



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 09:07 pm GMT

PDB ID : 2YFH
Title : Structure of a Chimeric Glutamate Dehydrogenase
Authors : Oliveira, T.; Panjekar, S.; Sharkey, M.A.; Carrigan, J.B.; Hamza, M.; Engel, P.C.; Khan, A.R.
Deposited on : 2011-04-05
Resolution : 2.69 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 : 4.02b-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

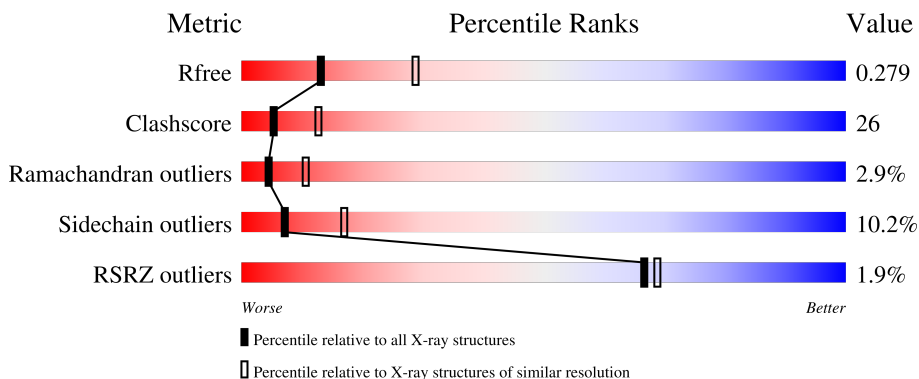
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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.



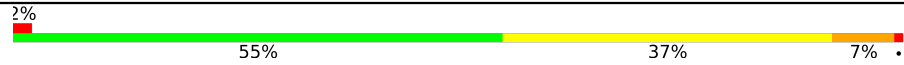
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	448	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the far left labeled '2%', a large green segment labeled '55%', a large yellow segment labeled '37%', and a small red segment at the far right labeled '7%'. A small black dot is located at the end of the bar.</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20640 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 GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3371	2135	577	641	18			
1	B	447	Total	C	N	O	S	0	0	0
			3395	2149	584	645	17			
1	C	447	Total	C	N	O	S	0	0	0
			3395	2149	584	645	17			
1	D	444	Total	C	N	O	S	0	0	0
			3370	2136	578	639	17			
1	E	448	Total	C	N	O	S	0	0	0
			3403	2154	585	646	18			
1	F	447	Total	C	N	O	S	0	0	0
			3393	2148	583	645	17			

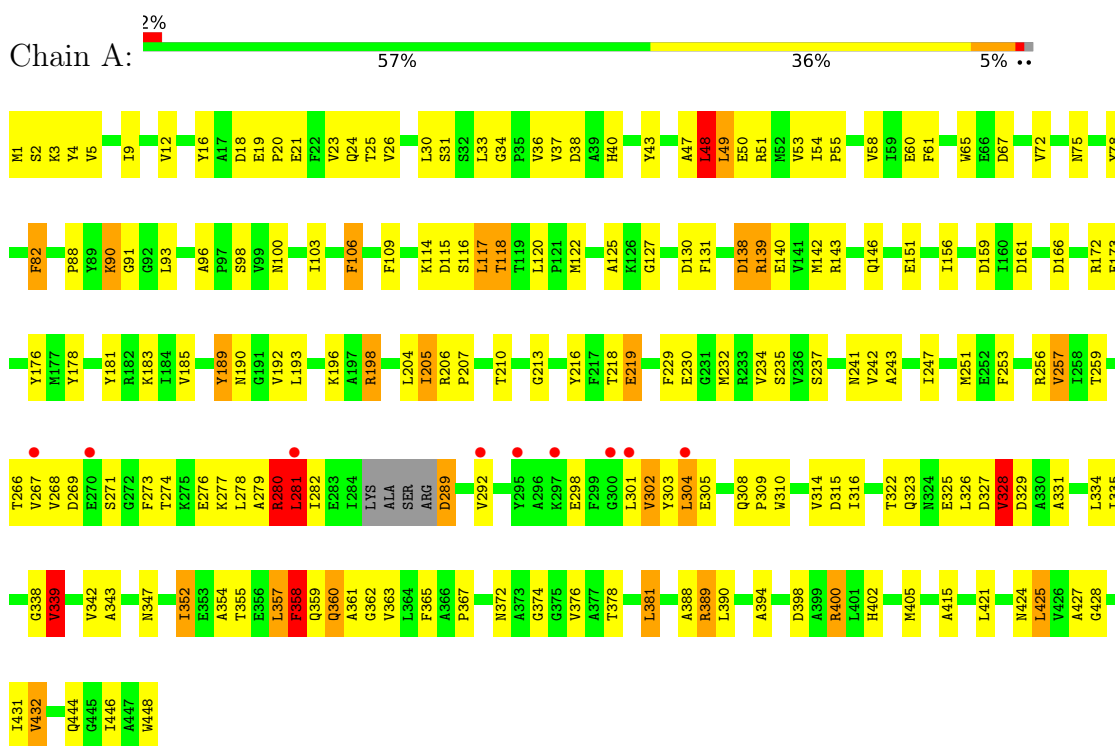
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	55	Total	O	0	0
			55	55		
2	C	61	Total	O	0	0
			61	61		
2	D	60	Total	O	0	0
			60	60		
2	E	46	Total	O	0	0
			46	46		
2	F	46	Total	O	0	0
			46	46		

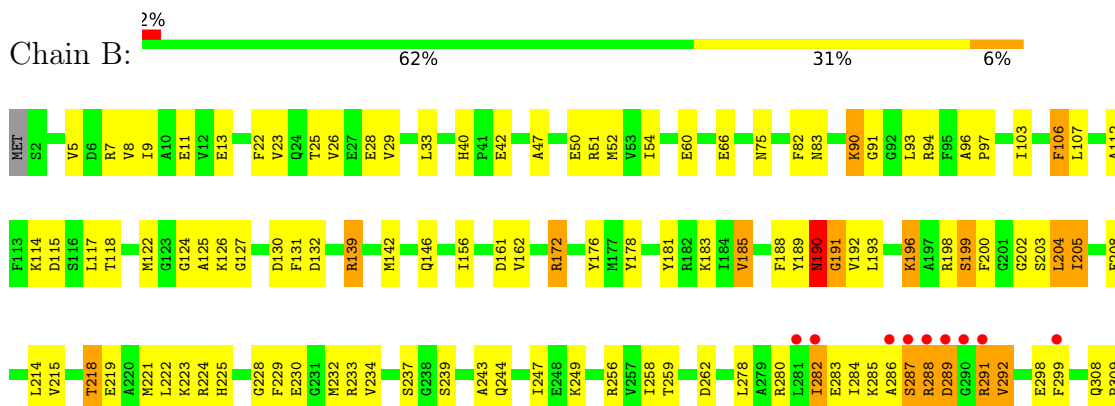
3 Residue-property plots [i](#)

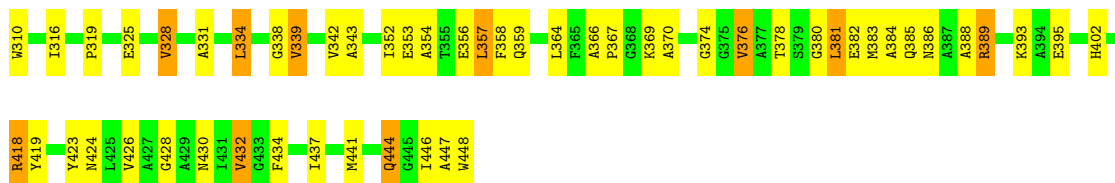
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE

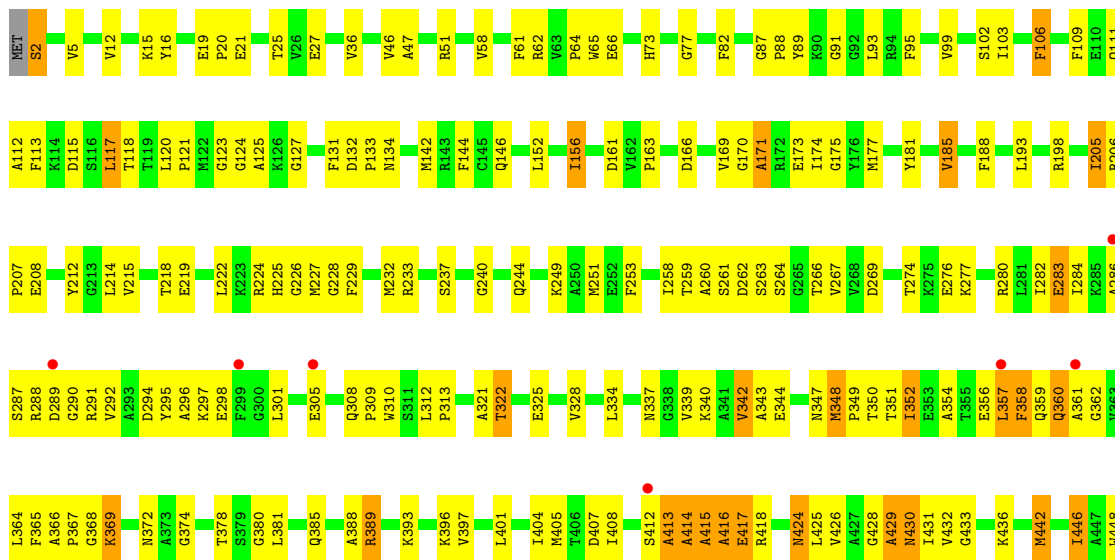


- Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE

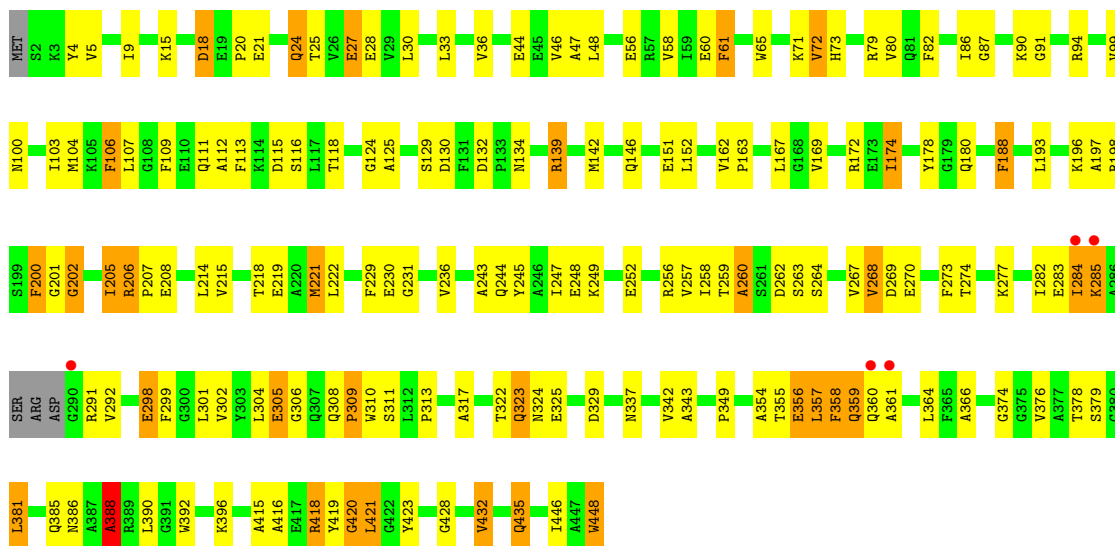




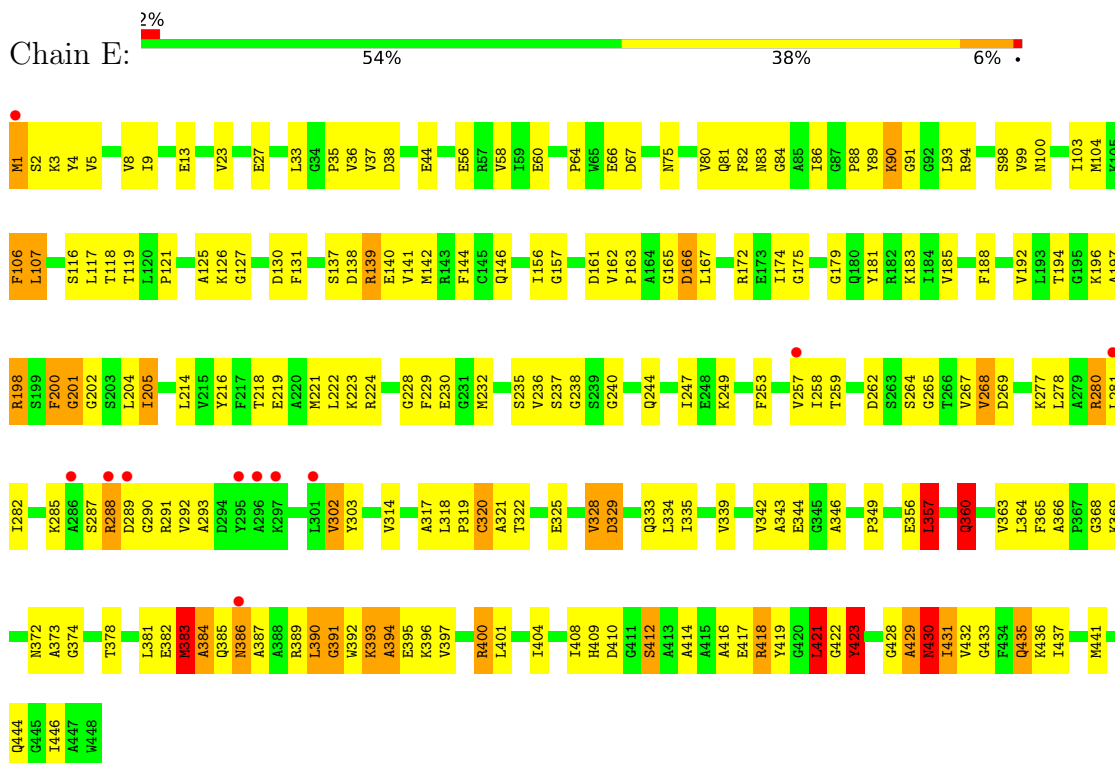
• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE



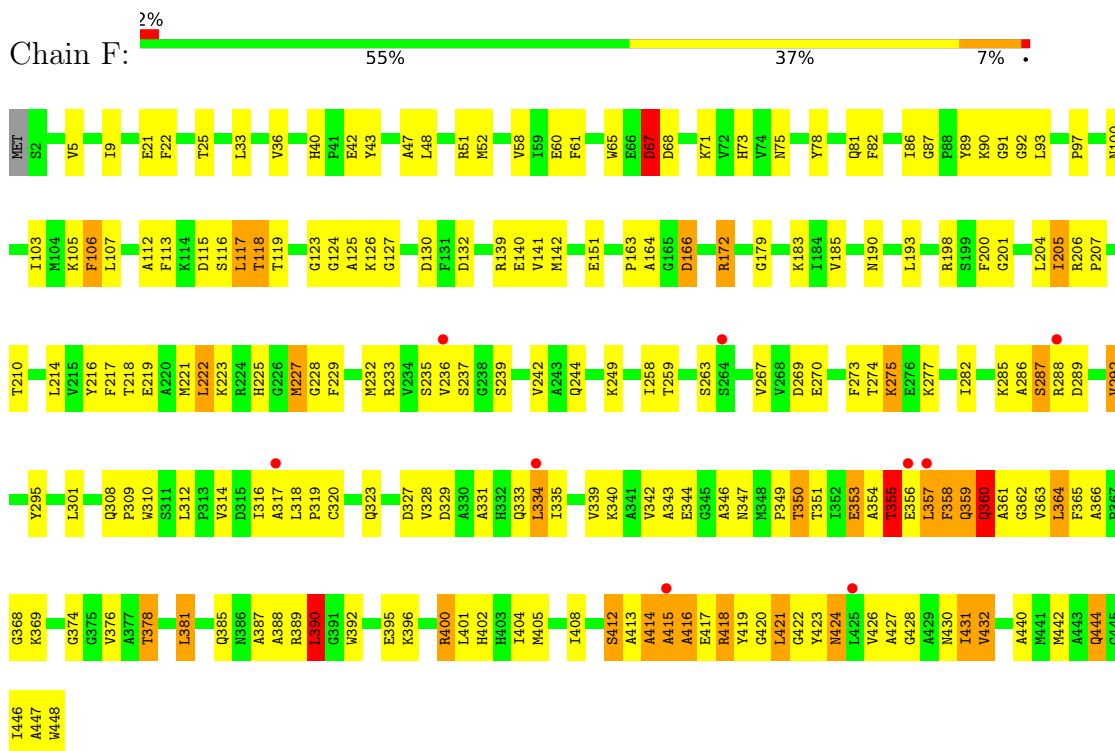
• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE



• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE



• Molecule 1: GLUTAMATE DEHYDROGENASE, NAD-SPECIFIC GLUTAMATE DEHYDROGENASE, GLUTAMATE DEHYDROGENASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.10Å 113.86Å 109.58Å 116.54° 101.54° 104.09°	Depositor
Resolution (Å)	36.52 – 2.69 47.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.6 (36.52-2.69) 93.6 (47.47-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.215 , 0.282 0.213 , 0.279	Depositor DCC
R_{free} test set	5046 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20640	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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 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	0.47	1/3440 (0.0%)	0.66	1/4649 (0.0%)
1	B	0.45	0/3464	0.64	2/4681 (0.0%)
1	C	0.45	0/3464	0.65	0/4681
1	D	0.44	0/3438	0.62	0/4645
1	E	0.45	0/3472	0.64	0/4691
1	F	0.40	0/3462	0.61	1/4679 (0.0%)
All	All	0.44	1/20740 (0.0%)	0.64	4/28026 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	SER	CB-OG	8.11	1.52	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ASN	N-CA-C	6.72	129.15	111.00
1	B	191	GLY	N-CA-C	-5.61	99.07	113.10
1	F	390	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	281	LEU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLN	Peptide
1	C	429	ALA	Peptide
1	D	388	ALA	Peptide
1	E	383	MET	Peptide
1	E	423	TYR	Peptide
1	E	429	ALA	Peptide

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	3371	0	3304	166	0
1	B	3395	0	3332	140	0
1	C	3395	0	3332	200	0
1	D	3370	0	3309	175	0
1	E	3403	0	3344	208	0
1	F	3393	0	3325	216	0
2	A	45	0	0	5	0
2	B	55	0	0	7	0
2	C	61	0	0	12	0
2	D	60	0	0	2	0
2	E	46	0	0	6	0
2	F	46	0	0	1	0
All	All	20640	0	19946	1065	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 26.

All (1065) 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:355:THR:C	1:F:357:LEU:HA	1.62	1.18
1:D:283:GLU:HA	1:D:284:ILE:HB	1.27	1.13
1:D:356:GLU:HA	1:D:358:PHE:N	1.62	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:GLU:HA	1:D:358:PHE:H	1.01	1.11
1:C:356:GLU:HB3	1:C:357:LEU:C	1.73	1.08
1:E:356:GLU:O	1:E:357:LEU:HB2	1.50	1.06
1:F:357:LEU:HG	1:F:357:LEU:O	1.27	1.04
1:D:259:THR:HG22	1:D:260:ALA:H	1.24	1.01
1:E:235:SER:HB3	1:E:314:VAL:HG11	1.42	1.01
1:C:313:PRO:HB3	1:C:337:ASN:HB3	1.42	0.99
1:E:104:MET:HB3	2:E:2012:HOH:O	1.64	0.97
1:B:287:SER:HA	1:B:288:ARG:O	1.66	0.96
1:D:415:ALA:HB2	1:D:432:VAL:HG13	1.47	0.95
1:A:361:ALA:HB1	1:A:362:GLY:HA3	1.48	0.95
1:F:357:LEU:O	1:F:357:LEU:CG	2.16	0.94
1:C:356:GLU:HB3	1:C:357:LEU:CA	1.98	0.92
1:F:227:MET:SD	1:F:340:LYS:HD2	2.10	0.92
1:F:359:GLN:HB2	1:F:362:GLY:H	1.36	0.91
1:B:196:LYS:HZ3	1:B:386:ASN:HD21	1.16	0.91
1:E:240:GLY:O	1:E:244:GLN:HG3	1.73	0.88
1:C:389:ARG:HD2	2:E:2011:HOH:O	1.74	0.87
1:B:196:LYS:NZ	1:B:386:ASN:HD21	1.71	0.86
1:A:58:VAL:HB	1:D:60:GLU:HB2	1.56	0.86
1:C:374:GLY:O	1:C:378:THR:HG23	1.74	0.86
1:C:416:ALA:HB2	1:C:428:GLY:HA3	1.58	0.85
1:D:118:THR:HG21	1:D:376:VAL:HG12	1.57	0.85
1:E:428:GLY:HA3	1:E:429:ALA:HB3	1.58	0.85
1:D:356:GLU:CA	1:D:358:PHE:H	1.86	0.85
1:D:360:GLN:N	1:D:361:ALA:HA	1.91	0.84
1:F:65:TRP:HE1	1:F:75:ASN:ND2	1.76	0.84
1:F:356:GLU:N	1:F:357:LEU:HA	1.85	0.84
1:B:356:GLU:HA	1:B:357:LEU:C	1.98	0.84
1:E:360:GLN:O	1:E:360:GLN:HG3	1.78	0.84
1:A:269:ASP:OD2	1:A:277:LYS:HE2	1.77	0.84
1:C:219:GLU:HG2	1:C:229:PHE:HD2	1.44	0.83
1:A:247:ILE:HG23	1:A:257:VAL:HG21	1.58	0.83
1:F:357:LEU:HB3	1:F:359:GLN:O	1.79	0.83
1:D:283:GLU:CA	1:D:284:ILE:HB	2.09	0.83
1:A:142:MET:O	1:A:146:GLN:HG3	1.78	0.82
1:B:219:GLU:HG2	1:B:229:PHE:HD2	1.41	0.82
1:E:372:ASN:O	1:E:374:GLY:N	2.12	0.82
1:C:277:LYS:HG2	1:C:295:TYR:OH	1.78	0.82
1:F:418:ARG:H	1:F:419:TYR:CA	1.93	0.81
1:A:230:GLU:HG3	1:A:253:PHE:O	1.80	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:LEU:HB3	1:F:126:LYS:HD3	1.63	0.80
1:C:123:GLY:HA3	2:C:2019:HOH:O	1.80	0.80
1:D:385:GLN:HE21	1:D:392:TRP:H	1.27	0.80
1:F:359:GLN:HB2	1:F:362:GLY:N	1.97	0.80
1:C:408:ILE:O	1:C:412:SER:HB2	1.82	0.79
1:F:374:GLY:O	1:F:378:THR:HG23	1.82	0.79
1:B:356:GLU:HB3	1:B:359:GLN:HG2	1.64	0.79
1:F:358:PHE:HB3	1:F:363:VAL:CG1	2.12	0.79
1:E:374:GLY:O	1:E:378:THR:HG23	1.82	0.79
1:C:412:SER:HB3	1:C:432:VAL:HG11	1.62	0.79
1:B:381:LEU:O	1:B:384:ALA:O	2.00	0.78
1:E:408:ILE:O	1:E:412:SER:HB2	1.82	0.78
1:F:239:SER:HB2	1:F:285:LYS:HG2	1.63	0.78
1:F:359:GLN:HA	1:F:360:GLN:C	2.03	0.78
1:F:328:VAL:HG12	1:F:353:GLU:HB3	1.63	0.78
1:F:350:THR:HG23	1:F:354:ALA:O	1.83	0.78
1:F:418:ARG:H	1:F:419:TYR:C	1.86	0.78
1:D:283:GLU:HA	1:D:284:ILE:CB	2.11	0.77
1:E:139:ARG:HG2	1:E:139:ARG:HH11	1.49	0.77
1:E:392:TRP:HB3	1:E:396:LYS:HB3	1.67	0.77
1:A:218:THR:HG21	1:A:343:ALA:CB	2.14	0.77
1:F:227:MET:HE1	1:F:232:MET:SD	2.24	0.77
1:C:280:ARG:NH1	1:C:283:GLU:HB3	2.00	0.77
1:D:374:GLY:O	1:D:378:THR:HG23	1.83	0.77
1:C:408:ILE:HG13	2:C:2057:HOH:O	1.85	0.77
1:D:268:VAL:HG21	1:D:304:LEU:HD12	1.64	0.77
1:A:198:ARG:H	1:A:198:ARG:NE	1.83	0.77
1:E:91:GLY:HA3	1:E:125:ALA:O	1.85	0.76
1:F:267:VAL:HG22	1:F:292:VAL:HG13	1.66	0.76
1:A:21:GLU:O	1:A:24:GLN:HG2	1.85	0.76
1:A:51:ARG:NH1	1:A:448:TRP:O	2.15	0.76
1:D:196:LYS:NZ	1:D:201:GLY:HA3	2.00	0.76
1:E:262:ASP:OD2	1:E:292:VAL:HB	1.84	0.76
1:F:328:VAL:HG23	1:F:329:ASP:H	1.50	0.76
1:F:359:GLN:HA	1:F:361:ALA:N	2.00	0.75
1:E:428:GLY:CA	1:E:429:ALA:HB3	2.16	0.75
1:A:257:VAL:HG23	1:A:273:PHE:HB2	1.68	0.75
1:E:392:TRP:HB2	1:E:397:VAL:HG23	1.69	0.75
1:D:91:GLY:HA3	1:D:125:ALA:O	1.86	0.75
1:D:142:MET:SD	1:F:446:ILE:HD12	2.27	0.75
1:E:437:ILE:HG23	1:E:441:MET:HE1	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HD2	2:C:2028:HOH:O	1.86	0.74
1:D:308:GLN:HB2	1:D:309:PRO:HD2	1.67	0.74
1:E:1:MET:HA	1:E:38:ASP:OD1	1.87	0.74
1:F:417:GLU:HB3	1:F:418:ARG:HA	1.67	0.74
1:B:262:ASP:H	1:B:292:VAL:HG21	1.52	0.74
1:F:141:VAL:HG21	1:F:172:ARG:NH1	2.01	0.74
1:F:357:LEU:HD23	1:F:359:GLN:O	1.88	0.74
1:E:390:LEU:HD12	1:E:390:LEU:O	1.88	0.74
1:A:328:VAL:HG23	1:A:329:ASP:H	1.53	0.73
1:F:65:TRP:HE1	1:F:75:ASN:HD22	1.35	0.73
1:D:219:GLU:HG2	1:D:229:PHE:HD2	1.53	0.73
1:D:236:VAL:H	1:D:259:THR:HB	1.54	0.73
1:D:357:LEU:N	1:D:360:GLN:HG2	2.03	0.73
1:E:60:GLU:HB2	1:F:58:VAL:HB	1.69	0.73
1:F:418:ARG:H	1:F:420:GLY:N	1.86	0.73
1:C:297:LYS:HG2	1:C:298:GLU:N	2.03	0.72
1:E:223:LYS:HB3	1:E:224:ARG:NH1	2.04	0.72
1:F:359:GLN:CB	1:F:362:GLY:H	2.01	0.72
1:F:417:GLU:CB	1:F:418:ARG:HA	2.19	0.72
1:A:198:ARG:H	1:A:198:ARG:HE	1.36	0.72
1:F:417:GLU:N	1:F:418:ARG:HB2	2.04	0.72
1:A:48:LEU:O	1:A:50:GLU:N	2.22	0.72
1:F:396:LYS:HE2	1:F:400:ARG:HH12	1.54	0.72
1:E:83:ASN:HD21	1:E:441:MET:CE	2.02	0.72
1:E:90:LYS:HD2	1:E:383:MET:HE1	1.70	0.72
1:A:400:ARG:HG2	1:A:400:ARG:HH11	1.55	0.72
1:D:193:LEU:O	1:D:196:LYS:HE2	1.90	0.71
1:C:356:GLU:HB3	1:C:358:PHE:N	2.04	0.71
1:E:216:TYR:OH	1:E:249:LYS:HE2	1.89	0.71
1:E:83:ASN:HD21	1:E:441:MET:HE1	1.53	0.71
1:F:447:ALA:HB1	1:F:448:TRP:HA	1.72	0.71
1:B:214:LEU:O	1:B:218:THR:HG23	1.90	0.71
1:F:239:SER:CB	1:F:285:LYS:HG2	2.19	0.71
1:B:90:LYS:HD2	1:B:383:MET:HE1	1.71	0.71
1:A:427:ALA:O	1:A:431:ILE:HG13	1.90	0.71
1:E:116:SER:HB2	1:E:437:ILE:CD1	2.21	0.70
1:E:200:PHE:HD1	1:E:200:PHE:H	1.39	0.70
1:B:52:MET:HG2	1:B:441:MET:CE	2.21	0.70
1:E:139:ARG:HH11	1:E:139:ARG:CG	2.03	0.70
1:F:118:THR:O	1:F:119:THR:OG1	2.09	0.70
1:E:1:MET:HG3	1:E:4:TYR:H	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:LEU:CB	1:F:359:GLN:O	2.39	0.70
1:E:267:VAL:CG2	1:E:292:VAL:HG13	2.22	0.70
1:C:288:ARG:C	1:C:290:GLY:H	1.92	0.70
1:E:391:GLY:O	1:E:392:TRP:CD1	2.45	0.69
1:A:400:ARG:HH11	1:A:400:ARG:CG	2.05	0.69
1:C:415:ALA:N	1:C:417:GLU:HB3	2.07	0.69
1:F:221:MET:HG3	1:F:423:TYR:OH	1.92	0.69
1:E:431:ILE:O	1:E:432:VAL:HG12	1.90	0.69
1:F:357:LEU:H	1:F:358:PHE:C	1.95	0.69
1:E:429:ALA:H	1:E:432:VAL:HG12	1.56	0.69
1:B:437:ILE:O	1:B:441:MET:HG3	1.93	0.69
1:D:196:LYS:HZ2	1:D:201:GLY:HA3	1.56	0.69
1:E:446:ILE:O	1:E:446:ILE:HG22	1.93	0.69
1:F:267:VAL:CG2	1:F:292:VAL:HG13	2.21	0.69
1:F:91:GLY:HA3	1:F:125:ALA:O	1.92	0.69
1:F:359:GLN:HB2	1:F:362:GLY:CA	2.23	0.69
1:F:378:THR:HG22	1:F:401:LEU:HD13	1.75	0.68
1:F:415:ALA:HA	1:F:418:ARG:HG3	1.74	0.68
1:D:283:GLU:HB3	1:D:284:ILE:CG2	2.24	0.68
1:F:381:LEU:O	1:F:385:GLN:HG3	1.92	0.68
1:E:267:VAL:HG23	1:E:292:VAL:HG13	1.76	0.68
1:B:374:GLY:O	1:B:378:THR:HG23	1.92	0.68
1:C:240:GLY:O	1:C:244:GLN:HG3	1.93	0.68
1:C:393:LYS:HG2	2:C:2054:HOH:O	1.94	0.68
1:B:388:ALA:N	1:B:389:ARG:HA	2.06	0.68
1:D:259:THR:HG22	1:D:260:ALA:N	2.05	0.68
1:D:146:GLN:HA	1:D:180:GLN:HG2	1.75	0.68
1:D:385:GLN:NE2	1:D:392:TRP:H	1.90	0.68
1:B:219:GLU:HG2	1:B:229:PHE:CD2	2.28	0.68
1:A:51:ARG:HB2	2:A:2009:HOH:O	1.94	0.67
1:F:90:LYS:HG3	1:F:91:GLY:N	2.09	0.67
1:E:319:PRO:HD2	1:E:343:ALA:O	1.93	0.67
1:F:357:LEU:N	1:F:358:PHE:C	2.47	0.67
1:C:424:ASN:HD21	1:C:426:VAL:HB	1.60	0.67
1:C:21:GLU:HG2	1:C:102:SER:OG	1.95	0.67
1:D:9:ILE:HD13	1:D:27:GLU:HA	1.76	0.67
1:C:258:ILE:HB	1:C:269:ASP:O	1.94	0.67
1:D:180:GLN:HA	1:D:180:GLN:OE1	1.95	0.67
1:C:356:GLU:CB	1:C:358:PHE:N	2.58	0.67
1:E:36:VAL:HG21	1:E:431:ILE:HG12	1.77	0.67
1:F:216:TYR:OH	1:F:249:LYS:HE3	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLY:O	2:C:2019:HOH:O	2.11	0.67
1:E:33:LEU:O	1:E:37:VAL:HG23	1.94	0.67
1:E:194:THR:HA	1:E:382:GLU:OE1	1.95	0.66
1:E:165:GLY:O	1:E:166:ASP:HB2	1.95	0.66
1:A:361:ALA:CB	1:A:362:GLY:HA3	2.23	0.66
1:C:412:SER:O	1:C:429:ALA:HB2	1.96	0.66
1:F:418:ARG:HB3	1:F:419:TYR:HB2	1.78	0.66
1:A:206:ARG:HB3	1:A:207:PRO:HD3	1.77	0.66
1:B:444:GLN:OE1	2:B:2054:HOH:O	2.12	0.66
1:E:103:ILE:O	1:E:107:LEU:HD23	1.96	0.66
1:F:328:VAL:HG12	1:F:353:GLU:CB	2.26	0.66
1:A:327:ASP:O	1:A:328:VAL:HG13	1.96	0.66
1:E:90:LYS:CD	1:E:383:MET:HE1	2.26	0.66
1:F:354:ALA:O	1:F:355:THR:OG1	2.11	0.66
1:C:88:PRO:C	2:C:2019:HOH:O	2.33	0.66
1:C:274:THR:HB	1:C:276:GLU:OE1	1.97	0.65
1:C:342:VAL:HG22	1:C:365:PHE:HD1	1.61	0.65
1:E:428:GLY:HA3	1:E:429:ALA:CB	2.27	0.65
1:F:428:GLY:O	1:F:432:VAL:HG23	1.97	0.65
1:E:393:LYS:O	1:E:394:ALA:HB3	1.96	0.65
1:F:328:VAL:HG23	1:F:329:ASP:N	2.10	0.65
1:D:99:VAL:HG12	1:D:130:ASP:HA	1.78	0.65
1:E:218:THR:HG21	1:E:343:ALA:CB	2.27	0.65
1:A:43:TYR:HA	1:A:48:LEU:HD23	1.78	0.65
1:D:61:PHE:N	1:D:61:PHE:CD1	2.63	0.65
1:E:400:ARG:HG2	1:E:400:ARG:HH11	1.62	0.65
1:C:369:LYS:NZ	1:C:430:ASN:HD22	1.94	0.65
1:D:139:ARG:CG	1:D:139:ARG:HH11	2.11	0.64
1:E:200:PHE:CD1	1:E:200:PHE:N	2.66	0.64
1:F:353:GLU:O	1:F:356:GLU:N	2.30	0.64
1:E:75:ASN:HB3	1:E:130:ASP:OD1	1.98	0.64
1:C:354:ALA:C	1:C:356:GLU:N	2.48	0.64
1:E:390:LEU:O	1:E:391:GLY:C	2.35	0.64
1:C:46:VAL:HG21	1:C:442:MET:CE	2.27	0.64
1:D:71:LYS:O	1:D:72:VAL:HB	1.97	0.64
1:C:266:THR:OG1	1:C:308:GLN:HA	1.98	0.64
1:D:359:GLN:C	1:D:361:ALA:HA	2.19	0.63
1:F:417:GLU:H	1:F:418:ARG:HB2	1.62	0.63
1:B:444:GLN:HG2	1:F:179:GLY:HA2	1.79	0.63
1:A:5:VAL:O	1:A:9:ILE:HG13	1.98	0.63
1:B:90:LYS:HE2	1:B:162:VAL:HB	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:THR:CG2	1:D:260:ALA:H	2.06	0.63
1:D:356:GLU:H	1:D:357:LEU:HB2	1.62	0.63
1:A:355:THR:O	1:A:359:GLN:HG3	1.98	0.63
1:C:214:LEU:O	1:C:218:THR:HG23	1.99	0.63
1:A:48:LEU:C	2:A:2009:HOH:O	2.35	0.63
1:D:343:ALA:CB	1:D:366:ALA:HB3	2.29	0.63
1:B:196:LYS:NZ	1:B:386:ASN:ND2	2.45	0.63
1:C:424:ASN:C	1:C:424:ASN:HD22	2.01	0.63
1:D:196:LYS:CE	1:D:201:GLY:HA3	2.29	0.63
1:F:36:VAL:O	1:F:40:HIS:HD2	1.81	0.63
1:B:9:ILE:O	1:B:13:GLU:HG3	1.99	0.62
1:C:446:ILE:O	1:C:446:ILE:HG13	1.97	0.62
1:E:317:ALA:HB3	1:E:342:VAL:HG23	1.81	0.62
1:D:99:VAL:HG11	1:D:129:SER:C	2.19	0.62
1:F:141:VAL:HG21	1:F:172:ARG:HH12	1.64	0.62
1:A:361:ALA:HB3	1:A:363:VAL:HG23	1.81	0.62
1:C:206:ARG:HB3	1:C:207:PRO:HD3	1.82	0.62
1:E:5:VAL:O	1:E:9:ILE:HG13	1.98	0.62
1:B:234:VAL:HG22	1:B:316:ILE:HB	1.82	0.62
1:E:381:LEU:O	1:E:384:ALA:HB3	1.99	0.62
1:A:218:THR:CG2	1:A:343:ALA:CB	2.77	0.62
1:C:413:ALA:HB1	1:C:425:LEU:CD1	2.29	0.62
1:E:107:LEU:HD12	1:E:126:LYS:HE2	1.81	0.62
1:F:90:LYS:HG3	1:F:91:GLY:H	1.65	0.62
1:F:331:ALA:O	1:F:335:ILE:HG13	2.00	0.62
1:A:234:VAL:HG22	1:A:316:ILE:HB	1.82	0.62
1:C:118:THR:HA	1:C:408:ILE:HD11	1.81	0.62
1:D:205:ILE:HG23	1:D:205:ILE:O	2.00	0.62
1:C:414:ALA:H	1:C:416:ALA:HB3	1.64	0.61
1:F:218:THR:OG1	1:F:229:PHE:CE2	2.52	0.61
1:B:52:MET:HG2	1:B:441:MET:HE1	1.82	0.61
1:C:356:GLU:HB3	1:C:357:LEU:CB	2.30	0.61
1:D:357:LEU:H	1:D:360:GLN:HG2	1.65	0.61
1:A:72:VAL:HG22	1:D:446:ILE:HD13	1.81	0.61
1:C:429:ALA:HA	1:C:432:VAL:HG12	1.81	0.61
1:F:219:GLU:HG2	1:F:229:PHE:HD2	1.65	0.61
1:F:358:PHE:HB3	1:F:363:VAL:HG11	1.81	0.61
1:B:428:GLY:O	1:B:432:VAL:HG22	2.00	0.61
1:B:13:GLU:HG2	1:B:23:VAL:HG13	1.82	0.61
1:E:35:PRO:O	1:E:38:ASP:HB2	2.00	0.61
1:E:342:VAL:O	1:E:365:PHE:HA	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:SER:CB	1:C:432:VAL:HG11	2.30	0.61
1:D:354:ALA:O	1:D:357:LEU:HB2	2.00	0.61
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.65	0.61
1:C:87:GLY:HA3	1:C:121:PRO:O	2.01	0.61
1:C:350:THR:HG22	1:C:351:THR:O	2.01	0.61
1:D:206:ARG:HG2	1:D:207:PRO:HD3	1.83	0.61
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.16	0.61
1:C:175:GLY:O	1:E:444:GLN:HA	2.00	0.61
1:F:416:ALA:H	1:F:418:ARG:HB2	1.66	0.61
1:F:235:SER:HB3	1:F:314:VAL:HG11	1.83	0.60
1:E:116:SER:HB2	1:E:437:ILE:HD11	1.83	0.60
1:B:319:PRO:HD2	1:B:343:ALA:O	2.02	0.60
1:E:131:PHE:HB2	1:E:144:PHE:CZ	2.36	0.60
1:A:218:THR:HG21	1:A:343:ALA:HB3	1.83	0.60
1:E:384:ALA:HA	1:E:386:ASN:OD1	2.01	0.60
1:F:418:ARG:N	1:F:419:TYR:HB2	2.16	0.60
1:A:277:LYS:NZ	1:A:301:LEU:HD11	2.16	0.60
1:C:163:PRO:HD2	1:C:193:LEU:HD23	1.84	0.60
1:D:196:LYS:NZ	1:D:386:ASN:OD1	2.34	0.60
1:E:219:GLU:HG3	1:E:253:PHE:CE2	2.37	0.60
1:B:258:ILE:HG13	1:B:259:THR:HG23	1.82	0.60
1:E:290:GLY:HA2	2:E:2030:HOH:O	2.00	0.60
1:E:435:GLN:HE21	1:E:435:GLN:HA	1.66	0.60
1:F:440:ALA:O	1:F:444:GLN:HG2	2.00	0.60
1:D:283:GLU:HB3	1:D:284:ILE:HG22	1.84	0.60
1:A:219:GLU:CG	1:A:229:PHE:HD2	2.14	0.59
1:A:219:GLU:HG2	1:A:229:PHE:HD2	1.65	0.59
1:D:214:LEU:O	1:D:218:THR:HG23	2.01	0.59
1:E:384:ALA:CA	1:E:386:ASN:OD1	2.50	0.59
1:E:390:LEU:O	1:E:391:GLY:O	2.20	0.59
1:F:308:GLN:HB3	1:F:309:PRO:HD2	1.82	0.59
1:A:280:ARG:HG2	1:A:298:GLU:OE2	2.01	0.59
1:C:20:PRO:HG2	1:C:21:GLU:OE2	2.02	0.59
1:B:54:ILE:HG22	1:C:62:ARG:HB2	1.83	0.59
1:C:120:LEU:HD13	1:C:380:GLY:HA3	1.85	0.59
1:C:152:LEU:HG	1:C:156:ILE:HD13	1.83	0.59
1:F:5:VAL:O	1:F:9:ILE:HG13	2.02	0.59
1:C:65:TRP:CH2	1:C:73:HIS:HD2	2.20	0.59
1:E:280:ARG:HH11	1:E:280:ARG:HB2	1.67	0.59
1:F:93:LEU:HA	1:F:127:GLY:O	2.02	0.59
1:B:202:GLY:HA2	1:B:382:GLU:CD	2.23	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HD12	1:B:278:LEU:O	2.03	0.59
1:E:386:ASN:OD1	1:E:387:ALA:N	2.35	0.59
1:F:421:LEU:HD22	1:F:424:ASN:HB2	1.85	0.59
1:A:5:VAL:CG2	1:A:37:VAL:HG11	2.33	0.59
1:B:378:THR:HA	1:B:381:LEU:HB2	1.82	0.59
1:C:308:GLN:HB2	1:C:309:PRO:HD2	1.84	0.59
1:A:308:GLN:HB3	1:A:309:PRO:HD2	1.84	0.58
1:D:283:GLU:CA	1:D:284:ILE:CB	2.77	0.58
1:C:368:GLY:HA3	2:C:2043:HOH:O	2.04	0.58
1:C:389:ARG:HB2	2:C:2051:HOH:O	2.01	0.58
1:F:342:VAL:HG23	1:F:365:PHE:HD1	1.68	0.58
1:B:215:VAL:HG13	1:B:229:PHE:CZ	2.39	0.58
1:C:414:ALA:O	1:C:415:ALA:HB3	2.03	0.58
1:A:5:VAL:HG23	1:A:37:VAL:HG11	1.84	0.58
1:A:118:THR:HG21	1:A:122:MET:CE	2.33	0.58
1:B:424:ASN:OD1	1:B:426:VAL:HG22	2.04	0.58
1:E:437:ILE:HG23	1:E:441:MET:CE	2.34	0.58
1:C:276:GLU:CD	1:C:276:GLU:H	2.05	0.58
1:D:284:ILE:O	1:D:285:LYS:HB2	2.02	0.58
1:D:269:ASP:HB2	1:D:301:LEU:HD13	1.84	0.58
1:A:342:VAL:HG13	1:A:365:PHE:HD1	1.68	0.58
1:D:205:ILE:O	1:D:205:ILE:CG2	2.51	0.58
1:B:393:LYS:HB2	2:B:2047:HOH:O	2.04	0.58
1:D:132:ASP:OD1	1:D:134:ASN:HB2	2.04	0.58
1:F:344:GLU:OE1	1:F:349:PRO:HD2	2.04	0.58
1:F:115:ASP:O	1:F:118:THR:OG1	2.22	0.57
1:F:418:ARG:C	1:F:418:ARG:HD2	2.24	0.57
1:A:256:ARG:NE	2:A:2025:HOH:O	2.37	0.57
1:B:291:ARG:HD2	1:B:291:ARG:N	2.18	0.57
1:D:259:THR:O	1:D:260:ALA:CB	2.52	0.57
1:D:305:GLU:CD	1:D:306:GLY:H	2.06	0.57
1:F:417:GLU:O	1:F:421:LEU:O	2.22	0.57
1:A:117:LEU:O	1:A:117:LEU:HD22	2.05	0.57
1:B:205:ILE:HA	1:B:208:GLU:OE1	2.04	0.57
1:C:215:VAL:HG21	1:C:249:LYS:HB3	1.87	0.57
1:E:106:PHE:CE1	1:E:107:LEU:HD22	2.39	0.57
1:A:277:LYS:HZ3	1:A:301:LEU:HD11	1.70	0.57
1:F:100:ASN:OD1	1:F:103:ILE:HD12	2.04	0.57
1:A:61:PHE:CG	1:A:151:GLU:HG2	2.39	0.57
1:B:60:GLU:HB2	1:C:58:VAL:HB	1.86	0.57
1:B:228:GLY:O	1:B:232:MET:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ALA:O	1:C:356:GLU:HB2	2.05	0.57
1:B:117:LEU:HD11	1:B:370:ALA:HA	1.87	0.56
1:C:95:PHE:HZ	1:C:177:MET:CE	2.18	0.56
1:D:5:VAL:O	1:D:9:ILE:HG13	2.05	0.56
1:B:7:ARG:O	1:B:8:VAL:HB	2.05	0.56
1:B:112:ALA:HA	1:B:124:GLY:HA3	1.86	0.56
1:B:142:MET:HB2	2:B:2020:HOH:O	2.05	0.56
1:D:200:PHE:N	1:D:200:PHE:CD1	2.73	0.56
1:A:60:GLU:HB2	1:D:58:VAL:HB	1.87	0.56
1:A:139:ARG:HH11	1:A:139:ARG:CG	2.18	0.56
1:A:267:VAL:HG23	1:A:292:VAL:CG1	2.35	0.56
1:C:258:ILE:HG13	1:C:258:ILE:O	2.05	0.56
1:D:308:GLN:HG3	1:D:310:TRP:CD1	2.40	0.56
1:E:67:ASP:HB2	1:E:140:GLU:OE2	2.06	0.56
1:E:90:LYS:HD2	1:E:383:MET:CE	2.35	0.56
1:D:259:THR:O	1:D:260:ALA:HB2	2.04	0.56
1:E:236:VAL:HG22	1:E:318:LEU:HB2	1.87	0.56
1:E:93:LEU:HA	1:E:127:GLY:O	2.04	0.56
1:E:269:ASP:OD2	1:E:277:LYS:HE2	2.06	0.56
1:A:172:ARG:HD3	1:A:173:GLU:OE2	2.06	0.56
1:D:259:THR:O	1:D:273:PHE:HE1	1.88	0.56
1:E:288:ARG:HA	1:E:290:GLY:H	1.71	0.56
1:F:97:PRO:HD3	1:F:132:ASP:HB2	1.88	0.56
1:F:210:THR:HG22	1:F:242:VAL:HG13	1.88	0.56
1:F:427:ALA:O	1:F:431:ILE:CG2	2.53	0.56
1:A:331:ALA:O	1:A:335:ILE:HG13	2.06	0.56
1:B:280:ARG:O	1:B:284:ILE:HG13	2.05	0.56
1:D:313:PRO:HB3	1:D:337:ASN:HD22	1.70	0.56
1:B:139:ARG:HH11	1:B:139:ARG:CG	2.19	0.56
1:C:25:THR:HG21	1:C:106:PHE:HB2	1.86	0.56
1:D:24:GLN:HG2	1:D:25:THR:N	2.21	0.56
1:C:132:ASP:OD1	1:C:134:ASN:HB2	2.06	0.56
1:C:415:ALA:H	1:C:417:GLU:HB3	1.68	0.56
1:D:219:GLU:HG2	1:D:229:PHE:CD2	2.38	0.56
1:F:355:THR:CA	1:F:357:LEU:HA	2.35	0.56
1:B:190:ASN:O	1:B:196:LYS:HE3	2.06	0.55
1:C:388:ALA:C	1:E:386:ASN:ND2	2.59	0.55
1:E:139:ARG:HG2	1:E:139:ARG:NH1	2.15	0.55
1:E:219:GLU:HG2	1:E:229:PHE:HD1	1.71	0.55
1:A:47:ALA:HB3	1:D:72:VAL:HG12	1.89	0.55
1:B:181:TYR:O	1:B:185:VAL:HG13	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:MET:SD	1:C:340:LYS:HD3	2.46	0.55
1:B:52:MET:HG2	1:B:441:MET:HE3	1.87	0.55
1:B:380:GLY:HA2	1:B:383:MET:HE3	1.87	0.55
1:D:178:TYR:HD2	1:F:444:GLN:NE2	2.04	0.55
1:D:418:ARG:HD3	1:D:419:TYR:CE1	2.41	0.55
1:F:418:ARG:N	1:F:420:GLY:N	2.53	0.55
1:F:418:ARG:HD2	1:F:418:ARG:O	2.07	0.55
1:C:413:ALA:O	1:C:414:ALA:CB	2.54	0.55
1:D:378:THR:HA	1:D:381:LEU:HB2	1.87	0.55
1:F:223:LYS:C	1:F:225:HIS:H	2.09	0.55
1:A:47:ALA:C	1:A:48:LEU:O	2.44	0.55
1:C:288:ARG:C	1:C:290:GLY:N	2.60	0.55
1:B:83:ASN:HD21	1:B:441:MET:HE2	1.71	0.55
1:E:342:VAL:CG1	1:E:365:PHE:HD1	2.20	0.55
1:C:388:ALA:C	1:E:386:ASN:HD21	2.09	0.55
1:E:247:ILE:HG12	1:E:257:VAL:HG11	1.89	0.55
1:A:67:ASP:HB2	1:A:140:GLU:OE2	2.08	0.54
1:A:91:GLY:HA3	1:A:125:ALA:O	2.07	0.54
1:B:446:ILE:HD12	1:F:142:MET:HE1	1.89	0.54
1:C:446:ILE:O	1:C:446:ILE:CG1	2.55	0.54
1:D:259:THR:HG21	1:D:309:PRO:HG3	1.89	0.54
1:A:374:GLY:O	1:A:378:THR:HG23	2.08	0.54
1:C:413:ALA:O	1:C:414:ALA:HB3	2.07	0.54
1:D:392:TRP:HB3	1:D:396:LYS:HD3	1.89	0.54
1:D:420:GLY:C	1:D:421:LEU:HG	2.27	0.54
1:C:228:GLY:O	1:C:232:MET:HG3	2.07	0.54
1:D:262:ASP:OD2	1:D:292:VAL:HB	2.07	0.54
1:D:283:GLU:CB	1:D:284:ILE:HG22	2.36	0.54
1:D:357:LEU:H	1:D:360:GLN:CG	2.20	0.54
1:E:2:SER:HA	1:E:5:VAL:HB	1.90	0.54
1:E:200:PHE:HD1	1:E:200:PHE:N	2.06	0.54
1:F:48:LEU:O	1:F:52:MET:HG3	2.07	0.54
1:C:415:ALA:HA	1:C:416:ALA:O	2.07	0.54
1:E:214:LEU:O	1:E:218:THR:HG23	2.07	0.54
1:E:223:LYS:HB3	1:E:224:ARG:HH11	1.73	0.54
1:B:243:ALA:O	1:B:247:ILE:HG13	2.08	0.54
1:C:429:ALA:O	1:C:430:ASN:HB2	2.08	0.54
1:B:282:ILE:HG13	1:B:283:GLU:N	2.21	0.53
1:B:286:ALA:O	1:B:287:SER:HB2	2.07	0.53
1:C:170:GLY:O	1:C:173:GLU:N	2.39	0.53
1:C:413:ALA:HB1	1:C:425:LEU:HD12	1.88	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLY:HA3	1:C:125:ALA:O	2.08	0.53
1:E:197:ALA:O	1:E:202:GLY:HA3	2.08	0.53
1:F:217:PHE:CE2	1:F:366:ALA:HB1	2.43	0.53
1:C:430:ASN:H	1:C:432:VAL:HG12	1.73	0.53
1:D:56:GLU:HG2	1:D:448:TRP:CD2	2.43	0.53
1:E:58:VAL:HG13	1:E:80:VAL:HG22	1.89	0.53
1:C:356:GLU:OE2	1:C:357:LEU:HB3	2.09	0.53
1:F:227:MET:SD	1:F:340:LYS:NZ	2.79	0.53
1:A:204:LEU:O	1:A:205:ILE:HB	2.07	0.53
1:B:114:LYS:O	1:B:117:LEU:HB3	2.08	0.53
1:D:416:ALA:O	1:D:420:GLY:O	2.27	0.53
1:E:429:ALA:H	1:E:432:VAL:CG1	2.20	0.53
1:F:334:LEU:HB3	1:F:339:VAL:HG11	1.90	0.53
1:C:156:ILE:HB	1:C:161:ASP:O	2.09	0.53
1:C:215:VAL:HG11	1:C:249:LYS:HG3	1.89	0.53
1:F:227:MET:SD	1:F:340:LYS:CD	2.92	0.53
1:C:46:VAL:HG21	1:C:442:MET:HE2	1.89	0.53
1:D:109:PHE:O	1:D:112:ALA:HB3	2.09	0.53
1:F:216:TYR:CZ	1:F:249:LYS:HE3	2.44	0.53
1:A:303:TYR:C	1:A:304:LEU:HD23	2.29	0.53
1:B:183:LYS:HE3	1:D:448:TRP:CE3	2.44	0.53
1:A:72:VAL:CG2	1:D:446:ILE:HD13	2.39	0.52
1:A:82:PHE:CE1	1:A:109:PHE:HD1	2.27	0.52
1:E:106:PHE:CZ	1:E:107:LEU:CD2	2.92	0.52
1:F:319:PRO:HD2	1:F:343:ALA:O	2.09	0.52
1:A:24:GLN:NE2	2:A:2003:HOH:O	2.41	0.52
1:B:5:VAL:O	1:B:9:ILE:HG13	2.09	0.52
1:C:62:ARG:HG2	1:C:64:PRO:HD3	1.91	0.52
1:F:286:ALA:O	1:F:287:SER:HB2	2.08	0.52
1:D:248:GLU:O	1:D:252:GLU:HG3	2.09	0.52
1:E:201:GLY:O	1:E:385:GLN:NE2	2.42	0.52
1:F:206:ARG:HB3	1:F:207:PRO:HD3	1.90	0.52
1:F:225:HIS:CB	1:F:364:LEU:HD21	2.39	0.52
1:F:427:ALA:O	1:F:431:ILE:HG23	2.09	0.52
1:B:51:ARG:NH1	1:B:448:TRP:O	2.38	0.52
1:B:156:ILE:HA	1:B:161:ASP:HB3	1.91	0.52
1:F:417:GLU:CB	1:F:418:ARG:CA	2.87	0.52
1:D:80:VAL:O	1:D:125:ALA:HB1	2.10	0.52
1:D:355:THR:O	1:D:356:GLU:CB	2.57	0.52
1:E:393:LYS:O	1:E:394:ALA:CB	2.57	0.52
1:E:400:ARG:HG2	1:E:400:ARG:NH1	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:SER:O	1:F:416:ALA:CB	2.58	0.52
1:A:232:MET:HB3	1:A:315:ASP:HB2	1.91	0.52
1:A:327:ASP:O	1:A:328:VAL:HG22	2.09	0.52
1:C:219:GLU:HG2	1:C:229:PHE:CD2	2.34	0.52
1:C:412:SER:O	1:C:413:ALA:HB2	2.09	0.52
1:F:426:VAL:HG12	1:F:427:ALA:N	2.25	0.52
1:A:181:TYR:O	1:A:185:VAL:HG13	2.09	0.52
1:C:408:ILE:CG1	2:C:2057:HOH:O	2.51	0.52
1:D:262:ASP:HB3	1:D:292:VAL:HG23	1.92	0.52
1:E:267:VAL:HG23	1:E:292:VAL:CG1	2.40	0.52
1:F:357:LEU:HD23	1:F:359:GLN:NE2	2.25	0.52
1:B:239:SER:OG	1:B:285:LYS:HG3	2.09	0.52
1:B:418:ARG:HD2	1:B:419:TYR:CE2	2.45	0.52
1:D:90:LYS:HD2	1:D:162:VAL:O	2.09	0.52
1:D:118:THR:HG21	1:D:376:VAL:CG1	2.34	0.52
1:E:36:VAL:HG13	1:E:419:TYR:CZ	2.44	0.52
1:E:437:ILE:CG2	1:E:441:MET:HE1	2.38	0.52
2:B:2054:HOH:O	1:F:200:PHE:HB3	2.08	0.52
1:A:327:ASP:C	1:A:328:VAL:HG22	2.30	0.52
1:C:297:LYS:CG	1:C:298:GLU:N	2.72	0.52
1:D:196:LYS:HZ2	1:D:201:GLY:CA	2.23	0.52
1:E:216:TYR:CZ	1:E:249:LYS:HE2	2.45	0.52
1:E:343:ALA:CB	1:E:366:ALA:HB3	2.40	0.52
1:C:267:VAL:CG2	1:C:292:VAL:HG12	2.39	0.51
1:F:327:ASP:O	1:F:354:ALA:HB2	2.10	0.51
1:A:378:THR:HA	1:A:381:LEU:HB2	1.92	0.51
1:E:224:ARG:HG2	1:E:409:HIS:HE1	1.74	0.51
1:F:424:ASN:C	1:F:424:ASN:HD22	2.12	0.51
1:C:313:PRO:CB	1:C:337:ASN:HB3	2.29	0.51
1:C:360:GLN:C	1:C:362:GLY:H	2.12	0.51
1:F:65:TRP:NE1	1:F:75:ASN:ND2	2.54	0.51
1:F:190:ASN:ND2	1:F:201:GLY:HA3	2.25	0.51
1:F:359:GLN:HB2	1:F:362:GLY:HA2	1.91	0.51
1:F:369:LYS:HB2	2:F:2041:HOH:O	2.10	0.51
1:B:388:ALA:H	1:B:389:ARG:HA	1.73	0.51
1:C:36:VAL:HG21	1:C:431:ILE:HG23	1.93	0.51
1:C:432:VAL:HG13	1:C:433:GLY:N	2.26	0.51
1:D:423:TYR:O	1:D:423:TYR:CD1	2.64	0.51
1:A:402:HIS:HB2	2:A:2023:HOH:O	2.10	0.51
1:C:334:LEU:HB3	1:C:339:VAL:HG11	1.92	0.51
1:E:383:MET:O	1:E:384:ALA:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:ILE:O	1:E:433:GLY:N	2.40	0.51
1:A:267:VAL:HG23	1:A:292:VAL:HG13	1.92	0.51
1:B:52:MET:CE	1:B:441:MET:HE3	2.40	0.51
1:D:65:TRP:O	1:D:72:VAL:HA	2.09	0.51
1:F:244:GLN:NE2	1:F:282:ILE:HG12	2.25	0.51
1:A:269:ASP:HB2	1:A:301:LEU:HD13	1.92	0.51
1:F:401:LEU:O	1:F:405:MET:HG2	2.11	0.51
1:F:412:SER:O	1:F:416:ALA:HB1	2.11	0.51
1:F:418:ARG:N	1:F:419:TYR:CA	2.67	0.51
1:C:208:GLU:HB3	1:C:212:TYR:CE1	2.46	0.51
1:E:56:GLU:OE2	1:E:83:ASN:HA	2.09	0.51
1:A:266:THR:HG21	1:A:309:PRO:HB3	1.93	0.51
1:D:356:GLU:CB	1:D:358:PHE:HB2	2.41	0.51
1:A:204:LEU:HD13	1:A:394:ALA:HB2	1.92	0.51
1:C:360:GLN:C	1:C:362:GLY:N	2.64	0.51
1:D:390:LEU:HD11	1:F:392:TRP:HH2	1.76	0.51
1:B:298:GLU:OE1	2:B:2033:HOH:O	2.20	0.50
1:E:430:ASN:O	1:E:431:ILE:HB	2.11	0.50
1:A:49:LEU:HD23	1:A:49:LEU:H	1.76	0.50
1:D:91:GLY:O	1:D:163:PRO:HA	2.11	0.50
1:B:97:PRO:HG3	1:B:132:ASP:HB2	1.93	0.50
1:E:335:ILE:CD1	1:E:357:LEU:HD23	2.41	0.50
1:A:213:GLY:HA2	1:A:405:MET:HG3	1.92	0.50
1:D:247:ILE:HG23	1:D:257:VAL:HG11	1.93	0.50
1:E:204:LEU:HD13	1:E:394:ALA:HB2	1.94	0.50
1:E:224:ARG:NH2	1:E:410:ASP:OD1	2.44	0.50
1:F:228:GLY:O	1:F:232:MET:HG3	2.12	0.50
1:F:418:ARG:CB	1:F:419:TYR:HB2	2.41	0.50
1:A:276:GLU:O	1:A:279:ALA:HB3	2.12	0.50
1:A:342:VAL:HG13	1:A:365:PHE:CD1	2.46	0.50
1:D:356:GLU:HG3	1:D:356:GLU:O	2.12	0.50
1:E:181:TYR:CZ	1:E:185:VAL:HG11	2.46	0.50
1:F:86:ILE:HD11	1:F:116:SER:HA	1.94	0.50
1:B:244:GLN:HG2	1:B:282:ILE:HG22	1.94	0.50
1:D:268:VAL:CG2	1:D:304:LEU:HD12	2.40	0.50
1:D:304:LEU:O	1:D:305:GLU:O	2.29	0.50
1:F:357:LEU:CD2	1:F:359:GLN:O	2.59	0.50
1:F:415:ALA:O	1:F:416:ALA:HB2	2.11	0.50
1:A:118:THR:CG2	1:A:120:LEU:H	2.25	0.50
1:D:152:LEU:O	1:D:152:LEU:HG	2.11	0.50
1:D:215:VAL:HG11	1:D:249:LYS:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLN:N	1:D:361:ALA:CA	2.71	0.50
1:E:9:ILE:HG21	1:E:27:GLU:HG2	1.94	0.50
1:E:142:MET:O	1:E:146:GLN:HG3	2.10	0.50
1:B:203:SER:HB3	1:B:204:LEU:O	2.12	0.50
1:D:71:LYS:HD3	1:D:73:HIS:CE1	2.47	0.50
1:D:299:PHE:HB3	1:D:301:LEU:HG	1.93	0.50
1:F:106:PHE:CE1	1:F:107:LEU:HD23	2.47	0.50
1:A:388:ALA:N	1:A:389:ARG:HA	2.27	0.50
1:D:103:ILE:HG22	1:D:107:LEU:HD12	1.92	0.50
1:D:313:PRO:HA	1:D:337:ASN:HB3	1.94	0.50
1:D:355:THR:O	1:D:356:GLU:HB3	2.12	0.50
1:A:139:ARG:NH1	1:A:139:ARG:HG2	2.27	0.49
1:C:280:ARG:HH12	1:C:283:GLU:HB3	1.72	0.49
1:C:369:LYS:HZ3	1:C:430:ASN:HD22	1.60	0.49
1:C:414:ALA:O	1:C:415:ALA:CB	2.59	0.49
1:E:392:TRP:HB2	1:E:397:VAL:CG2	2.41	0.49
1:F:204:LEU:O	1:F:205:ILE:HB	2.11	0.49
1:B:162:VAL:HG13	1:B:192:VAL:C	2.32	0.49
1:D:206:ARG:CG	1:D:207:PRO:HD3	2.42	0.49
1:A:88:PRO:HD3	1:E:188:PHE:CD2	2.48	0.49
1:B:156:ILE:HB	1:B:161:ASP:O	2.12	0.49
1:C:95:PHE:CZ	1:C:177:MET:HE3	2.46	0.49
1:D:256:ARG:HD3	1:D:270:GLU:O	2.12	0.49
1:F:342:VAL:HG23	1:F:365:PHE:CD1	2.46	0.49
1:A:235:SER:HB3	1:A:314:VAL:HG11	1.94	0.49
1:B:96:ALA:O	1:B:130:ASP:HA	2.13	0.49
1:D:360:GLN:HA	1:D:361:ALA:HB2	1.94	0.49
2:B:2054:HOH:O	1:F:200:PHE:CB	2.61	0.49
1:C:429:ALA:HA	1:C:432:VAL:CG1	2.42	0.49
1:E:214:LEU:HD21	1:E:318:LEU:HD22	1.94	0.49
1:E:335:ILE:HD12	1:E:357:LEU:HD23	1.94	0.49
1:F:139:ARG:HG3	1:F:139:ARG:O	2.12	0.49
1:F:323:GLN:HG2	1:F:347:ASN:O	2.13	0.49
1:F:396:LYS:HE2	1:F:400:ARG:NH1	2.24	0.49
1:C:95:PHE:HZ	1:C:177:MET:HE3	1.77	0.49
1:C:244:GLN:NE2	1:C:282:ILE:HG12	2.27	0.49
1:C:258:ILE:O	1:C:259:THR:HG23	2.12	0.49
1:E:5:VAL:CG2	1:E:37:VAL:HG21	2.43	0.49
1:F:269:ASP:HB2	1:F:301:LEU:HD13	1.94	0.49
1:F:418:ARG:N	1:F:419:TYR:CB	2.75	0.49
1:A:90:LYS:HG3	1:A:115:ASP:OD2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG21	1:C:442:MET:HE1	1.93	0.49
1:D:259:THR:O	1:D:273:PHE:CE1	2.66	0.49
1:A:116:SER:C	1:A:118:THR:H	2.16	0.49
1:C:297:LYS:HG2	1:C:298:GLU:H	1.75	0.49
1:C:401:LEU:O	1:C:405:MET:HG2	2.13	0.49
1:D:322:THR:O	1:D:325:GLU:HG2	2.13	0.49
1:E:385:GLN:C	1:E:387:ALA:N	2.66	0.49
1:A:24:GLN:HG3	1:A:25:THR:N	2.27	0.49
1:B:75:ASN:HB3	1:B:130:ASP:OD1	2.13	0.49
1:B:91:GLY:HA3	1:B:125:ALA:O	2.12	0.49
1:A:143:ARG:HD3	1:B:66:GLU:OE2	2.13	0.49
1:D:4:TYR:CE1	1:D:44:GLU:HG3	2.48	0.49
1:F:287:SER:O	1:F:288:ARG:C	2.51	0.49
1:D:324:ASN:HA	1:D:349:PRO:O	2.13	0.48
1:A:192:VAL:HG13	1:A:193:LEU:HG	1.95	0.48
1:B:221:MET:HG3	1:B:423:TYR:OH	2.13	0.48
1:D:109:PHE:CE2	1:D:113:PHE:HE2	2.31	0.48
1:D:298:GLU:O	1:D:298:GLU:HG3	2.12	0.48
1:E:58:VAL:HB	1:F:60:GLU:HB2	1.95	0.48
1:E:198:ARG:H	1:E:198:ARG:NH1	2.11	0.48
1:F:106:PHE:CD1	1:F:106:PHE:C	2.87	0.48
1:F:447:ALA:HA	1:F:448:TRP:C	2.33	0.48
1:A:219:GLU:HG2	1:A:229:PHE:CD2	2.47	0.48
1:C:142:MET:O	1:C:146:GLN:HG3	2.13	0.48
1:C:215:VAL:CG1	1:C:249:LYS:HG3	2.44	0.48
1:D:356:GLU:CA	1:D:358:PHE:N	2.54	0.48
1:E:287:SER:O	1:E:288:ARG:C	2.51	0.48
1:F:65:TRP:CE2	1:F:73:HIS:HB2	2.48	0.48
1:F:344:GLU:HG3	1:F:368:GLY:N	2.27	0.48
1:A:49:LEU:O	1:A:53:VAL:HG22	2.13	0.48
1:F:36:VAL:O	1:F:40:HIS:CD2	2.64	0.48
1:F:214:LEU:O	1:F:218:THR:HG23	2.14	0.48
1:A:49:LEU:HD23	1:A:49:LEU:N	2.28	0.48
1:A:178:TYR:HB2	1:A:193:LEU:HD12	1.95	0.48
1:B:310:TRP:O	1:B:334:LEU:HD13	2.13	0.48
1:C:109:PHE:CE2	1:C:113:PHE:HE2	2.32	0.48
1:C:262:ASP:CG	1:C:263:SER:H	2.17	0.48
1:C:342:VAL:HG22	1:C:365:PHE:CD1	2.47	0.48
1:C:385:GLN:HE22	1:C:397:VAL:HG22	1.78	0.48
1:D:356:GLU:H	1:D:357:LEU:CB	2.25	0.48
1:E:156:ILE:HG22	1:E:161:ASP:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HG	1:A:278:LEU:O	2.13	0.48
1:A:446:ILE:HD12	1:E:142:MET:SD	2.54	0.48
1:C:205:ILE:O	1:C:205:ILE:HG22	2.13	0.48
1:C:401:LEU:O	1:C:401:LEU:HD12	2.14	0.48
1:C:412:SER:O	1:C:413:ALA:CB	2.61	0.48
1:D:317:ALA:HB3	1:D:342:VAL:HG22	1.95	0.48
1:F:413:ALA:O	1:F:414:ALA:O	2.31	0.48
1:A:361:ALA:CB	1:A:363:VAL:HG23	2.43	0.48
1:B:7:ARG:NH1	1:B:11:GLU:OE2	2.47	0.48
1:F:68:ASP:HB2	1:F:140:GLU:OE2	2.13	0.48
1:A:237:SER:HB3	1:A:310:TRP:CZ2	2.48	0.48
1:B:444:GLN:NE2	2:B:2054:HOH:O	2.47	0.48
1:F:100:ASN:CG	1:F:103:ILE:HD12	2.34	0.48
1:A:448:TRP:NE1	1:E:183:LYS:HD2	2.29	0.48
1:C:344:GLU:CD	1:C:349:PRO:HD2	2.34	0.48
1:F:21:GLU:HB3	1:F:106:PHE:CD2	2.49	0.48
1:A:114:LYS:NZ	1:A:372:ASN:OD1	2.37	0.48
1:B:90:LYS:HE2	1:B:162:VAL:O	2.13	0.48
1:C:267:VAL:HG21	1:C:292:VAL:HG12	1.95	0.48
1:C:404:ILE:C	2:C:2057:HOH:O	2.52	0.48
1:E:13:GLU:HG2	1:E:23:VAL:HG13	1.96	0.48
1:F:273:PHE:CE1	1:F:295:TYR:OH	2.67	0.48
1:B:142:MET:O	1:B:146:GLN:HG3	2.14	0.47
1:B:172:ARG:HD3	1:B:176:TYR:CE2	2.49	0.47
1:B:446:ILE:O	1:B:448:TRP:O	2.31	0.47
1:F:368:GLY:O	1:F:369:LYS:C	2.52	0.47
1:C:274:THR:H	1:C:277:LYS:HB3	1.79	0.47
1:C:287:SER:HA	1:C:288:ARG:HA	1.66	0.47
1:C:404:ILE:O	1:C:407:ASP:N	2.47	0.47
1:A:415:ALA:HB2	1:A:432:VAL:HG13	1.95	0.47
1:C:424:ASN:ND2	1:C:426:VAL:HB	2.29	0.47
1:E:356:GLU:O	1:E:357:LEU:CB	2.38	0.47
1:A:278:LEU:O	1:A:281:LEU:O	2.32	0.47
1:B:356:GLU:HA	1:B:357:LEU:O	2.14	0.47
1:C:415:ALA:HA	1:C:416:ALA:C	2.35	0.47
1:F:218:THR:OG1	1:F:229:PHE:HE2	1.98	0.47
1:F:310:TRP:CE3	1:F:310:TRP:HA	2.49	0.47
1:C:51:ARG:NH1	1:C:448:TRP:O	2.48	0.47
1:C:260:ALA:O	1:C:261:SER:HB3	2.15	0.47
1:C:294:ASP:HA	1:C:297:LYS:HD3	1.97	0.47
1:C:416:ALA:O	1:C:418:ARG:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:VAL:O	1:E:125:ALA:HB1	2.15	0.47
1:B:83:ASN:HD21	1:B:441:MET:CE	2.27	0.47
1:B:199:SER:HB2	1:B:200:PHE:HD1	1.79	0.47
1:B:262:ASP:HB3	1:B:285:LYS:HZ3	1.80	0.47
1:D:112:ALA:HA	1:D:124:GLY:HA3	1.97	0.47
1:E:218:THR:CG2	1:E:343:ALA:CB	2.92	0.47
1:F:395:GLU:HG3	1:F:396:LYS:N	2.29	0.47
1:A:139:ARG:HH11	1:A:139:ARG:HG2	1.79	0.47
1:A:328:VAL:HG23	1:A:329:ASP:N	2.25	0.47
1:D:18:ASP:C	1:D:20:PRO:HD3	2.34	0.47
1:D:61:PHE:N	1:D:61:PHE:HD1	2.10	0.47
1:E:268:VAL:HG23	1:E:302:VAL:O	2.15	0.47
1:E:293:ALA:N	2:E:2028:HOH:O	2.48	0.47
1:E:342:VAL:HG13	1:E:365:PHE:HD1	1.79	0.47
1:E:383:MET:O	1:E:384:ALA:CB	2.62	0.47
1:F:267:VAL:HG22	1:F:292:VAL:CG1	2.40	0.47
1:A:142:MET:SD	1:C:446:ILE:HG23	2.55	0.47
1:A:280:ARG:O	1:A:282:ILE:O	2.33	0.47
1:C:280:ARG:O	1:C:284:ILE:HG13	2.15	0.47
1:C:389:ARG:HG2	1:E:121:PRO:HG2	1.96	0.47
1:D:99:VAL:CG1	1:D:130:ASP:HA	2.44	0.47
1:D:260:ALA:O	1:D:267:VAL:HG12	2.14	0.47
1:F:163:PRO:HD2	1:F:193:LEU:HD23	1.97	0.47
1:C:233:ARG:NH1	1:C:313:PRO:O	2.48	0.47
1:F:426:VAL:O	1:F:427:ALA:HB3	2.15	0.47
1:A:18:ASP:O	1:A:20:PRO:HD2	2.15	0.47
1:A:282:ILE:H	1:A:282:ILE:HG13	1.37	0.47
1:C:112:ALA:HA	1:C:124:GLY:HA3	1.97	0.47
1:E:258:ILE:HG13	1:E:259:THR:HG23	1.96	0.47
1:F:426:VAL:O	1:F:428:GLY:N	2.48	0.47
1:A:118:THR:HG21	1:A:122:MET:HE2	1.95	0.46
1:B:40:HIS:HB3	1:B:42:GLU:OE2	2.15	0.46
1:E:228:GLY:O	1:E:232:MET:HG3	2.14	0.46
1:F:424:ASN:HD21	1:F:426:VAL:HB	1.81	0.46
1:A:90:LYS:HG2	1:A:122:MET:HB3	1.97	0.46
1:C:237:SER:HB3	1:C:310:TRP:CZ2	2.50	0.46
1:D:61:PHE:CB	1:D:151:GLU:HG2	2.45	0.46
1:D:244:GLN:NE2	1:D:282:ILE:HG12	2.29	0.46
1:E:328:VAL:CG1	1:E:329:ASP:N	2.78	0.46
1:E:414:ALA:O	1:E:418:ARG:HB2	2.15	0.46
1:F:275:LYS:H	1:F:275:LYS:HD3	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ARG:NH2	1:B:258:ILE:HD13	2.30	0.46
1:F:359:GLN:CA	1:F:360:GLN:C	2.79	0.46
1:A:36:VAL:O	1:A:40:HIS:HD2	1.98	0.46
1:A:267:VAL:CG2	1:A:292:VAL:HG13	2.46	0.46
1:B:338:GLY:O	1:B:339:VAL:C	2.53	0.46
1:C:120:LEU:CD1	1:C:380:GLY:HA3	2.46	0.46
1:D:146:GLN:NE2	1:F:446:ILE:O	2.36	0.46
1:E:219:GLU:HG2	1:E:229:PHE:CD1	2.51	0.46
1:F:259:THR:HA	1:F:267:VAL:O	2.15	0.46
1:F:288:ARG:HA	1:F:289:ASP:HA	1.56	0.46
1:F:310:TRP:HA	1:F:310:TRP:HE3	1.81	0.46
1:A:47:ALA:O	1:A:48:LEU:O	2.34	0.46
1:A:65:TRP:CZ2	1:A:131:PHE:HE1	2.32	0.46
1:B:115:ASP:HB3	1:B:122:MET:HB2	1.97	0.46
1:C:188:PHE:CD2	1:E:88:PRO:HD3	2.51	0.46
1:E:428:GLY:CA	1:E:429:ALA:CB	2.85	0.46
1:E:441:MET:HB2	1:E:441:MET:HE3	1.38	0.46
1:A:338:GLY:O	1:A:339:VAL:C	2.54	0.46
1:D:61:PHE:HB3	1:D:151:GLU:HG2	1.98	0.46
1:D:104:MET:HA	1:D:104:MET:CE	2.45	0.46
1:E:90:LYS:HE3	1:E:162:VAL:HG12	1.97	0.46
1:E:342:VAL:HG13	1:E:365:PHE:CD1	2.50	0.46
1:A:75:ASN:HB3	1:A:130:ASP:OD1	2.16	0.46
1:A:120:LEU:CD2	1:E:390:LEU:HD23	2.45	0.46
1:A:359:GLN:HE22	1:A:424:ASN:ND2	2.14	0.46
1:D:197:ALA:O	1:D:202:GLY:N	2.48	0.46
1:F:236:VAL:HG22	1:F:318:LEU:HB2	1.98	0.46
1:F:358:PHE:CB	1:F:363:VAL:HG13	2.46	0.46
1:A:60:GLU:HG2	1:A:78:TYR:CD2	2.51	0.46
1:A:118:THR:HG23	1:A:120:LEU:H	1.80	0.46
1:C:12:VAL:HG13	1:C:16:TYR:HD2	1.81	0.46
1:D:36:VAL:HA	1:D:419:TYR:CE2	2.50	0.46
1:E:106:PHE:CZ	1:E:107:LEU:HD22	2.51	0.46
1:A:243:ALA:O	1:A:247:ILE:HG13	2.15	0.46
1:E:196:LYS:NZ	1:E:385:GLN:HE22	2.14	0.46
1:F:118:THR:HG21	1:F:376:VAL:HG12	1.98	0.46
1:A:190:ASN:HB2	1:A:196:LYS:HE2	1.97	0.45
1:A:205:ILE:O	1:A:205:ILE:HG22	2.15	0.45
1:A:218:THR:CG2	1:A:343:ALA:HB2	2.46	0.45
1:B:103:ILE:HA	1:B:106:PHE:HD2	1.80	0.45
1:B:287:SER:HA	1:B:288:ARG:C	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ILE:HG22	1:B:441:MET:HE2	1.97	0.45
1:C:249:LYS:HD2	1:C:253:PHE:HE1	1.81	0.45
1:E:116:SER:OG	1:E:436:LYS:HB3	2.15	0.45
1:B:402:HIS:O	1:B:402:HIS:CD2	2.68	0.45
1:D:356:GLU:O	1:D:356:GLU:CG	2.64	0.45
1:B:112:ALA:CA	1:B:124:GLY:HA3	2.46	0.45
1:E:435:GLN:HA	1:E:435:GLN:NE2	2.31	0.45
1:C:369:LYS:HZ1	1:C:430:ASN:HD22	1.63	0.45
1:D:111:GLN:HG3	1:D:115:ASP:OD2	2.16	0.45
1:E:218:THR:HG21	1:E:343:ALA:HB3	1.98	0.45
1:F:117:LEU:O	1:F:117:LEU:HD22	2.16	0.45
1:A:139:ARG:CG	1:A:139:ARG:NH1	2.79	0.45
1:B:13:GLU:HG2	1:B:23:VAL:CG1	2.45	0.45
1:C:111:GLN:HG3	1:C:115:ASP:OD2	2.16	0.45
1:D:208:GLU:HG3	1:D:245:TYR:CD1	2.52	0.45
1:D:448:TRP:CE3	1:D:448:TRP:HA	2.50	0.45
1:E:157:GLY:HA2	1:E:192:VAL:HG23	1.97	0.45
1:A:361:ALA:CB	1:A:362:GLY:CA	2.91	0.45
1:B:188:PHE:CZ	1:D:87:GLY:HA2	2.52	0.45
1:B:196:LYS:HZ1	1:B:386:ASN:ND2	2.13	0.45
1:B:285:LYS:HZ3	1:B:292:VAL:HG22	1.82	0.45
1:C:47:ALA:O	1:C:51:ARG:HG3	2.17	0.45
1:E:360:GLN:O	1:E:360:GLN:CG	2.60	0.45
1:F:218:THR:HG22	1:F:343:ALA:CB	2.47	0.45
1:C:218:THR:HG22	1:C:343:ALA:CB	2.46	0.45
1:D:99:VAL:HG11	1:D:129:SER:O	2.17	0.45
1:D:139:ARG:CG	1:D:139:ARG:NH1	2.74	0.45
1:D:392:TRP:CB	1:D:396:LYS:HD3	2.47	0.45
1:E:1:MET:O	1:E:4:TYR:HB3	2.16	0.45
1:A:115:ASP:O	1:A:118:THR:HB	2.16	0.45
1:B:334:LEU:HD12	1:B:334:LEU:HA	1.88	0.45
1:C:262:ASP:CG	1:C:263:SER:N	2.70	0.45
1:D:188:PHE:CE2	1:F:87:GLY:HA2	2.52	0.45
1:D:269:ASP:OD1	1:D:269:ASP:C	2.55	0.45
1:D:274:THR:OG1	1:D:277:LYS:HG3	2.16	0.45
1:E:389:ARG:O	1:E:391:GLY:N	2.49	0.45
1:F:309:PRO:O	1:F:312:LEU:HB2	2.16	0.45
1:C:262:ASP:N	1:C:292:VAL:HG21	2.32	0.45
1:C:404:ILE:HG22	2:C:2057:HOH:O	2.17	0.45
1:C:408:ILE:O	1:C:412:SER:CB	2.59	0.45
1:F:328:VAL:CG2	1:F:329:ASP:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:GLU:HG2	1:B:299:PHE:CE2	2.52	0.45
1:B:369:LYS:HD2	1:B:369:LYS:HA	1.75	0.45
1:C:66:GLU:CD	1:F:139:ARG:HH11	2.21	0.45
1:A:448:TRP:CE2	1:E:183:LYS:HD2	2.52	0.44
1:C:266:THR:HG1	1:C:308:GLN:HA	1.82	0.44
1:D:100:ASN:O	1:D:104:MET:HG2	2.18	0.44
1:E:64:PRO:HG2	1:F:447:ALA:HB1	1.98	0.44
1:E:416:ALA:O	1:E:417:GLU:C	2.55	0.44
1:E:430:ASN:C	1:E:431:ILE:O	2.54	0.44
1:F:217:PHE:HE2	1:F:366:ALA:HB1	1.82	0.44
1:F:327:ASP:O	1:F:331:ALA:HB2	2.17	0.44
1:B:118:THR:HG21	1:B:376:VAL:HG22	1.99	0.44
1:D:385:GLN:HG2	1:D:392:TRP:CD2	2.52	0.44
1:F:219:GLU:HG2	1:F:229:PHE:CD2	2.48	0.44
1:A:33:LEU:O	1:A:37:VAL:HG12	2.17	0.44
1:C:25:THR:CG2	1:C:106:PHE:HB2	2.48	0.44
1:C:372:ASN:OD1	1:C:372:ASN:C	2.55	0.44
1:C:415:ALA:CA	1:C:416:ALA:C	2.86	0.44
1:E:1:MET:HG3	1:E:4:TYR:N	2.28	0.44
1:F:273:PHE:HE1	1:F:295:TYR:OH	1.99	0.44
1:F:427:ALA:O	1:F:431:ILE:HG22	2.16	0.44
1:B:308:GLN:HB3	1:B:309:PRO:CD	2.47	0.44
1:C:15:LYS:HD3	1:C:16:TYR:CZ	2.53	0.44
1:D:139:ARG:HH11	1:D:139:ARG:HG3	1.82	0.44
1:D:264:SER:HB2	1:D:291:ARG:HH21	1.82	0.44
1:E:221:MET:HG3	1:E:423:TYR:HE2	1.83	0.44
1:B:189:TYR:O	1:B:191:GLY:HA3	2.18	0.44
1:B:356:GLU:CD	1:B:356:GLU:O	2.56	0.44
1:C:360:GLN:O	1:C:362:GLY:N	2.51	0.44
1:C:369:LYS:HB2	1:C:369:LYS:HE3	1.76	0.44
1:D:106:PHE:CD1	1:D:106:PHE:C	2.91	0.44
1:C:280:ARG:HH11	1:C:283:GLU:HB3	1.77	0.44
1:C:356:GLU:CB	1:C:357:LEU:HB2	2.47	0.44
1:E:237:SER:OG	1:E:319:PRO:HA	2.18	0.44
1:F:381:LEU:HD12	1:F:381:LEU:HA	1.78	0.44
1:A:1:MET:O	1:A:38:ASP:OD2	2.36	0.44
1:A:138:ASP:OD2	1:A:176:TYR:OH	2.33	0.44
1:C:103:ILE:HA	1:C:106:PHE:HD2	1.83	0.44
1:C:267:VAL:HG22	1:C:296:ALA:HB2	2.00	0.44
1:C:357:LEU:C	1:C:359:GLN:N	2.68	0.44
1:E:1:MET:HG3	1:E:3:LYS:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:ALA:N	1:E:346:ALA:HB2	2.32	0.44
1:E:390:LEU:C	1:E:391:GLY:O	2.56	0.44
1:F:237:SER:O	1:F:320:CYS:HB2	2.17	0.44
1:A:100:ASN:OD1	1:A:103:ILE:HD12	2.17	0.44
1:B:25:THR:O	1:B:29:VAL:HG23	2.18	0.44
1:C:181:TYR:O	1:C:185:VAL:HG13	2.18	0.44
1:E:86:ILE:HG12	2:E:2008:HOH:O	2.18	0.44
1:E:196:LYS:HB2	1:E:196:LYS:HE2	1.81	0.44
1:A:12:VAL:HG12	1:A:23:VAL:HG22	2.00	0.44
1:A:357:LEU:O	1:A:358:PHE:CG	2.70	0.44
1:B:202:GLY:HA2	1:B:382:GLU:HG3	2.00	0.44
1:C:414:ALA:N	1:C:416:ALA:HB3	2.31	0.44
1:E:81:GLN:HB3	1:E:89:TYR:CD1	2.52	0.44
1:E:205:ILE:HG22	1:E:205:ILE:O	2.18	0.44
1:E:432:VAL:CG1	1:E:433:GLY:N	2.80	0.44
1:F:222:LEU:HD21	1:F:316:ILE:HD11	1.99	0.44
1:F:239:SER:HB3	1:F:285:LYS:HG2	1.98	0.44
1:F:317:ALA:HB3	1:F:342:VAL:HG12	1.98	0.44
1:C:356:GLU:CB	1:C:358:PHE:H	2.30	0.43
1:E:432:VAL:HG13	1:E:433:GLY:N	2.32	0.43
1:F:334:LEU:O	1:F:339:VAL:HG12	2.17	0.43
1:B:380:GLY:HA2	1:B:383:MET:CE	2.47	0.43
1:F:233:ARG:HH12	1:F:270:GLU:CD	2.21	0.43
1:E:81:GLN:HA	1:E:125:ALA:HB2	2.00	0.43
1:E:137:SER:OG	1:E:140:GLU:HG3	2.19	0.43
1:A:352:ILE:H	1:A:352:ILE:HG13	1.52	0.43
1:B:93:LEU:HA	1:B:127:GLY:O	2.17	0.43
1:C:117:LEU:HD22	1:C:408:ILE:HG23	2.01	0.43
1:C:237:SER:HB3	1:C:310:TRP:CH2	2.54	0.43
1:D:79:ARG:HH22	1:D:163:PRO:HA	1.82	0.43
1:E:396:LYS:O	1:E:400:ARG:HD3	2.19	0.43
1:A:26:VAL:HG12	1:A:30:LEU:HD12	2.00	0.43
1:A:189:TYR:C	1:A:190:ASN:O	2.55	0.43
1:A:367:PRO:CD	1:A:425:LEU:HB3	2.48	0.43
1:B:178:TYR:HB2	1:B:193:LEU:HD12	2.01	0.43
1:B:366:ALA:HA	1:B:367:PRO:HD3	1.75	0.43
1:E:163:PRO:HD2	1:E:192:VAL:O	2.18	0.43
1:E:238:GLY:HA3	1:E:320:CYS:O	2.18	0.43
1:F:258:ILE:HG13	1:F:259:THR:HG23	2.01	0.43
1:A:5:VAL:HG13	1:A:30:LEU:HB3	2.00	0.43
1:B:224:ARG:HG3	1:B:225:HIS:CD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ASN:N	1:B:430:ASN:HD22	2.16	0.43
1:C:218:THR:OG1	1:C:229:PHE:CE2	2.71	0.43
1:C:357:LEU:HA	1:C:359:GLN:HB3	1.99	0.43
1:E:100:ASN:OD1	1:E:103:ILE:HG13	2.18	0.43
1:E:221:MET:HA	1:E:423:TYR:OH	2.18	0.43
1:E:249:LYS:HD2	1:E:249:LYS:HA	1.78	0.43
1:E:265:GLY:HA3	1:E:303:TYR:CZ	2.52	0.43
1:E:320:CYS:HA	1:E:346:ALA:N	2.33	0.43
1:B:287:SER:CA	1:B:288:ARG:O	2.51	0.43
1:C:347:ASN:O	1:C:348:MET:C	2.56	0.43
1:D:356:GLU:HA	1:D:358:PHE:HB2	2.01	0.43
1:D:435:GLN:HE21	1:D:435:GLN:HB3	1.57	0.43
1:F:369:LYS:HE3	1:F:430:ASN:OD1	2.19	0.43
1:A:90:LYS:HE2	1:A:90:LYS:HB2	1.70	0.43
1:A:444:GLN:HA	1:E:175:GLY:O	2.19	0.43
1:B:139:ARG:HA	1:B:139:ARG:HD3	1.84	0.43
1:C:2:SER:HB3	1:C:5:VAL:H	1.83	0.43
1:C:448:TRP:HA	1:C:448:TRP:CE3	2.53	0.43
1:D:46:VAL:HG23	1:D:46:VAL:O	2.18	0.43
1:E:400:ARG:O	1:E:404:ILE:HG13	2.18	0.43
1:F:320:CYS:C	1:F:346:ALA:HB2	2.39	0.43
1:F:447:ALA:HB1	1:F:448:TRP:CA	2.47	0.43
1:A:289:ASP:C	1:A:289:ASP:OD1	2.57	0.43
1:B:94:ARG:HE	1:B:94:ARG:HB2	1.57	0.43
1:C:131:PHE:HB2	1:C:144:PHE:CZ	2.54	0.43
1:C:269:ASP:HB2	1:C:301:LEU:HD13	2.01	0.43
1:E:360:GLN:HE21	1:E:360:GLN:HB2	1.64	0.43
1:E:429:ALA:N	1:E:432:VAL:HG12	2.30	0.43
1:A:93:LEU:HA	1:A:127:GLY:O	2.18	0.43
1:A:274:THR:OG1	1:A:277:LYS:HG3	2.18	0.43
1:B:181:TYR:CZ	1:B:185:VAL:HG11	2.54	0.43
1:C:385:GLN:NE2	1:C:397:VAL:HG22	2.34	0.43
1:D:376:VAL:O	1:D:379:SER:HB2	2.18	0.43
1:D:381:LEU:HD12	1:D:381:LEU:HA	1.85	0.43
1:B:225:HIS:HE1	1:B:423:TYR:CE2	2.37	0.42
1:B:289:ASP:O	1:B:291:ARG:NH1	2.52	0.42
1:B:448:TRP:CE2	1:F:183:LYS:HD2	2.53	0.42
1:D:188:PHE:CD2	1:F:87:GLY:HA2	2.54	0.42
1:B:47:ALA:HA	1:B:50:GLU:OE1	2.19	0.42
1:C:378:THR:HG21	1:C:401:LEU:HD22	2.02	0.42
1:E:56:GLU:OE2	1:E:84:GLY:N	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ILE:HD13	1:E:174:ILE:HA	1.83	0.42
1:F:378:THR:HA	1:F:381:LEU:HD22	2.01	0.42
1:A:96:ALA:O	1:A:130:ASP:HA	2.18	0.42
1:D:428:GLY:O	1:D:432:VAL:HG22	2.18	0.42
1:F:22:PHE:CE2	1:F:105:LYS:HE2	2.55	0.42
1:F:92:GLY:HA2	1:F:164:ALA:H	1.84	0.42
1:A:88:PRO:HB3	1:A:159:ASP:O	2.20	0.42
1:A:421:LEU:HD23	1:A:427:ALA:CB	2.50	0.42
1:D:206:ARG:HB2	2:D:2035:HOH:O	2.19	0.42
1:E:429:ALA:O	1:E:430:ASN:CG	2.58	0.42
1:F:355:THR:C	1:F:357:LEU:CA	2.58	0.42
1:F:359:GLN:CA	1:F:362:GLY:H	2.33	0.42
1:A:183:LYS:HD2	1:C:448:TRP:CE2	2.54	0.42
1:B:328:VAL:HG22	1:B:357:LEU:HD11	2.00	0.42
1:D:218:THR:CG2	1:D:343:ALA:CB	2.98	0.42
1:D:218:THR:HG21	1:D:343:ALA:HB3	2.02	0.42
1:D:243:ALA:O	1:D:247:ILE:HG13	2.20	0.42
1:A:360:GLN:C	1:A:361:ALA:O	2.55	0.42
1:D:388:ALA:HA	1:F:387:ALA:HB3	2.01	0.42
1:E:127:GLY:HA2	2:E:2012:HOH:O	2.19	0.42
1:E:244:GLN:CD	1:E:282:ILE:HD12	2.40	0.42
1:F:402:HIS:HD2	1:F:402:HIS:O	2.01	0.42
1:B:33:LEU:HD13	1:B:434:PHE:CG	2.55	0.42
1:D:198:ARG:HA	1:D:202:GLY:HA3	2.02	0.42
1:D:284:ILE:HG12	1:D:285:LYS:N	2.34	0.42
1:E:94:ARG:HG2	1:E:99:VAL:CG2	2.49	0.42
1:E:201:GLY:HA2	1:E:202:GLY:HA3	1.69	0.42
1:F:71:LYS:HE3	1:F:71:LYS:HB2	1.88	0.42
1:F:342:VAL:CG2	1:F:365:PHE:HD1	2.32	0.42
1:B:122:MET:SD	1:B:383:MET:HE1	2.60	0.42
1:B:331:ALA:HB3	1:B:357:LEU:HD12	2.01	0.42
1:C:16:TYR:HB3	1:C:19:GLU:HB2	2.02	0.42
1:C:61:PHE:CZ	1:C:77:GLY:HA3	2.54	0.42
1:E:13:GLU:HG2	1:E:23:VAL:CG1	2.50	0.42
1:E:288:ARG:HA	1:E:289:ASP:HA	1.83	0.42
1:A:12:VAL:HG13	1:A:16:TYR:HD2	1.84	0.42
1:A:198:ARG:HE	1:A:198:ARG:N	2.10	0.42
1:C:93:LEU:HA	1:C:127:GLY:O	2.20	0.42
1:D:230:GLU:O	1:D:231:GLY:C	2.58	0.42
1:F:67:ASP:HB2	1:F:71:LYS:O	2.20	0.42
1:F:426:VAL:HG12	1:F:427:ALA:H	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:HB3	1:A:19:GLU:HB2	2.01	0.42
1:C:88:PRO:O	1:C:89:TYR:C	2.58	0.42
1:C:322:THR:HG22	2:C:2041:HOH:O	2.20	0.42
1:E:224:ARG:HA	1:E:224:ARG:HD3	1.80	0.42
1:F:275:LYS:H	1:F:275:LYS:CD	2.33	0.42
1:A:361:ALA:HB1	1:A:362:GLY:CA	2.32	0.41
1:A:444:GLN:O	1:E:179:GLY:HA3	2.20	0.41
1:B:354:ALA:C	1:B:356:GLU:N	2.70	0.41
1:C:61:PHE:CE2	1:C:77:GLY:HA3	2.55	0.41
1:C:288:ARG:O	1:C:290:GLY:N	2.52	0.41
1:C:352:ILE:H	1:C:352:ILE:HG13	1.52	0.41
1:D:21:GLU:HB3	1:D:106:PHE:CD2	2.55	0.41
1:E:278:LEU:O	1:E:281:LEU:HB3	2.20	0.41
1:B:178:TYR:HB2	1:B:193:LEU:CD1	2.49	0.41
1:B:200:PHE:CD1	1:B:200:PHE:N	2.88	0.41
1:B:202:GLY:HA2	1:B:382:GLU:CG	2.50	0.41
1:C:132:ASP:C	1:C:134:ASN:H	2.23	0.41
1:C:207:PRO:HD2	1:C:208:GLU:OE1	2.19	0.41
1:C:267:VAL:CG2	1:C:296:ALA:HB2	2.49	0.41
1:E:4:TYR:CE1	1:E:44:GLU:HG3	2.55	0.41
1:E:4:TYR:O	1:E:8:VAL:HG23	2.19	0.41
1:E:325:GLU:HG2	1:E:349:PRO:HB3	2.01	0.41
1:F:274:THR:HG23	1:F:277:LYS:HE3	2.02	0.41
1:A:82:PHE:CZ	1:A:109:PHE:HD1	2.38	0.41
1:A:216:TYR:CE1	1:A:402:HIS:CD2	3.08	0.41
1:A:280:ARG:HD2	1:A:280:ARG:HA	1.86	0.41
1:A:323:GLN:HG3	1:A:347:ASN:O	2.20	0.41
1:B:308:GLN:NE2	1:B:325:GLU:O	2.46	0.41
1:D:245:TYR:HD1	1:D:248:GLU:OE1	2.03	0.41
1:F:43:TYR:HA	1:F:442:MET:HE3	2.02	0.41
1:F:388:ALA:O	1:F:390:LEU:HD22	2.20	0.41
1:B:90:LYS:CD	1:B:383:MET:HE1	2.45	0.41
1:B:237:SER:OG	1:B:319:PRO:HA	2.21	0.41
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.89	0.41
1:A:400:ARG:HE	1:E:390:LEU:HD21	1.85	0.41
1:C:95:PHE:CZ	1:C:177:MET:CE	3.02	0.41
1:C:173:GLU:C	1:C:174:ILE:O	2.55	0.41
1:C:366:ALA:HA	1:C:367:PRO:HD3	1.88	0.41
1:E:221:MET:HG3	1:E:423:TYR:CE2	2.55	0.41
1:F:60:GLU:HG2	1:F:78:TYR:CD1	2.55	0.41
1:F:358:PHE:HB3	1:F:363:VAL:HG13	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASN:ND2	1:B:131:PHE:HA	2.36	0.41
1:D:139:ARG:NH1	1:D:139:ARG:HG2	2.34	0.41
1:D:388:ALA:HA	1:F:387:ALA:CB	2.50	0.41
1:E:428:GLY:N	1:E:429:ALA:HB3	2.36	0.41
1:E:430:ASN:O	1:E:431:ILE:CB	2.69	0.41
1:F:47:ALA:O	1:F:51:ARG:HG3	2.20	0.41
1:F:205:ILE:O	1:F:205:ILE:HG22	2.20	0.41
1:D:46:VAL:O	1:D:48:LEU:N	2.54	0.41
1:D:196:LYS:HE3	1:D:196:LYS:HB2	1.95	0.41
1:D:309:PRO:C	1:D:311:SER:H	2.23	0.41
1:E:94:ARG:O	1:E:99:VAL:HG21	2.21	0.41
1:E:118:THR:O	1:E:119:THR:OG1	2.28	0.41
1:A:1:MET:HG3	1:A:2:SER:H	1.84	0.41
1:A:218:THR:HG21	1:A:343:ALA:HB2	2.00	0.41
1:A:428:GLY:O	1:A:432:VAL:HG22	2.21	0.41
1:B:47:ALA:O	1:B:51:ARG:HG3	2.20	0.41
1:D:322:THR:OG1	1:D:323:GLN:N	2.54	0.41
1:E:378:THR:CG2	1:E:401:LEU:HD13	2.51	0.41
1:F:115:ASP:OD2	1:F:123:GLY:O	2.39	0.41
1:A:4:TYR:HD2	1:A:37:VAL:CG2	2.34	0.41
1:A:54:ILE:HA	1:A:55:PRO:HD3	1.96	0.41
1:A:354:ALA:O	1:A:357:LEU:O	2.38	0.41
1:A:367:PRO:HD3	1:A:425:LEU:HB3	2.03	0.41
1:B:223:LYS:C	1:B:225:HIS:N	2.73	0.41
1:C:171:ALA:O	1:C:174:ILE:O	2.39	0.41
1:C:237:SER:OG	1:C:325:GLU:OE1	2.37	0.41
1:C:321:ALA:HB3	1:C:325:GLU:CD	2.41	0.41
1:D:218:THR:HA	1:D:221:MET:HB3	2.02	0.41
1:D:313:PRO:HB3	1:D:337:ASN:ND2	2.34	0.41
1:D:416:ALA:O	1:D:419:TYR:O	2.39	0.41
1:F:81:GLN:HG2	1:F:89:TYR:CG	2.56	0.41
1:F:334:LEU:C	1:F:339:VAL:HG12	2.41	0.41
1:F:388:ALA:O	1:F:389:ARG:HB2	2.21	0.41
1:B:215:VAL:HG21	1:B:249:LYS:HB3	2.03	0.41
1:C:312:LEU:H	1:C:312:LEU:HD22	1.86	0.41
1:E:285:LYS:HD2	1:E:285:LYS:HA	1.91	0.41
1:E:328:VAL:HG12	1:E:329:ASP:N	2.36	0.41
1:F:358:PHE:CB	1:F:363:VAL:CG1	2.91	0.41
1:A:106:PHE:CD1	1:A:106:PHE:C	2.95	0.40
1:A:156:ILE:HB	1:A:161:ASP:O	2.21	0.40
1:A:210:THR:HG21	1:A:242:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:O	1:A:302:VAL:HG13	2.21	0.40
1:B:22:PHE:O	1:B:26:VAL:HG23	2.20	0.40
1:C:132:ASP:HA	1:C:133:PRO:HD3	1.92	0.40
1:C:218:THR:CG2	1:C:343:ALA:CB	2.99	0.40
1:C:282:ILE:O	1:C:286:ALA:HB2	2.21	0.40
1:D:30:LEU:HD23	1:D:33:LEU:HD12	2.02	0.40
1:E:205:ILE:O	1:E:205:ILE:CG2	2.69	0.40
1:E:344:GLU:HB2	1:E:368:GLY:N	2.36	0.40
1:F:225:HIS:HB2	1:F:364:LEU:HD21	2.03	0.40
1:F:357:LEU:C	1:F:359:GLN:N	2.74	0.40
1:C:225:HIS:ND1	1:C:364:LEU:HD21	2.36	0.40
1:C:357:LEU:H	1:C:359:GLN:HB2	1.86	0.40
1:E:422:GLY:O	1:E:423:TYR:C	2.58	0.40
1:F:351:THR:O	1:F:354:ALA:O	2.39	0.40
1:B:107:LEU:CB	1:B:126:LYS:HG2	2.51	0.40
1:B:278:LEU:HD12	1:B:278:LEU:C	2.41	0.40
1:C:212:TYR:CD2	1:C:249:LYS:HE3	2.56	0.40
1:D:94:ARG:HD3	2:D:2020:HOH:O	2.21	0.40
1:D:244:GLN:HE21	1:D:282:ILE:HG12	1.85	0.40
1:E:268:VAL:HG23	1:E:302:VAL:HG22	2.03	0.40
1:F:61:PHE:CG	1:F:151:GLU:HG2	2.57	0.40
1:F:404:ILE:O	1:F:408:ILE:HG13	2.20	0.40
1:A:1:MET:HA	1:A:34:GLY:HA3	2.04	0.40
1:A:216:TYR:OH	1:A:398:ASP:OD1	2.34	0.40
1:A:342:VAL:CG1	1:A:365:PHE:HD1	2.34	0.40
1:D:169:VAL:HG12	1:D:174:ILE:HD12	2.03	0.40
1:E:264:SER:HB3	1:E:291:ARG:NH2	2.37	0.40
1:F:223:LYS:C	1:F:225:HIS:N	2.73	0.40
1:B:424:ASN:OD1	1:B:426:VAL:CG2	2.70	0.40
1:C:169:VAL:HG13	1:C:173:GLU:HB2	2.02	0.40
1:C:206:ARG:N	1:C:207:PRO:CD	2.85	0.40
1:D:27:GLU:HG3	1:D:28:GLU:N	2.37	0.40
1:D:86:ILE:HD11	1:D:116:SER:HA	2.03	0.40
1:E:364:LEU:HD23	1:E:364:LEU:HA	1.75	0.40
1:E:421:LEU:HB3	1:E:422:GLY:H	1.54	0.40
1:F:112:ALA:HA	1:F:124:GLY:HA3	2.04	0.40
1:F:113:PHE:O	1:F:117:LEU:HB2	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	442/448 (99%)	399 (90%)	33 (8%)	10 (2%)	6	16
1	B	445/448 (99%)	407 (92%)	29 (6%)	9 (2%)	7	19
1	C	445/448 (99%)	390 (88%)	43 (10%)	12 (3%)	5	12
1	D	440/448 (98%)	380 (86%)	44 (10%)	16 (4%)	3	7
1	E	446/448 (100%)	386 (86%)	42 (9%)	18 (4%)	3	6
1	F	445/448 (99%)	377 (85%)	56 (13%)	12 (3%)	5	12
All	All	2663/2688 (99%)	2339 (88%)	247 (9%)	77 (3%)	4	10

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	49	LEU
1	A	205	ILE
1	A	289	ASP
1	A	328	VAL
1	A	358	PHE
1	B	190	ASN
1	B	205	ILE
1	B	287	SER
1	B	288	ARG
1	B	358	PHE
1	B	385	GLN
1	C	205	ILE
1	C	413	ALA
1	C	414	ALA
1	C	415	ALA
1	C	417	GLU
1	D	47	ALA
1	D	260	ALA
1	D	284	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	305	GLU
1	D	356	GLU
1	E	166	ASP
1	E	201	GLY
1	E	205	ILE
1	E	357	LEU
1	E	360	GLN
1	E	363	VAL
1	E	373	ALA
1	E	384	ALA
1	E	390	LEU
1	E	431	ILE
1	F	205	ILE
1	F	287	SER
1	F	355	THR
1	F	414	ALA
1	F	416	ALA
1	A	280	ARG
1	C	99	VAL
1	C	226	GLY
1	C	361	ALA
1	C	430	ASN
1	D	202	GLY
1	D	309	PRO
1	D	358	PHE
1	E	391	GLY
1	E	394	ALA
1	E	423	TYR
1	F	166	ASP
1	F	360	GLN
1	F	422	GLY
1	A	189	TYR
1	C	416	ALA
1	D	285	LYS
1	D	388	ALA
1	D	418	ARG
1	F	67	ASP
1	F	418	ARG
1	A	339	VAL
1	B	447	ALA
1	D	72	VAL
1	E	386	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	421	LEU
1	C	171	ALA
1	D	188	PHE
1	D	205	ILE
1	E	288	ARG
1	E	393	LYS
1	F	415	ALA
1	A	241	ASN
1	B	357	LEU
1	D	420	GLY
1	E	430	ASN
1	F	292	VAL
1	B	339	VAL
1	C	348	MET
1	D	302	VAL

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	340/343 (99%)	302 (89%)	38 (11%)	6	13
1	B	342/343 (100%)	309 (90%)	33 (10%)	8	19
1	C	342/343 (100%)	310 (91%)	32 (9%)	8	20
1	D	339/343 (99%)	310 (91%)	29 (9%)	10	24
1	E	343/343 (100%)	304 (89%)	39 (11%)	5	13
1	F	341/343 (99%)	304 (89%)	37 (11%)	6	14
All	All	2047/2058 (100%)	1839 (90%)	208 (10%)	7	17

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	48	LEU
1	A	82	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	90	LYS
1	A	98	SER
1	A	106	PHE
1	A	117	LEU
1	A	118	THR
1	A	138	ASP
1	A	139	ARG
1	A	166	ASP
1	A	198	ARG
1	A	219	GLU
1	A	251	MET
1	A	257	VAL
1	A	259	THR
1	A	271	SER
1	A	280	ARG
1	A	281	LEU
1	A	302	VAL
1	A	304	LEU
1	A	305	GLU
1	A	322	THR
1	A	325	GLU
1	A	326	LEU
1	A	328	VAL
1	A	334	LEU
1	A	339	VAL
1	A	352	ILE
1	A	357	LEU
1	A	358	PHE
1	A	376	VAL
1	A	381	LEU
1	A	389	ARG
1	A	390	LEU
1	A	400	ARG
1	A	425	LEU
1	A	432	VAL
1	B	28	GLU
1	B	82	PHE
1	B	90	LYS
1	B	106	PHE
1	B	139	ARG
1	B	172	ARG
1	B	185	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	190	ASN
1	B	196	LYS
1	B	198	ARG
1	B	199	SER
1	B	204	LEU
1	B	218	THR
1	B	222	LEU
1	B	230	GLU
1	B	256	ARG
1	B	282	ILE
1	B	289	ASP
1	B	291	ARG
1	B	292	VAL
1	B	328	VAL
1	B	334	LEU
1	B	342	VAL
1	B	352	ILE
1	B	353	GLU
1	B	364	LEU
1	B	376	VAL
1	B	381	LEU
1	B	389	ARG
1	B	395	GLU
1	B	418	ARG
1	B	432	VAL
1	B	444	GLN
1	C	2	SER
1	C	27	GLU
1	C	82	PHE
1	C	106	PHE
1	C	117	LEU
1	C	156	ILE
1	C	166	ASP
1	C	185	VAL
1	C	198	ARG
1	C	222	LEU
1	C	224	ARG
1	C	251	MET
1	C	264	SER
1	C	283	GLU
1	C	289	ASP
1	C	291	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	305	GLU
1	C	322	THR
1	C	328	VAL
1	C	342	VAL
1	C	352	ILE
1	C	357	LEU
1	C	358	PHE
1	C	360	GLN
1	C	369	LYS
1	C	381	LEU
1	C	389	ARG
1	C	396	LYS
1	C	424	ASN
1	C	436	LYS
1	C	442	MET
1	C	446	ILE
1	D	15	LYS
1	D	18	ASP
1	D	24	GLN
1	D	27	GLU
1	D	61	PHE
1	D	82	PHE
1	D	106	PHE
1	D	139	ARG
1	D	167	LEU
1	D	172	ARG
1	D	174	ILE
1	D	200	PHE
1	D	206	ARG
1	D	221	MET
1	D	222	LEU
1	D	258	ILE
1	D	263	SER
1	D	268	VAL
1	D	298	GLU
1	D	323	GLN
1	D	329	ASP
1	D	357	LEU
1	D	359	GLN
1	D	364	LEU
1	D	381	LEU
1	D	421	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	432	VAL
1	D	435	GLN
1	D	448	TRP
1	E	1	MET
1	E	66	GLU
1	E	82	PHE
1	E	90	LYS
1	E	98	SER
1	E	106	PHE
1	E	107	LEU
1	E	117	LEU
1	E	138	ASP
1	E	139	ARG
1	E	141	VAL
1	E	167	LEU
1	E	172	ARG
1	E	198	ARG
1	E	200	PHE
1	E	222	LEU
1	E	230	GLU
1	E	268	VAL
1	E	280	ARG
1	E	302	VAL
1	E	320	CYS
1	E	322	THR
1	E	328	VAL
1	E	329	ASP
1	E	333	GLN
1	E	334	LEU
1	E	339	VAL
1	E	357	LEU
1	E	360	GLN
1	E	369	LYS
1	E	383	MET
1	E	395	GLU
1	E	400	ARG
1	E	412	SER
1	E	418	ARG
1	E	421	LEU
1	E	423	TYR
1	E	430	ASN
1	E	435	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	25	THR
1	F	33	LEU
1	F	42	GLU
1	F	67	ASP
1	F	82	PHE
1	F	106	PHE
1	F	117	LEU
1	F	118	THR
1	F	130	ASP
1	F	166	ASP
1	F	172	ARG
1	F	185	VAL
1	F	198	ARG
1	F	222	LEU
1	F	227	MET
1	F	263	SER
1	F	275	LYS
1	F	333	GLN
1	F	334	LEU
1	F	350	THR
1	F	353	GLU
1	F	355	THR
1	F	357	LEU
1	F	358	PHE
1	F	359	GLN
1	F	360	GLN
1	F	364	LEU
1	F	378	THR
1	F	381	LEU
1	F	390	LEU
1	F	400	ARG
1	F	412	SER
1	F	421	LEU
1	F	424	ASN
1	F	431	ILE
1	F	432	VAL
1	F	444	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	GLN
1	A	337	ASN
1	A	359	GLN
1	A	430	ASN
1	B	73	HIS
1	B	190	ASN
1	B	323	GLN
1	B	324	ASN
1	B	385	GLN
1	B	386	ASN
1	B	402	HIS
1	B	435	GLN
1	B	444	GLN
1	C	69	ASN
1	C	73	HIS
1	C	244	GLN
1	C	307	GLN
1	C	308	GLN
1	C	385	GLN
1	C	424	ASN
1	C	430	ASN
1	C	444	GLN
1	D	241	ASN
1	D	244	GLN
1	D	323	GLN
1	D	337	ASN
1	D	385	GLN
1	D	402	HIS
1	D	435	GLN
1	E	83	ASN
1	E	359	GLN
1	E	360	GLN
1	E	385	GLN
1	E	435	GLN
1	F	40	HIS
1	F	75	ASN
1	F	244	GLN
1	F	359	GLN
1	F	402	HIS
1	F	424	ASN
1	F	444	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	444/448 (99%)	-0.42	9 (2%) 65 67	42, 66, 105, 141	0
1	B	447/448 (99%)	-0.35	9 (2%) 65 67	41, 64, 92, 147	0
1	C	447/448 (99%)	-0.31	7 (1%) 72 74	44, 62, 109, 156	0
1	D	444/448 (99%)	-0.46	5 (1%) 80 82	43, 66, 105, 148	0
1	E	448/448 (100%)	-0.23	11 (2%) 57 59	47, 66, 98, 144	0
1	F	447/448 (99%)	-0.17	9 (2%) 65 67	47, 73, 107, 145	0
All	All	2677/2688 (99%)	-0.32	50 (1%) 66 69	41, 66, 104, 156	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	289	ASP	5.5
1	B	290	GLY	4.6
1	B	281	LEU	4.5
1	B	286	ALA	4.0
1	B	288	ARG	3.8
1	C	412	SER	3.8
1	A	304	LEU	3.7
1	C	361	ALA	3.7
1	F	357	LEU	3.4
1	C	299	PHE	3.4
1	A	292	VAL	3.3
1	A	297	LYS	3.3
1	F	356	GLU	3.3
1	E	295	TYR	3.2
1	C	305	GLU	3.0
1	F	334	LEU	2.9
1	D	284	ILE	2.9
1	E	288	ARG	2.9
1	F	415	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	281	LEU	2.7
1	A	300	GLY	2.7
1	F	288	ARG	2.7
1	B	287	SER	2.7
1	F	317	ALA	2.7
1	D	361	ALA	2.6
1	A	267	VAL	2.6
1	D	290	GLY	2.5
1	A	295	TYR	2.5
1	A	301	LEU	2.5
1	E	281	LEU	2.4
1	F	425	LEU	2.4
1	E	257	VAL	2.4
1	D	285	LYS	2.3
1	E	297	LYS	2.3
1	B	282	ILE	2.3
1	B	289	ASP	2.3
1	B	299	PHE	2.3
1	C	289	ASP	2.3
1	C	357	LEU	2.3
1	E	386	ASN	2.2
1	F	264	SER	2.2
1	B	291	ARG	2.2
1	C	286	ALA	2.1
1	A	270	GLU	2.1
1	E	296	ALA	2.1
1	F	236	VAL	2.1
1	E	301	LEU	2.1
1	E	286	ALA	2.1
1	E	1	MET	2.1
1	D	360	GLN	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.