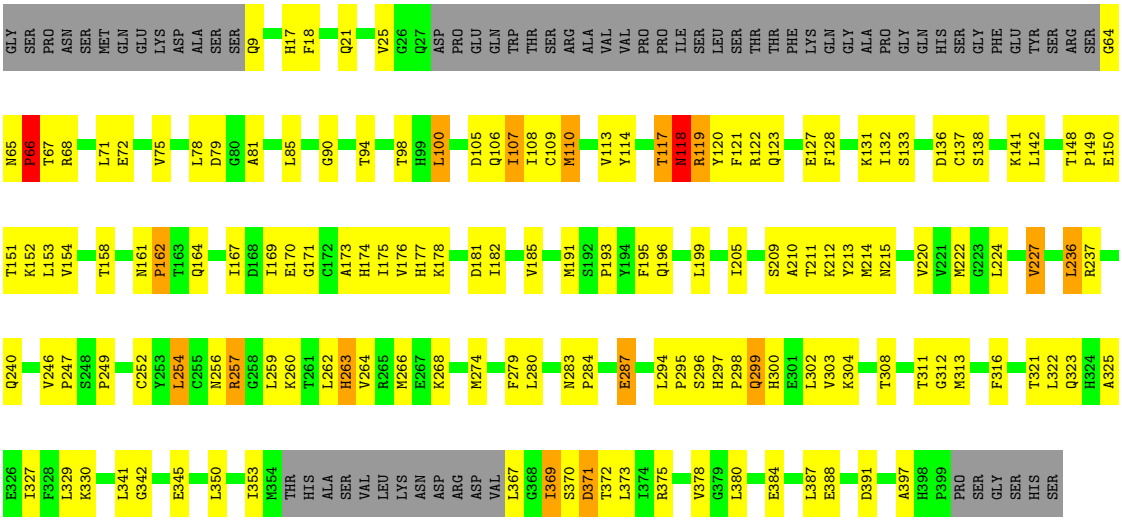




HIS
SER

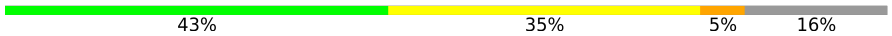
• Molecule 1: Cystathionine gamma-lyase

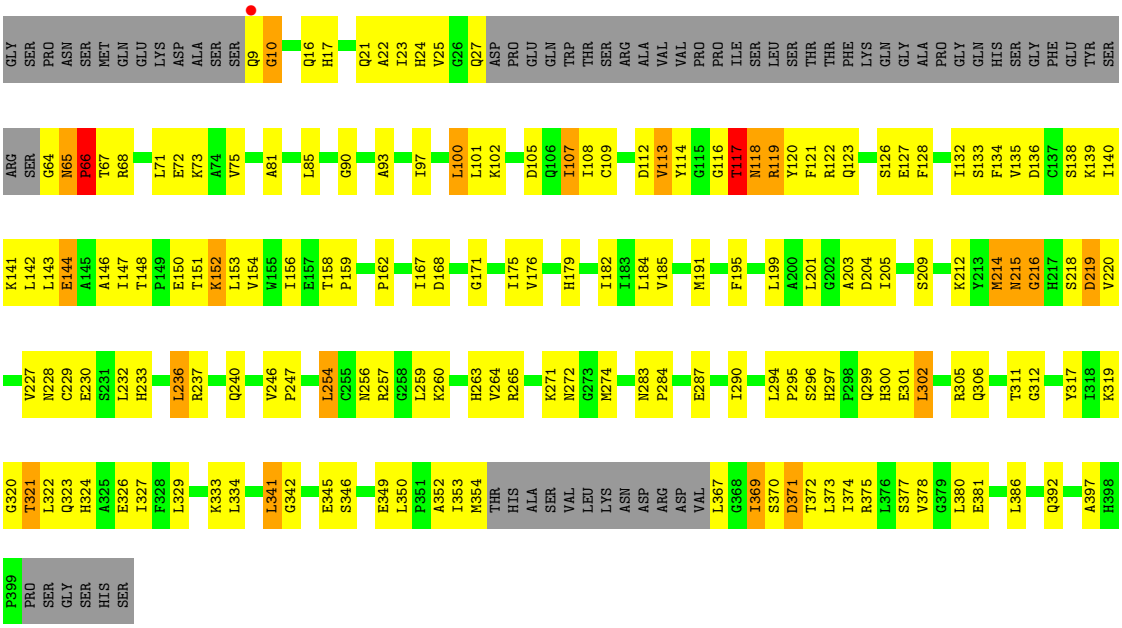
Chain C:



• Molecule 1: Cystathionine gamma-lyase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α, β, γ	121.30Å 121.30Å 125.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 49.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.40) 99.8 (49.80-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.236 0.224 , 0.232	Depositor DCC
R_{free} test set	3588 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.036 for -h,-l,-k 0.034 for -h,l,k 0.036 for l,-k,h 0.038 for -l,-k,-h 0.488 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11083	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.40	0/2710	0.67	3/3671 (0.1%)
1	B	0.39	1/2710 (0.0%)	0.67	2/3671 (0.1%)
1	C	0.37	0/2710	0.66	0/3671
1	D	0.39	0/2710	0.66	3/3671 (0.1%)
All	All	0.39	1/10840 (0.0%)	0.67	8/14684 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	GLN	CB-CG	-5.33	1.38	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	GLY	N-CA-C	11.27	141.28	113.10
1	D	10	GLY	N-CA-C	10.41	139.14	113.10
1	B	9	GLN	CB-CA-C	-7.35	95.70	110.40
1	B	9	GLN	CA-CB-CG	5.27	125.00	113.40
1	A	214	MET	N-CA-C	5.15	124.90	111.00
1	D	216	GLY	N-CA-C	-5.12	100.29	113.10
1	A	216	GLY	N-CA-C	-5.10	100.35	113.10
1	D	214	MET	N-CA-C	5.09	124.74	111.00

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	2654	0	2662	165	0
1	B	2654	0	2662	154	0
1	C	2654	0	2662	156	0
1	D	2654	0	2662	165	0
2	A	120	0	0	17	0
2	B	126	0	0	17	0
2	C	116	0	0	17	0
2	D	105	0	0	23	0
All	All	11083	0	10648	629	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 30.

All (629) 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:B:65:ASN:HB3	1:B:66:PRO:HD2	1.42	1.01
1:C:210:ALA:HB3	2:C:520:HOH:O	1.59	1.00
1:B:68:ARG:HH11	1:B:246:VAL:HG11	1.29	0.97
1:C:68:ARG:HH11	1:C:246:VAL:HG11	1.27	0.96
1:C:369:ILE:HD12	1:C:369:ILE:H	1.29	0.96
1:B:369:ILE:HD12	1:B:369:ILE:H	1.31	0.96
1:D:65:ASN:HB3	1:D:66:PRO:HD2	1.48	0.96
1:C:65:ASN:HB3	1:C:66:PRO:HD2	1.46	0.95
1:A:65:ASN:HB3	1:A:66:PRO:HD2	1.48	0.93
1:A:237:ARG:HG2	2:A:511:HOH:O	1.70	0.90
1:A:117:THR:O	1:A:118:ASN:HB2	1.72	0.89
1:D:369:ILE:H	1:D:369:ILE:HD12	1.39	0.88
1:B:148:THR:HG23	1:B:149:PRO:HD2	1.57	0.86
1:C:148:THR:HG23	1:C:149:PRO:HD2	1.57	0.85
1:D:117:THR:O	1:D:118:ASN:HB2	1.72	0.85
1:A:369:ILE:HD12	1:A:369:ILE:H	1.43	0.83
1:C:9:GLN:HG3	2:C:494:HOH:O	1.77	0.83
1:D:214:MET:HG2	2:D:472:HOH:O	1.79	0.83
1:A:120:TYR:O	1:A:121:PHE:HB2	1.78	0.82
1:B:65:ASN:HB3	1:B:66:PRO:CD	2.12	0.80
1:C:107:ILE:HG23	1:C:132:ILE:HG13	1.62	0.80
1:A:65:ASN:HB3	1:A:66:PRO:CD	2.11	0.80
1:A:85:LEU:HD13	1:A:236:LEU:HB3	1.64	0.80
1:A:97:ILE:O	1:A:100:LEU:HB2	1.81	0.80
1:D:85:LEU:HD13	1:D:236:LEU:HB3	1.63	0.79
1:D:120:TYR:O	1:D:121:PHE:HB2	1.78	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ARG:HH11	1:B:240:GLN:HE22	1.30	0.79
1:A:141:LYS:HE3	2:A:480:HOH:O	1.83	0.79
1:D:97:ILE:O	1:D:100:LEU:HB2	1.83	0.79
1:D:65:ASN:HB3	1:D:66:PRO:CD	2.11	0.79
1:D:214:MET:O	1:D:216:GLY:N	2.17	0.78
1:B:311:THR:HG22	1:B:312:GLY:N	1.98	0.78
1:A:214:MET:O	1:A:216:GLY:N	2.16	0.78
1:A:81:ALA:HB2	1:A:199:LEU:CD1	2.13	0.78
1:D:81:ALA:HB2	1:D:199:LEU:CD1	2.13	0.78
1:B:107:ILE:HG23	1:B:132:ILE:HG13	1.64	0.77
1:B:214:MET:HG3	1:B:215:ASN:H	1.48	0.77
1:A:114:TYR:CD2	1:A:369:ILE:HG13	2.19	0.77
1:A:278:GLN:HG2	2:A:469:HOH:O	1.84	0.77
1:D:120:TYR:HA	2:D:456:HOH:O	1.85	0.77
1:C:311:THR:HG22	1:C:312:GLY:N	2.00	0.76
1:D:114:TYR:CD2	1:D:369:ILE:HG13	2.20	0.76
1:A:214:MET:SD	1:A:342:GLY:O	2.43	0.76
1:A:85:LEU:CD1	1:A:236:LEU:HB3	2.15	0.76
1:B:9:GLN:HG2	2:B:517:HOH:O	1.85	0.75
1:B:214:MET:N	2:B:557:HOH:O	2.20	0.75
1:C:68:ARG:NH1	1:C:246:VAL:HG11	2.01	0.75
1:C:214:MET:HG3	1:C:215:ASN:H	1.50	0.75
1:C:220:VAL:HG21	1:C:254:LEU:HB3	1.68	0.75
1:B:220:VAL:HG21	1:B:254:LEU:HB3	1.67	0.75
1:C:90:GLY:HA3	1:C:209:SER:HB2	1.68	0.75
1:C:117:THR:O	1:C:118:ASN:HB2	1.87	0.75
1:B:311:THR:HG22	1:B:312:GLY:H	1.52	0.74
1:B:90:GLY:HA3	1:B:209:SER:HB2	1.67	0.74
1:C:65:ASN:HB3	1:C:66:PRO:CD	2.16	0.74
1:C:237:ARG:HH11	1:C:240:GLN:HE22	1.31	0.74
1:D:214:MET:SD	1:D:342:GLY:O	2.44	0.74
1:B:117:THR:O	1:B:118:ASN:HB2	1.86	0.74
1:A:214:MET:HG2	2:A:490:HOH:O	1.88	0.74
1:C:68:ARG:HH11	1:C:246:VAL:CG1	2.00	0.74
1:D:85:LEU:CD1	1:D:236:LEU:HB3	2.17	0.73
1:B:64:GLY:O	1:B:65:ASN:HB2	1.88	0.73
1:C:329:LEU:HD11	1:C:350:LEU:HB2	1.71	0.73
1:B:214:MET:HG3	1:B:215:ASN:N	2.03	0.73
1:A:122:ARG:HD3	1:A:134:PHE:HE2	1.54	0.73
1:B:68:ARG:HH11	1:B:246:VAL:CG1	2.02	0.72
1:C:311:THR:HG22	1:C:312:GLY:H	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ARG:HD3	1:D:134:PHE:HE2	1.54	0.72
1:C:119:ARG:O	1:C:123:GLN:HG3	1.89	0.72
1:B:81:ALA:HB2	1:B:199:LEU:CD1	2.20	0.71
1:B:68:ARG:NH1	1:B:246:VAL:HG11	2.03	0.71
1:B:119:ARG:O	1:B:123:GLN:HG3	1.90	0.71
1:A:214:MET:CE	1:A:265:ARG:HH11	2.03	0.71
1:C:81:ALA:HB2	1:C:199:LEU:CD1	2.20	0.71
1:B:329:LEU:HD11	1:B:350:LEU:HB2	1.72	0.71
1:C:17:HIS:O	1:C:21:GLN:HG3	1.89	0.71
1:C:151:THR:HG22	1:C:182:ILE:HD12	1.73	0.71
1:C:214:MET:HG3	1:C:215:ASN:N	2.06	0.71
1:D:237:ARG:NH1	1:D:240:GLN:HE22	1.89	0.70
1:D:369:ILE:HD12	1:D:369:ILE:N	2.06	0.70
1:B:151:THR:HG22	1:B:182:ILE:HD12	1.72	0.70
1:C:321:THR:HG22	1:C:322:LEU:N	2.07	0.70
1:D:141:LYS:HE3	2:D:468:HOH:O	1.91	0.70
1:B:237:ARG:NH1	1:B:240:GLN:HE22	1.90	0.69
1:D:214:MET:CE	1:D:265:ARG:HH11	2.04	0.69
1:B:322:LEU:HD13	1:B:371:ASP:HB3	1.75	0.69
1:B:321:THR:HG22	1:B:322:LEU:N	2.07	0.68
1:D:176:VAL:HG13	1:D:182:ILE:HD13	1.73	0.68
1:A:176:VAL:HG13	1:A:182:ILE:HD13	1.75	0.68
1:B:120:TYR:O	1:B:121:PHE:HB2	1.94	0.68
1:A:107:ILE:HD13	1:A:153:LEU:HD23	1.76	0.68
1:A:237:ARG:NH1	1:A:240:GLN:HE22	1.91	0.68
1:C:322:LEU:HD13	1:C:371:ASP:HB3	1.76	0.68
1:A:311:THR:HG22	1:A:312:GLY:H	1.58	0.67
1:C:120:TYR:O	1:C:121:PHE:HB2	1.94	0.67
1:D:204:ASP:O	1:D:227:VAL:HG23	1.95	0.67
1:B:110:MET:HE2	1:B:167:ILE:HD11	1.75	0.67
1:B:17:HIS:O	1:B:21:GLN:HG3	1.94	0.67
1:B:154:VAL:HG23	1:B:182:ILE:HD11	1.76	0.67
1:C:154:VAL:HG23	1:C:182:ILE:HD11	1.77	0.67
1:C:237:ARG:NH1	1:C:240:GLN:HE22	1.93	0.67
1:A:369:ILE:HD12	1:A:369:ILE:N	2.10	0.66
1:D:290:ILE:HD11	1:D:317:TYR:HE1	1.60	0.66
1:D:154:VAL:HG23	1:D:182:ILE:HD11	1.78	0.66
1:A:204:ASP:O	1:A:227:VAL:HG23	1.96	0.66
1:C:214:MET:SD	1:C:342:GLY:O	2.54	0.66
1:C:345:GLU:HG3	1:D:24:HIS:HE1	1.60	0.65
1:D:311:THR:HG22	1:D:312:GLY:H	1.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ILE:HG21	1:B:397:ALA:HA	1.78	0.65
1:A:151:THR:HG22	1:A:182:ILE:HD12	1.78	0.65
1:A:119:ARG:O	1:A:123:GLN:HG3	1.96	0.65
1:C:327:ILE:HG21	1:C:397:ALA:HA	1.78	0.65
1:A:290:ILE:HD11	1:A:317:TYR:HE1	1.61	0.65
1:D:107:ILE:HD13	1:D:153:LEU:HD23	1.77	0.65
1:D:151:THR:HG22	1:D:182:ILE:HD12	1.78	0.65
1:A:154:VAL:HG23	1:A:182:ILE:HD11	1.79	0.65
1:C:369:ILE:HD12	1:C:369:ILE:N	2.08	0.65
1:D:119:ARG:O	1:D:123:GLN:HG3	1.97	0.64
1:A:227:VAL:HG21	1:A:232:LEU:HD23	1.78	0.64
1:C:110:MET:CE	1:C:167:ILE:HD11	2.27	0.64
1:B:345:GLU:HG3	1:A:24:HIS:HE1	1.63	0.64
1:B:148:THR:HG22	1:B:150:GLU:H	1.63	0.64
1:B:369:ILE:HD12	1:B:369:ILE:N	2.09	0.64
1:A:214:MET:HG3	1:A:265:ARG:NH1	2.12	0.64
1:C:369:ILE:H	1:C:369:ILE:CD1	1.98	0.63
1:B:214:MET:SD	1:B:342:GLY:O	2.56	0.63
1:D:219:ASP:N	2:D:426:HOH:O	2.31	0.63
1:A:139:LYS:HB2	1:A:142:LEU:HD12	1.78	0.63
1:C:148:THR:HG22	1:C:150:GLU:H	1.63	0.63
1:A:143:LEU:O	1:A:147:ILE:HG12	1.99	0.63
1:A:148:THR:HG22	1:A:150:GLU:OE2	1.99	0.63
1:D:333:LYS:HE3	2:D:481:HOH:O	1.99	0.63
1:B:110:MET:CE	1:B:167:ILE:HD11	2.27	0.63
1:B:350:LEU:HD22	1:B:353:ILE:HG12	1.81	0.63
1:D:148:THR:HG22	1:D:150:GLU:OE2	1.99	0.63
1:B:9:GLN:HG3	2:B:504:HOH:O	2.00	0.62
1:B:214:MET:CG	1:B:215:ASN:H	2.12	0.62
1:D:227:VAL:HG21	1:D:232:LEU:HD23	1.79	0.62
1:B:350:LEU:CD2	1:B:353:ILE:HG12	2.28	0.62
1:A:71:LEU:O	1:A:75:VAL:HG23	2.00	0.62
1:A:373:LEU:C	1:A:373:LEU:HD23	2.19	0.62
1:D:350:LEU:HD23	1:D:353:ILE:HD11	1.81	0.62
1:A:68:ARG:HH21	1:A:237:ARG:NH2	1.97	0.62
1:D:139:LYS:HB2	1:D:142:LEU:HD12	1.80	0.62
1:D:214:MET:HG3	1:D:265:ARG:NH1	2.14	0.62
1:D:68:ARG:HH21	1:D:237:ARG:NH2	1.97	0.62
1:D:141:LYS:HB2	2:D:468:HOH:O	1.99	0.62
1:C:148:THR:HG23	1:C:149:PRO:CD	2.30	0.61
1:C:350:LEU:HD22	1:C:353:ILE:HG12	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:O	1:D:147:ILE:HG12	2.00	0.61
1:C:106:GLN:NE2	1:C:108:ILE:HD11	2.16	0.61
1:C:67:THR:HG22	1:C:252:CYS:HB2	1.83	0.61
1:D:152:LYS:HE2	2:D:435:HOH:O	1.99	0.61
1:B:311:THR:CG2	1:B:312:GLY:H	2.14	0.61
1:D:220:VAL:HG21	1:D:254:LEU:HB3	1.83	0.61
1:D:373:LEU:C	1:D:373:LEU:HD23	2.20	0.61
1:D:102:LYS:HG3	1:D:105:ASP:OD1	2.00	0.61
1:B:81:ALA:HB2	1:B:199:LEU:HD12	1.83	0.61
1:A:350:LEU:HD23	1:A:353:ILE:HD11	1.83	0.61
1:B:68:ARG:O	1:B:72:GLU:HG3	2.00	0.60
1:B:90:GLY:HA3	1:B:209:SER:CB	2.31	0.60
1:B:257:ARG:HH22	1:A:216:GLY:HA3	1.66	0.60
1:C:214:MET:CG	1:C:215:ASN:H	2.14	0.60
1:C:81:ALA:HB2	1:C:199:LEU:HD12	1.82	0.60
1:C:350:LEU:CD2	1:C:353:ILE:HG12	2.31	0.60
1:D:215:ASN:O	1:D:218:SER:HB2	2.01	0.60
1:A:102:LYS:HG3	1:A:105:ASP:OD1	2.01	0.60
1:D:73:LYS:HE2	2:D:507:HOH:O	2.01	0.60
1:A:220:VAL:HG21	1:A:254:LEU:HB3	1.83	0.60
1:C:90:GLY:HA3	1:C:209:SER:CB	2.31	0.60
1:C:110:MET:HE2	1:C:167:ILE:HD11	1.84	0.60
1:B:311:THR:HG21	2:B:497:HOH:O	2.00	0.60
1:C:176:VAL:HG13	1:C:182:ILE:HD13	1.84	0.60
1:B:106:GLN:NE2	1:B:108:ILE:HD11	2.17	0.59
1:C:68:ARG:O	1:C:72:GLU:HG3	2.01	0.59
1:B:311:THR:CG2	1:B:312:GLY:N	2.65	0.59
1:B:369:ILE:H	1:B:369:ILE:CD1	2.00	0.59
1:C:311:THR:CG2	1:C:312:GLY:H	2.15	0.59
1:D:71:LEU:O	1:D:75:VAL:HG23	2.02	0.59
1:B:67:THR:HG22	1:B:252:CYS:HB2	1.83	0.59
1:C:141:LYS:HE2	2:C:519:HOH:O	2.01	0.59
1:C:257:ARG:HH22	1:D:216:GLY:HA3	1.67	0.59
1:D:23:ILE:O	1:D:27:GLN:HG3	2.02	0.59
1:C:263:HIS:CD2	1:C:264:VAL:H	2.21	0.59
1:C:311:THR:CG2	1:C:312:GLY:N	2.66	0.59
1:D:301:GLU:O	1:D:305:ARG:HG2	2.03	0.59
1:B:263:HIS:CD2	1:B:264:VAL:H	2.20	0.58
1:B:176:VAL:HG13	1:B:182:ILE:HD13	1.85	0.58
1:A:64:GLY:HA3	1:A:68:ARG:CZ	2.33	0.58
1:B:257:ARG:NH2	1:A:216:GLY:HA3	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASN:O	1:A:218:SER:HB2	2.02	0.58
1:A:295:PRO:HA	1:A:300:HIS:CG	2.39	0.58
1:B:295:PRO:HA	1:B:300:HIS:CD2	2.39	0.58
1:C:295:PRO:HA	1:C:300:HIS:CD2	2.38	0.58
1:D:64:GLY:O	1:D:65:ASN:HB2	2.04	0.58
1:A:301:GLU:O	1:A:305:ARG:HG2	2.04	0.58
1:D:311:THR:HG22	2:D:457:HOH:O	2.04	0.58
1:B:148:THR:HG23	1:B:149:PRO:CD	2.30	0.57
1:C:257:ARG:NH2	1:D:216:GLY:HA3	2.19	0.57
1:A:263:HIS:HD2	2:A:477:HOH:O	1.85	0.57
1:D:214:MET:HE2	1:D:265:ARG:HH11	1.69	0.57
1:D:295:PRO:HA	1:D:300:HIS:CG	2.39	0.57
1:A:112:ASP:OD1	1:A:117:THR:HG23	2.04	0.57
1:D:112:ASP:OD1	1:D:117:THR:HG23	2.05	0.57
1:C:21:GLN:HA	1:C:25:VAL:HG23	1.85	0.57
1:A:185:VAL:HG22	1:A:205:ILE:HB	1.87	0.57
1:A:21:GLN:HA	1:A:25:VAL:HG23	1.87	0.56
1:D:334:LEU:HD12	1:D:386:LEU:HD23	1.87	0.56
1:C:246:VAL:HG13	1:C:247:PRO:HD2	1.86	0.56
1:B:21:GLN:HA	1:B:25:VAL:HG23	1.86	0.56
1:C:114:TYR:CD2	1:C:369:ILE:HG13	2.40	0.56
1:D:68:ARG:HD3	2:D:483:HOH:O	2.05	0.56
1:B:170:GLU:O	1:B:173:ALA:HB3	2.06	0.56
1:B:100:LEU:HD11	1:B:236:LEU:HD13	1.88	0.56
1:C:100:LEU:HD11	1:C:236:LEU:HD13	1.87	0.56
1:C:170:GLU:O	1:C:173:ALA:HB3	2.06	0.56
1:B:246:VAL:HG13	1:B:247:PRO:HD2	1.88	0.56
1:B:323:GLN:O	1:B:327:ILE:HG12	2.05	0.56
1:B:68:ARG:HD3	2:B:489:HOH:O	2.06	0.56
1:A:341:LEU:HD23	1:A:341:LEU:N	2.21	0.55
1:D:21:GLN:HA	1:D:25:VAL:HG23	1.88	0.55
1:A:16:GLN:HB3	1:A:17:HIS:ND1	2.21	0.55
1:C:323:GLN:O	1:C:327:ILE:HG12	2.05	0.55
1:B:212:LYS:HE2	2:B:449:HOH:O	2.07	0.55
1:D:329:LEU:HD11	1:D:350:LEU:HB2	1.88	0.55
1:A:219:ASP:N	2:A:439:HOH:O	2.38	0.55
1:D:263:HIS:HD2	2:D:459:HOH:O	1.89	0.55
1:B:79:ASP:OD1	1:B:193:PRO:HB3	2.06	0.55
1:B:94:THR:O	1:B:98:THR:HG23	2.06	0.55
1:A:214:MET:HE3	1:A:265:ARG:HH11	1.71	0.55
1:C:79:ASP:OD1	1:C:193:PRO:HB3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HG3	1:A:265:ARG:HH12	1.71	0.55
1:A:230:GLU:OE2	1:A:230:GLU:HA	2.07	0.55
1:C:171:GLY:O	1:C:175:ILE:HG12	2.06	0.55
1:D:64:GLY:HA3	1:D:68:ARG:CZ	2.36	0.55
1:B:114:TYR:CD2	1:B:369:ILE:HG13	2.42	0.55
1:B:158:THR:HG21	1:B:169:ILE:HD11	1.89	0.55
1:A:334:LEU:HD12	1:A:386:LEU:HD23	1.88	0.55
1:C:94:THR:O	1:C:98:THR:HG23	2.07	0.55
1:A:214:MET:HE2	1:A:265:ARG:HH11	1.72	0.54
1:A:287:GLU:HG2	1:A:319:LYS:HG2	1.89	0.54
1:D:327:ILE:HG21	1:D:397:ALA:HA	1.89	0.54
1:A:246:VAL:HG13	1:A:247:PRO:HD2	1.88	0.54
1:B:214:MET:CG	1:B:215:ASN:N	2.70	0.54
1:A:272:ASN:HB3	1:A:378:VAL:HG11	1.89	0.54
1:D:246:VAL:HG13	1:D:247:PRO:HD2	1.88	0.54
1:B:119:ARG:HD3	2:B:562:HOH:O	2.06	0.54
1:C:9:GLN:HB2	2:C:440:HOH:O	2.07	0.54
1:C:274:MET:HE1	1:C:294:LEU:HD23	1.89	0.54
1:D:16:GLN:HB3	1:D:17:HIS:ND1	2.22	0.54
1:C:321:THR:CG2	1:C:322:LEU:N	2.70	0.54
1:D:341:LEU:N	1:D:341:LEU:HD23	2.21	0.54
1:C:158:THR:HG21	1:C:169:ILE:HD11	1.89	0.54
1:D:17:HIS:O	1:D:21:GLN:HG3	2.08	0.54
1:D:272:ASN:HB3	1:D:378:VAL:HG11	1.89	0.54
1:A:327:ILE:HG21	1:A:397:ALA:HA	1.90	0.54
1:D:287:GLU:HG2	1:D:319:LYS:HG2	1.90	0.54
1:B:171:GLY:O	1:B:175:ILE:HG12	2.08	0.54
1:D:113:VAL:HG13	1:D:114:TYR:H	1.73	0.54
1:B:321:THR:CG2	1:B:322:LEU:N	2.71	0.53
1:A:329:LEU:HD11	1:A:350:LEU:HB2	1.89	0.53
1:C:246:VAL:HG13	1:C:247:PRO:CD	2.38	0.53
1:D:150:GLU:OE2	1:D:150:GLU:N	2.41	0.53
1:A:17:HIS:O	1:A:21:GLN:HG3	2.08	0.53
1:A:113:VAL:HG13	1:A:114:TYR:H	1.72	0.53
1:A:126:SER:HB2	2:A:508:HOH:O	2.08	0.53
1:A:271:LYS:NZ	1:A:271:LYS:HB3	2.23	0.53
1:C:297:HIS:CD2	1:C:299:GLN:H	2.26	0.53
1:B:164:GLN:HG2	1:B:313:MET:HE3	1.89	0.53
1:D:185:VAL:HG22	1:D:205:ILE:HB	1.90	0.53
1:A:150:GLU:OE2	1:A:150:GLU:N	2.41	0.53
1:C:105:ASP:OD1	1:C:152:LYS:HD2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:THR:HG22	1:D:182:ILE:CD1	2.38	0.53
1:D:272:ASN:HB3	1:D:378:VAL:CG1	2.39	0.53
1:B:105:ASP:OD1	1:B:152:LYS:HD2	2.08	0.53
1:B:297:HIS:CD2	1:B:299:GLN:H	2.27	0.53
1:A:23:ILE:O	1:A:27:GLN:HG3	2.07	0.53
1:A:109:CYS:HB2	1:A:134:PHE:HD1	1.73	0.53
1:D:109:CYS:HB2	1:D:134:PHE:HD1	1.73	0.53
1:B:280:LEU:HD13	1:B:316:PHE:CD2	2.45	0.52
1:A:272:ASN:HB3	1:A:378:VAL:CG1	2.40	0.52
1:C:164:GLN:HG2	1:C:313:MET:HE3	1.90	0.52
1:C:313:MET:HB2	2:C:481:HOH:O	2.08	0.52
1:D:297:HIS:CD2	1:D:299:GLN:H	2.28	0.52
1:B:71:LEU:HA	1:B:256:ASN:HD22	1.73	0.52
1:B:246:VAL:HG13	1:B:247:PRO:CD	2.39	0.52
1:B:296:SER:HA	1:C:296:SER:HA	1.91	0.52
1:A:151:THR:HG22	1:A:182:ILE:CD1	2.38	0.52
1:D:118:ASN:O	1:D:122:ARG:HB2	2.09	0.52
1:C:90:GLY:CA	1:C:209:SER:HB2	2.38	0.52
1:A:118:ASN:O	1:A:122:ARG:HB2	2.09	0.52
1:D:109:CYS:HB2	1:D:134:PHE:CD1	2.45	0.52
1:D:214:MET:HG3	1:D:265:ARG:HH12	1.74	0.52
1:D:373:LEU:HD23	1:D:374:ILE:N	2.25	0.52
1:B:246:VAL:CG1	1:B:247:PRO:CD	2.88	0.52
1:A:373:LEU:HD23	1:A:374:ILE:N	2.25	0.52
1:C:64:GLY:HA3	1:C:68:ARG:NH2	2.25	0.52
1:C:246:VAL:CG1	1:C:247:PRO:HD2	2.40	0.52
1:A:136:ASP:OD2	1:A:138:SER:HB3	2.09	0.52
1:C:18:PHE:CZ	1:C:78:LEU:HD13	2.45	0.52
1:D:295:PRO:HA	1:D:300:HIS:CD2	2.45	0.52
1:D:271:LYS:NZ	1:D:271:LYS:HB3	2.26	0.51
1:B:82:LYS:HD2	2:B:551:HOH:O	2.09	0.51
1:A:109:CYS:HB2	1:A:134:PHE:CD1	2.46	0.51
1:D:101:LEU:HD22	1:D:152:LYS:HB3	1.93	0.51
1:D:274:MET:CE	1:D:294:LEU:HD23	2.40	0.51
1:C:67:THR:HG21	1:C:249:PRO:O	2.10	0.51
1:D:140:ILE:HD12	1:D:140:ILE:H	1.76	0.51
1:A:64:GLY:O	1:A:65:ASN:HB2	2.10	0.51
1:C:71:LEU:HA	1:C:256:ASN:HD22	1.74	0.51
1:C:153:LEU:HD11	1:C:185:VAL:HG23	1.92	0.51
1:C:214:MET:CG	1:C:215:ASN:N	2.72	0.51
1:C:246:VAL:CG1	1:C:247:PRO:CD	2.88	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:HIS:CD2	1:A:299:GLN:H	2.29	0.51
1:C:215:ASN:O	1:D:257:ARG:NH2	2.43	0.51
1:B:246:VAL:CG1	1:B:247:PRO:HD2	2.41	0.51
1:A:107:ILE:HD13	1:A:153:LEU:CD2	2.41	0.51
1:A:163:THR:HB	2:A:425:HOH:O	2.10	0.51
1:A:295:PRO:HA	1:A:300:HIS:CD2	2.45	0.51
1:C:191:MET:HG3	1:C:196:GLN:NE2	2.26	0.51
1:D:230:GLU:OE2	1:D:230:GLU:HA	2.09	0.51
1:A:65:ASN:ND2	2:A:502:HOH:O	2.43	0.51
1:A:274:MET:CE	1:A:294:LEU:HD23	2.40	0.51
1:B:370:SER:HB2	1:B:372:THR:HG22	1.93	0.51
1:C:373:LEU:HD23	1:C:373:LEU:C	2.31	0.51
1:C:167:ILE:HD12	1:C:167:ILE:N	2.26	0.50
1:D:158:THR:HA	1:D:159:PRO:C	2.32	0.50
1:A:101:LEU:HD22	1:A:152:LYS:HB3	1.93	0.50
1:A:140:ILE:HD12	1:A:140:ILE:H	1.76	0.50
1:D:257:ARG:HG2	1:D:257:ARG:HH11	1.77	0.50
1:B:67:THR:HB	2:B:452:HOH:O	2.10	0.50
1:B:90:GLY:CA	1:B:209:SER:HB2	2.37	0.50
1:A:350:LEU:H	1:A:354:MET:CE	2.25	0.50
1:C:75:VAL:HG21	1:C:224:LEU:HD13	1.94	0.50
1:B:106:GLN:HG2	1:B:107:ILE:N	2.27	0.50
1:B:153:LEU:HD11	1:B:185:VAL:HG23	1.92	0.50
1:D:375:ARG:NH1	2:D:458:HOH:O	2.44	0.50
1:B:341:LEU:N	1:B:341:LEU:HD23	2.27	0.50
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.76	0.50
1:C:341:LEU:HD23	1:C:341:LEU:N	2.27	0.50
1:C:106:GLN:HG2	1:C:107:ILE:N	2.26	0.50
1:B:167:ILE:N	1:B:167:ILE:HD12	2.26	0.49
1:A:158:THR:HA	1:A:159:PRO:C	2.31	0.49
1:C:65:ASN:CB	1:C:66:PRO:CD	2.85	0.49
1:C:174:HIS:O	1:C:178:LYS:HB2	2.12	0.49
1:C:222:MET:HB3	2:C:520:HOH:O	2.12	0.49
1:D:23:ILE:HA	1:D:260:LYS:HD3	1.92	0.49
1:D:136:ASP:OD2	1:D:138:SER:HB3	2.12	0.49
1:A:135:VAL:HG21	1:A:146:ALA:CB	2.43	0.49
1:C:280:LEU:HD13	1:C:316:PHE:CD2	2.46	0.49
1:A:263:HIS:CE1	1:A:264:VAL:HG13	2.47	0.49
1:D:127:GLU:O	1:D:128:PHE:HB2	2.12	0.49
1:D:237:ARG:CZ	1:D:240:GLN:HE22	2.25	0.49
1:A:237:ARG:CZ	1:A:240:GLN:HE22	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ILE:HA	1:D:260:LYS:CD	2.43	0.49
1:A:23:ILE:HA	1:A:260:LYS:HD3	1.94	0.49
1:A:349:GLU:HG2	1:A:350:LEU:N	2.28	0.49
1:C:370:SER:HB2	1:C:372:THR:HG22	1.95	0.49
1:B:67:THR:HG21	1:B:249:PRO:O	2.12	0.49
1:B:215:ASN:O	1:A:257:ARG:NH2	2.46	0.49
1:A:246:VAL:HG13	1:A:247:PRO:CD	2.43	0.49
1:A:369:ILE:H	1:A:369:ILE:CD1	2.08	0.49
1:C:304:LYS:HD3	2:C:480:HOH:O	2.13	0.49
1:D:323:GLN:O	1:D:327:ILE:HG12	2.13	0.49
1:B:85:LEU:HD12	1:B:85:LEU:N	2.28	0.49
1:B:119:ARG:HG3	1:B:120:TYR:N	2.28	0.49
1:B:321:THR:HG22	1:B:322:LEU:H	1.76	0.49
1:A:171:GLY:O	1:A:175:ILE:HG12	2.12	0.49
1:D:327:ILE:CG2	1:D:397:ALA:HA	2.43	0.49
1:B:373:LEU:C	1:B:373:LEU:HD23	2.32	0.49
1:A:23:ILE:HA	1:A:260:LYS:CD	2.43	0.49
1:C:262:LEU:O	1:C:266:MET:HG2	2.13	0.49
1:D:107:ILE:HD13	1:D:153:LEU:CD2	2.42	0.49
1:B:64:GLY:O	1:B:65:ASN:CB	2.59	0.48
1:B:191:MET:HG3	1:B:196:GLN:NE2	2.26	0.48
1:B:330:LYS:NZ	2:B:491:HOH:O	2.45	0.48
1:C:108:ILE:HD13	1:C:133:SER:HB3	1.94	0.48
1:C:298:PRO:HG2	1:C:299:GLN:NE2	2.28	0.48
1:D:212:LYS:HB2	1:D:219:ASP:HA	1.95	0.48
1:D:271:LYS:NZ	2:D:482:HOH:O	2.46	0.48
1:A:81:ALA:HB2	1:A:199:LEU:HD11	1.94	0.48
1:B:75:VAL:HG21	1:B:224:LEU:HD13	1.94	0.48
1:A:327:ILE:CG2	1:A:397:ALA:HA	2.43	0.48
1:A:370:SER:C	1:A:372:THR:H	2.17	0.48
1:C:108:ILE:HB	1:C:154:VAL:HG22	1.95	0.48
1:D:140:ILE:HD12	1:D:140:ILE:N	2.29	0.48
1:D:214:MET:CE	1:D:265:ARG:HD2	2.43	0.48
1:D:135:VAL:HG21	1:D:146:ALA:CB	2.43	0.48
1:D:350:LEU:H	1:D:354:MET:CE	2.26	0.48
1:B:341:LEU:HB3	1:B:375:ARG:HH12	1.78	0.48
1:C:119:ARG:HG3	1:C:120:TYR:N	2.29	0.48
1:B:174:HIS:O	1:B:178:LYS:HB2	2.13	0.48
1:A:323:GLN:O	1:A:327:ILE:HG12	2.14	0.48
1:D:122:ARG:HD3	1:D:134:PHE:CE2	2.42	0.48
1:B:120:TYR:O	1:B:122:ARG:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ILE:CG2	1:B:397:ALA:HA	2.44	0.48
1:B:18:PHE:CZ	1:B:78:LEU:HD13	2.49	0.48
1:B:108:ILE:HD13	1:B:133:SER:HB3	1.95	0.48
1:B:108:ILE:HB	1:B:154:VAL:HG22	1.96	0.48
1:D:153:LEU:HD11	1:D:185:VAL:HG23	1.95	0.48
1:D:263:HIS:CE1	1:D:264:VAL:HG13	2.49	0.48
1:D:350:LEU:HB3	1:D:354:MET:HE3	1.96	0.48
1:C:64:GLY:O	1:C:65:ASN:HB2	2.13	0.48
1:D:171:GLY:O	1:D:175:ILE:HG12	2.12	0.48
1:B:214:MET:HE2	1:B:215:ASN:H	1.79	0.47
1:C:110:MET:HE1	1:C:167:ILE:HD11	1.96	0.47
1:D:349:GLU:HG2	1:D:350:LEU:N	2.29	0.47
1:B:65:ASN:CB	1:B:66:PRO:CD	2.82	0.47
1:A:107:ILE:O	1:A:132:ILE:HD12	2.14	0.47
1:A:144:GLU:HG2	1:A:175:ILE:HG23	1.96	0.47
1:C:136:ASP:O	1:C:138:SER:N	2.47	0.47
1:D:144:GLU:HG2	1:D:175:ILE:HG23	1.96	0.47
1:D:153:LEU:HD11	1:D:185:VAL:CG2	2.43	0.47
1:D:246:VAL:HG13	1:D:247:PRO:CD	2.43	0.47
1:B:195:PHE:HA	1:B:308:THR:OG1	2.14	0.47
1:B:298:PRO:HG2	1:B:299:GLN:NE2	2.29	0.47
1:C:341:LEU:HB3	1:C:375:ARG:HH12	1.79	0.47
1:B:237:ARG:HD2	1:B:240:GLN:NE2	2.30	0.47
1:C:85:LEU:N	1:C:85:LEU:HD12	2.29	0.47
1:D:214:MET:HE3	1:D:265:ARG:HH11	1.75	0.47
1:B:313:MET:HB2	2:B:556:HOH:O	2.13	0.47
1:A:120:TYR:O	1:A:121:PHE:CB	2.52	0.47
1:A:81:ALA:HB2	1:A:199:LEU:HD12	1.95	0.47
1:A:367:LEU:N	2:A:427:HOH:O	2.47	0.47
1:C:117:THR:O	1:C:118:ASN:CB	2.61	0.47
1:C:268:LYS:HB3	1:C:380:LEU:HD22	1.97	0.47
1:D:64:GLY:HA2	2:D:483:HOH:O	2.15	0.47
1:A:122:ARG:HD3	1:A:134:PHE:CE2	2.42	0.47
1:C:106:GLN:HA	1:C:131:LYS:O	2.15	0.47
1:B:106:GLN:HA	1:B:131:LYS:O	2.15	0.47
1:A:140:ILE:HD12	1:A:140:ILE:N	2.29	0.47
1:A:214:MET:CE	1:A:265:ARG:HD2	2.44	0.47
1:A:127:GLU:O	1:A:128:PHE:HB2	2.15	0.47
1:A:212:LYS:HB2	1:A:219:ASP:HA	1.95	0.47
1:C:119:ARG:HH11	1:C:119:ARG:HG2	1.79	0.47
1:C:327:ILE:CG2	1:C:397:ALA:HA	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HD3	2:A:485:HOH:O	2.15	0.46
1:B:263:HIS:HE1	1:A:380:LEU:O	1.97	0.46
1:C:127:GLU:O	1:C:128:PHE:HB2	2.15	0.46
1:C:174:HIS:HB3	2:C:493:HOH:O	2.14	0.46
1:D:349:GLU:HA	2:D:499:HOH:O	2.13	0.46
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.79	0.46
1:A:152:LYS:HE2	2:A:451:HOH:O	2.15	0.46
1:C:321:THR:HG22	1:C:322:LEU:H	1.78	0.46
1:D:370:SER:C	1:D:372:THR:H	2.17	0.46
1:C:195:PHE:HA	1:C:308:THR:OG1	2.15	0.46
1:B:279:PHE:CZ	1:B:391:ASP:HB2	2.51	0.46
1:C:237:ARG:HD2	1:C:240:GLN:NE2	2.31	0.46
1:C:279:PHE:CZ	1:C:391:ASP:HB2	2.50	0.46
1:C:312:GLY:O	1:C:378:VAL:HG23	2.16	0.46
1:D:283:ASN:HA	1:D:284:PRO:HD3	1.85	0.46
1:A:68:ARG:O	1:A:72:GLU:HG3	2.16	0.46
1:A:322:LEU:O	1:A:326:GLU:HG2	2.16	0.46
1:C:67:THR:HG22	1:C:252:CYS:CB	2.46	0.46
1:C:330:LYS:NZ	2:C:415:HOH:O	2.41	0.46
1:D:229:CYS:HB3	1:D:232:LEU:HB2	1.98	0.46
1:B:295:PRO:HA	1:B:300:HIS:CG	2.51	0.46
1:D:107:ILE:O	1:D:132:ILE:HD12	2.15	0.46
1:D:123:GLN:HB2	2:D:456:HOH:O	2.16	0.46
1:A:227:VAL:HG22	1:A:228:ASN:N	2.31	0.46
1:B:113:VAL:HG13	1:B:114:TYR:H	1.81	0.45
1:A:153:LEU:HD11	1:A:185:VAL:HG23	1.98	0.45
1:A:153:LEU:HD11	1:A:185:VAL:CG2	2.45	0.45
1:C:263:HIS:HE1	1:D:380:LEU:O	1.99	0.45
1:C:295:PRO:HA	1:C:300:HIS:CG	2.51	0.45
1:B:136:ASP:O	1:B:138:SER:N	2.49	0.45
1:A:90:GLY:HA3	1:A:209:SER:HB2	1.97	0.45
1:C:260:LYS:NZ	2:C:425:HOH:O	2.36	0.45
1:D:179:HIS:HA	2:D:477:HOH:O	2.17	0.45
1:B:127:GLU:O	1:B:128:PHE:HB2	2.15	0.45
1:B:268:LYS:HB3	1:B:380:LEU:HD22	1.97	0.45
1:A:375:ARG:NH1	2:A:494:HOH:O	2.49	0.45
1:C:113:VAL:HG13	1:C:114:TYR:H	1.81	0.45
1:D:322:LEU:O	1:D:326:GLU:HG2	2.16	0.45
1:B:85:LEU:HD22	1:B:236:LEU:HB3	1.99	0.45
1:A:107:ILE:HD13	1:A:153:LEU:CG	2.46	0.45
1:C:85:LEU:HD22	1:C:236:LEU:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:HIS:HB3	2:B:483:HOH:O	2.17	0.45
1:D:81:ALA:HB2	1:D:199:LEU:HD11	1.95	0.45
1:D:81:ALA:HB2	1:D:199:LEU:HD12	1.94	0.45
1:B:262:LEU:O	1:B:266:MET:HG2	2.16	0.45
1:A:229:CYS:HB3	1:A:232:LEU:HB2	1.99	0.45
1:C:119:ARG:C	1:C:120:TYR:O	2.53	0.45
1:B:120:TYR:HA	2:B:520:HOH:O	2.17	0.45
1:D:232:LEU:HD12	1:D:232:LEU:HA	1.83	0.45
1:A:311:THR:HG22	2:A:479:HOH:O	2.16	0.45
1:A:101:LEU:CD2	1:A:152:LYS:HB3	2.47	0.45
1:A:113:VAL:HG22	1:A:114:TYR:N	2.32	0.45
1:C:283:ASN:HA	1:C:284:PRO:HD3	1.81	0.45
1:D:352:ALA:HB2	1:D:371:ASP:HA	1.99	0.45
1:C:279:PHE:HZ	1:C:391:ASP:HB2	1.81	0.44
1:B:298:PRO:HB2	1:B:299:GLN:HE21	1.83	0.44
1:B:312:GLY:O	1:B:378:VAL:HG23	2.17	0.44
1:C:177:HIS:HD2	2:C:509:HOH:O	2.00	0.44
1:D:227:VAL:HG22	1:D:228:ASN:N	2.33	0.44
1:B:174:HIS:HE1	2:B:567:HOH:O	2.01	0.44
1:A:116:GLY:O	1:A:117:THR:O	2.35	0.44
1:A:352:ALA:HB2	1:A:371:ASP:HA	1.99	0.44
1:C:64:GLY:HA3	1:C:68:ARG:CZ	2.48	0.44
1:D:101:LEU:CD2	1:D:152:LYS:HB3	2.48	0.44
1:D:113:VAL:HG22	1:D:114:TYR:N	2.33	0.44
1:D:139:LYS:HB3	2:D:468:HOH:O	2.17	0.44
1:A:22:ALA:O	1:A:260:LYS:HD3	2.18	0.44
1:A:201:LEU:CD1	1:A:306:GLN:HG3	2.47	0.44
1:B:233:HIS:HD2	2:B:532:HOH:O	1.99	0.44
1:A:184:LEU:HD23	1:A:203:ALA:HA	2.00	0.44
1:D:320:GLY:HA3	1:D:324:HIS:ND1	2.33	0.44
1:C:298:PRO:HB2	1:C:299:GLN:HE21	1.83	0.44
1:C:321:THR:CG2	1:C:322:LEU:H	2.31	0.44
1:A:140:ILE:H	1:A:140:ILE:CD1	2.30	0.44
1:D:201:LEU:CD1	1:D:306:GLN:HG3	2.47	0.44
1:B:67:THR:HG22	1:B:252:CYS:CB	2.47	0.44
1:B:205:ILE:HG12	1:B:227:VAL:CG2	2.48	0.44
1:D:140:ILE:H	1:D:140:ILE:CD1	2.30	0.44
1:D:168:ASP:OD1	1:D:171:GLY:N	2.43	0.44
1:D:184:LEU:HD23	1:D:203:ALA:HA	1.98	0.44
1:B:174:HIS:CE1	2:B:567:HOH:O	2.70	0.43
1:D:68:ARG:O	1:D:72:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:C	1:B:120:TYR:O	2.54	0.43
1:B:279:PHE:HZ	1:B:391:ASP:HB2	1.82	0.43
1:A:191:MET:HE3	1:A:195:PHE:HB3	1.99	0.43
1:A:218:SER:O	1:A:220:VAL:N	2.47	0.43
1:C:67:THR:HB	2:C:407:HOH:O	2.18	0.43
1:C:214:MET:HE2	1:C:215:ASN:H	1.84	0.43
1:D:107:ILE:HD13	1:D:153:LEU:CG	2.47	0.43
1:A:345:GLU:HA	1:A:381:GLU:OE1	2.19	0.43
1:C:161:ASN:HA	1:C:162:PRO:HA	1.78	0.43
1:C:384:GLU:O	1:C:388:GLU:HG3	2.18	0.43
1:D:22:ALA:O	1:D:260:LYS:HD3	2.18	0.43
1:B:341:LEU:HD23	1:B:341:LEU:H	1.84	0.43
1:D:296:SER:HB3	2:D:487:HOH:O	2.17	0.43
1:D:317:TYR:HD2	1:D:372:THR:HG23	1.83	0.43
1:B:72:GLU:OE2	1:B:85:LEU:HA	2.18	0.43
1:B:345:GLU:HB3	2:B:457:HOH:O	2.17	0.43
1:A:90:GLY:O	1:A:93:ALA:HB3	2.18	0.43
1:B:350:LEU:HD23	1:B:353:ILE:HG12	2.01	0.43
1:D:90:GLY:O	1:D:93:ALA:HB3	2.18	0.43
1:C:120:TYR:O	1:C:122:ARG:N	2.45	0.43
1:A:317:TYR:HD2	1:A:372:THR:HG23	1.83	0.43
1:A:320:GLY:HA3	1:A:324:HIS:ND1	2.32	0.43
1:D:114:TYR:HD2	1:D:369:ILE:HG13	1.81	0.43
1:C:341:LEU:HD23	1:C:341:LEU:H	1.84	0.43
1:D:108:ILE:HA	1:D:133:SER:O	2.18	0.43
1:A:64:GLY:HA2	2:A:485:HOH:O	2.19	0.43
1:C:72:GLU:OE2	1:C:85:LEU:HA	2.19	0.43
1:C:185:VAL:HG22	1:C:205:ILE:HB	2.01	0.43
1:D:201:LEU:HD11	1:D:306:GLN:HG3	2.01	0.43
1:D:345:GLU:HA	1:D:381:GLU:OE1	2.18	0.43
1:A:296:SER:HB3	2:A:443:HOH:O	2.19	0.42
1:D:90:GLY:HA3	1:D:209:SER:HB2	2.00	0.42
1:D:120:TYR:O	1:D:121:PHE:CB	2.52	0.42
1:D:233:HIS:HE1	2:D:475:HOH:O	2.02	0.42
1:B:71:LEU:HD22	1:B:252:CYS:HA	2.01	0.42
1:A:191:MET:HE3	1:A:195:PHE:CB	2.49	0.42
1:C:109:CYS:HB3	2:C:497:HOH:O	2.18	0.42
1:A:108:ILE:HA	1:A:133:SER:O	2.19	0.42
1:A:156:ILE:CD1	1:A:167:ILE:HG21	2.49	0.42
1:D:116:GLY:O	1:D:117:THR:O	2.37	0.42
1:B:321:THR:CG2	1:B:322:LEU:H	2.30	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:HG2	1:A:175:ILE:CG2	2.49	0.42
1:A:172:CYS:O	1:A:176:VAL:HG23	2.20	0.42
1:C:212:LYS:HE2	2:C:467:HOH:O	2.20	0.42
1:D:176:VAL:HG12	1:D:182:ILE:HG23	2.00	0.42
1:C:68:ARG:HD3	2:C:489:HOH:O	2.18	0.42
1:C:263:HIS:CD2	1:C:264:VAL:N	2.87	0.42
1:A:302:LEU:HD23	1:A:302:LEU:O	2.20	0.42
1:D:148:THR:HG22	1:D:150:GLU:H	1.84	0.42
1:C:18:PHE:HA	2:C:443:HOH:O	2.19	0.42
1:D:144:GLU:HG2	1:D:175:ILE:CG2	2.50	0.42
1:D:311:THR:HG22	1:D:312:GLY:N	2.30	0.42
1:B:263:HIS:CD2	1:B:264:VAL:N	2.87	0.42
1:B:371:ASP:OD1	1:B:371:ASP:N	2.52	0.42
1:A:148:THR:HG22	1:A:150:GLU:H	1.85	0.42
1:A:168:ASP:OD1	1:A:171:GLY:N	2.41	0.42
1:A:201:LEU:HD11	1:A:306:GLN:HG3	2.00	0.42
1:A:350:LEU:HD12	1:A:373:LEU:O	2.20	0.42
1:D:350:LEU:HD12	1:D:373:LEU:O	2.19	0.42
1:B:148:THR:CG2	1:B:150:GLU:OE2	2.68	0.42
1:B:211:THR:C	1:B:213:TYR:H	2.23	0.42
1:D:156:ILE:CD1	1:D:167:ILE:HG21	2.49	0.42
1:D:392:GLN:NE2	2:D:481:HOH:O	2.52	0.42
1:B:283:ASN:HA	1:B:284:PRO:HD3	1.81	0.42
1:B:384:GLU:O	1:B:388:GLU:HG3	2.19	0.42
1:A:283:ASN:HA	1:A:284:PRO:HD3	1.86	0.42
1:C:148:THR:CG2	1:C:150:GLU:OE2	2.68	0.42
1:C:211:THR:C	1:C:213:TYR:H	2.23	0.42
1:B:191:MET:HE3	1:B:195:PHE:HB3	2.01	0.41
1:C:297:HIS:HD2	1:C:299:GLN:H	1.66	0.41
1:D:191:MET:HE3	1:D:195:PHE:CB	2.50	0.41
1:B:153:LEU:HD11	1:B:185:VAL:CG2	2.50	0.41
1:C:174:HIS:HE1	2:C:502:HOH:O	2.02	0.41
1:D:218:SER:O	1:D:220:VAL:N	2.47	0.41
1:D:321:THR:HG22	2:D:443:HOH:O	2.19	0.41
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.94	0.41
1:C:191:MET:HE3	1:C:195:PHE:HB3	2.01	0.41
1:C:153:LEU:HD11	1:C:185:VAL:CG2	2.51	0.41
1:D:284:PRO:O	1:D:319:LYS:HD2	2.19	0.41
1:A:127:GLU:HG2	1:A:128:PHE:CD2	2.56	0.41
1:B:148:THR:CG2	1:B:149:PRO:N	2.84	0.41
1:A:176:VAL:HG12	1:A:182:ILE:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ILE:HB	1:B:315:THR:HB	2.03	0.41
1:B:297:HIS:HD2	1:B:299:GLN:H	1.67	0.41
1:A:114:TYR:HD2	1:A:369:ILE:HG13	1.81	0.41
1:A:311:THR:HG22	1:A:312:GLY:N	2.28	0.41
1:C:205:ILE:HG12	1:C:227:VAL:CG2	2.50	0.41
1:D:346:SER:HA	1:D:377:SER:O	2.19	0.41
1:B:117:THR:O	1:B:118:ASN:CB	2.61	0.41
1:B:185:VAL:HG22	1:B:205:ILE:HB	2.02	0.41
1:B:289:VAL:O	1:B:290:ILE:HD13	2.20	0.41
1:A:16:GLN:HB3	1:A:17:HIS:CE1	2.56	0.41
1:A:156:ILE:HD13	1:A:167:ILE:HG21	2.03	0.41
1:C:148:THR:CG2	1:C:149:PRO:N	2.84	0.41
1:C:287:GLU:OE2	1:C:287:GLU:HA	2.21	0.41
1:B:287:GLU:OE2	1:B:287:GLU:HA	2.21	0.41
1:A:85:LEU:HD11	1:A:236:LEU:HB3	2.00	0.41
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.84	0.41
1:A:284:PRO:O	1:A:319:LYS:HD2	2.21	0.41
1:D:156:ILE:HD13	1:D:167:ILE:HG21	2.03	0.41
1:B:161:ASN:HA	1:B:162:PRO:HA	1.78	0.40
1:D:302:LEU:HD23	1:D:302:LEU:O	2.21	0.40
1:A:232:LEU:O	1:A:236:LEU:HB2	2.22	0.40
1:A:341:LEU:N	1:A:341:LEU:CD2	2.83	0.40
1:C:148:THR:CG2	1:C:149:PRO:CD	2.99	0.40
1:C:313:MET:SD	1:C:375:ARG:HD2	2.62	0.40
1:D:367:LEU:N	2:D:486:HOH:O	2.55	0.40
1:A:148:THR:C	2:A:523:HOH:O	2.60	0.40
1:C:71:LEU:HD22	1:C:252:CYS:HA	2.03	0.40
1:C:325:ALA:HB1	1:C:350:LEU:CD1	2.51	0.40
1:D:341:LEU:N	1:D:341:LEU:CD2	2.84	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	337/410 (82%)	301 (89%)	25 (7%)	11 (3%)	4 3
1	B	337/410 (82%)	307 (91%)	22 (6%)	8 (2%)	6 6
1	C	337/410 (82%)	305 (90%)	27 (8%)	5 (2%)	10 14
1	D	337/410 (82%)	301 (89%)	26 (8%)	10 (3%)	4 3
All	All	1348/1640 (82%)	1214 (90%)	100 (7%)	34 (2%)	5 6

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	PRO
1	B	118	ASN
1	A	10	GLY
1	A	117	THR
1	A	118	ASN
1	C	66	PRO
1	C	118	ASN
1	D	10	GLY
1	D	117	THR
1	D	118	ASN
1	B	65	ASN
1	B	117	THR
1	B	137	CYS
1	A	219	ASP
1	C	117	THR
1	C	137	CYS
1	D	219	ASP
1	A	66	PRO
1	A	215	ASN
1	D	66	PRO
1	D	215	ASN
1	A	371	ASP
1	A	126	SER
1	A	146	ALA
1	D	126	SER
1	D	371	ASP
1	B	303	VAL
1	C	303	VAL
1	D	65	ASN
1	A	65	ASN
1	A	113	VAL
1	B	10	GLY
1	D	113	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	192	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	290/348 (83%)	271 (93%)	19 (7%)	16 26
1	B	290/348 (83%)	269 (93%)	21 (7%)	14 23
1	C	290/348 (83%)	268 (92%)	22 (8%)	13 20
1	D	290/348 (83%)	272 (94%)	18 (6%)	18 29
All	All	1160/1392 (83%)	1080 (93%)	80 (7%)	15 25

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

Mol	Chain	Res	Type
1	B	66	PRO
1	B	100	LEU
1	B	107	ILE
1	B	110	MET
1	B	118	ASN
1	B	119	ARG
1	B	142	LEU
1	B	162	PRO
1	B	181	ASP
1	B	227	VAL
1	B	236	LEU
1	B	254	LEU
1	B	257	ARG
1	B	259	LEU
1	B	263	HIS
1	B	287	GLU
1	B	299	GLN
1	B	302	LEU
1	B	369	ILE
1	B	371	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	387	LEU
1	A	9	GLN
1	A	66	PRO
1	A	67	THR
1	A	100	LEU
1	A	107	ILE
1	A	117	THR
1	A	119	ARG
1	A	144	GLU
1	A	152	LYS
1	A	162	PRO
1	A	236	LEU
1	A	254	LEU
1	A	256	ASN
1	A	259	LEU
1	A	302	LEU
1	A	321	THR
1	A	341	LEU
1	A	367	LEU
1	A	369	ILE
1	C	66	PRO
1	C	100	LEU
1	C	107	ILE
1	C	110	MET
1	C	118	ASN
1	C	119	ARG
1	C	142	LEU
1	C	162	PRO
1	C	181	ASP
1	C	227	VAL
1	C	236	LEU
1	C	254	LEU
1	C	257	ARG
1	C	259	LEU
1	C	263	HIS
1	C	287	GLU
1	C	299	GLN
1	C	302	LEU
1	C	367	LEU
1	C	369	ILE
1	C	371	ASP
1	C	387	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	9	GLN
1	D	66	PRO
1	D	67	THR
1	D	100	LEU
1	D	107	ILE
1	D	117	THR
1	D	119	ARG
1	D	144	GLU
1	D	152	LYS
1	D	162	PRO
1	D	236	LEU
1	D	254	LEU
1	D	256	ASN
1	D	259	LEU
1	D	302	LEU
1	D	321	THR
1	D	341	LEU
1	D	369	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	14	HIS
1	B	17	HIS
1	B	69	ASN
1	B	99	HIS
1	B	106	GLN
1	B	118	ASN
1	B	196	GLN
1	B	233	HIS
1	B	240	GLN
1	B	256	ASN
1	B	263	HIS
1	B	297	HIS
1	B	323	GLN
1	B	331	ASN
1	B	398	HIS
1	A	14	HIS
1	A	118	ASN
1	A	240	GLN
1	A	256	ASN
1	A	263	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	278	GLN
1	A	297	HIS
1	A	323	GLN
1	A	398	HIS
1	C	14	HIS
1	C	17	HIS
1	C	69	ASN
1	C	99	HIS
1	C	106	GLN
1	C	118	ASN
1	C	196	GLN
1	C	240	GLN
1	C	263	HIS
1	C	297	HIS
1	C	323	GLN
1	C	331	ASN
1	C	398	HIS
1	D	14	HIS
1	D	118	ASN
1	D	240	GLN
1	D	256	ASN
1	D	263	HIS
1	D	278	GLN
1	D	297	HIS
1	D	323	GLN
1	D	398	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	343/410 (83%)	-0.29	1 (0%)	94	93	29, 49, 78, 105	0
1	B	343/410 (83%)	-0.36	0	100	100	26, 43, 72, 94	0
1	C	343/410 (83%)	-0.37	0	100	100	27, 43, 73, 95	0
1	D	343/410 (83%)	-0.33	1 (0%)	94	93	28, 49, 78, 106	0
All	All	1372/1640 (83%)	-0.33	2 (0%)	95	95	26, 46, 77, 106	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ILE	2.4
1	D	9	GLN	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.