



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:11 AM UTC

PDB ID : 2PM6 / pdb_00002pm6
Title : Crystal Structure of yeast Sec13/31 edge element of the COPII vesicular coat, native version
Authors : Goldberg, J.; Fath, S.; Mancias, J.D.; Bi, X.
Deposited on : 2007-04-20
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

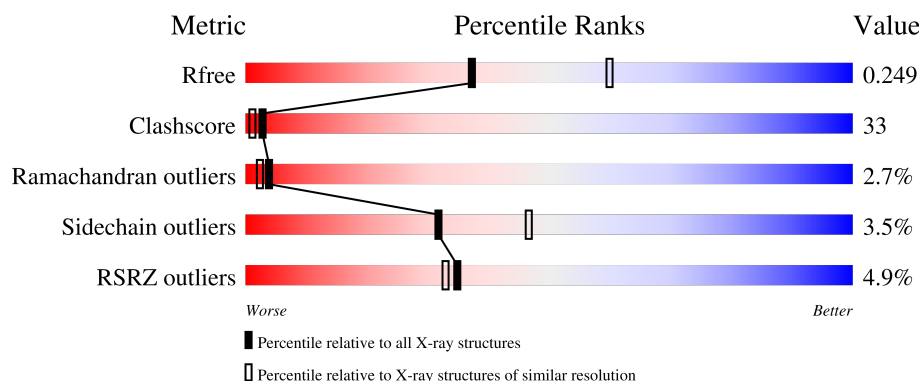
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	399	
1	C	399	
2	B	297	
2	D	297	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10195 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 Protein transport protein SEC31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2729	1728	449	547	5			
1	C	347	Total	C	N	O	S	0	0	0
			2746	1739	452	550	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	GLY	-	cloning artifact	UNP P38968
A	366	ALA	-	cloning artifact	UNP P38968
A	367	MET	-	cloning artifact	UNP P38968
A	368	GLY	-	cloning artifact	UNP P38968
A	369	SER	-	cloning artifact	UNP P38968
C	365	GLY	-	cloning artifact	UNP P38968
C	366	ALA	-	cloning artifact	UNP P38968
C	367	MET	-	cloning artifact	UNP P38968
C	368	GLY	-	cloning artifact	UNP P38968
C	369	SER	-	cloning artifact	UNP P38968

- Molecule 2 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2196	1403	375	415	3			
2	D	288	Total	C	N	O	S	0	0	0
			2263	1444	387	429	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		

Continued on next page...

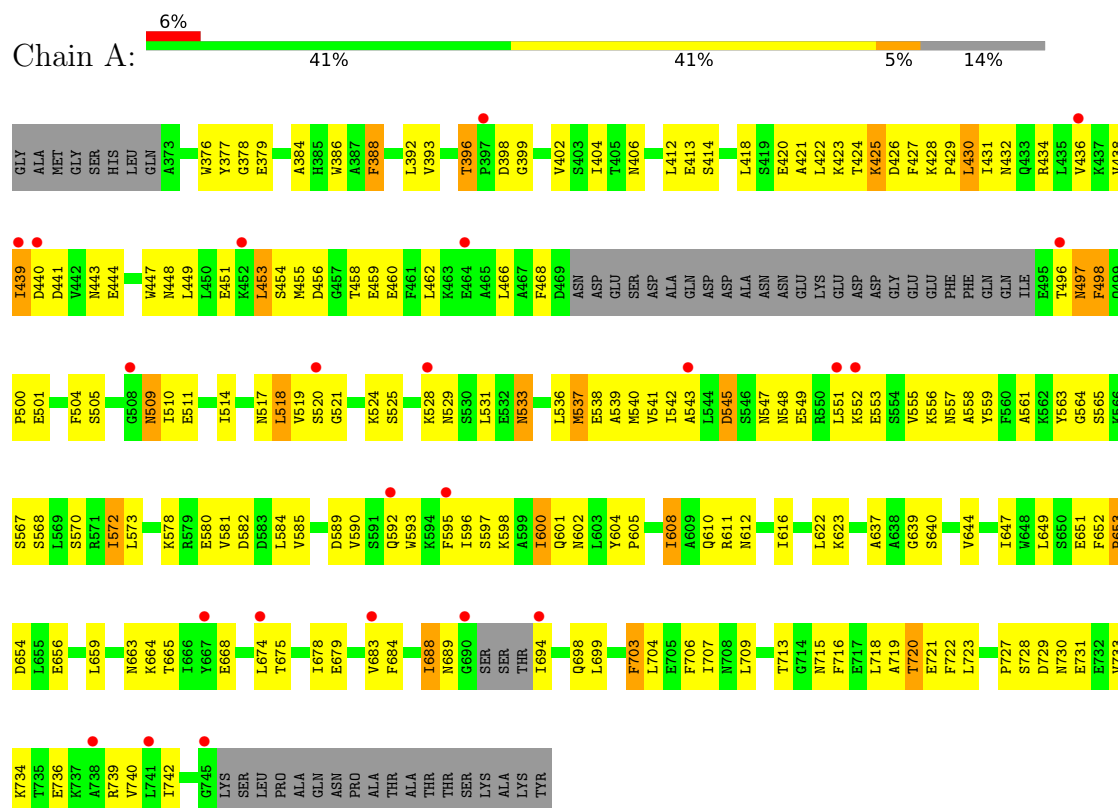
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	61	Total 61	O 61	0	0
3	C	51	Total 51	O 51	0	0
3	D	121	Total 121	O 121	0	0

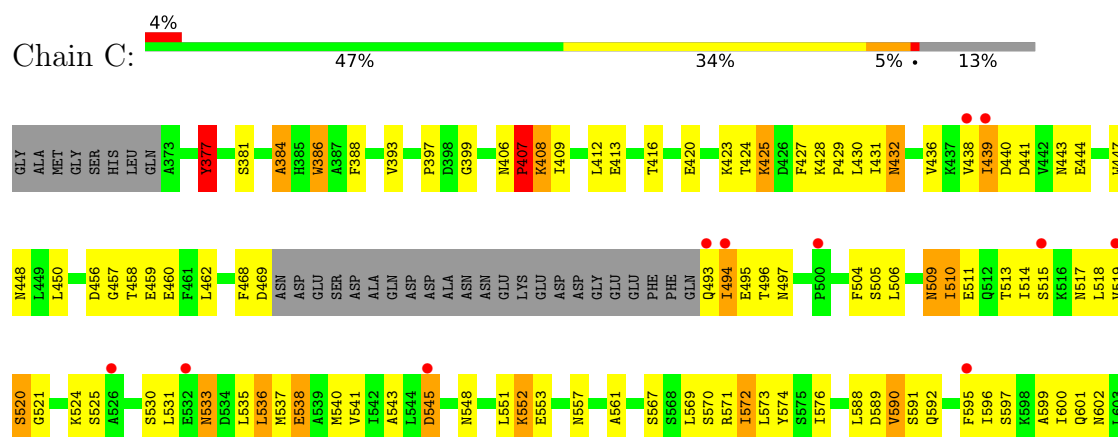
3 Residue-property plots

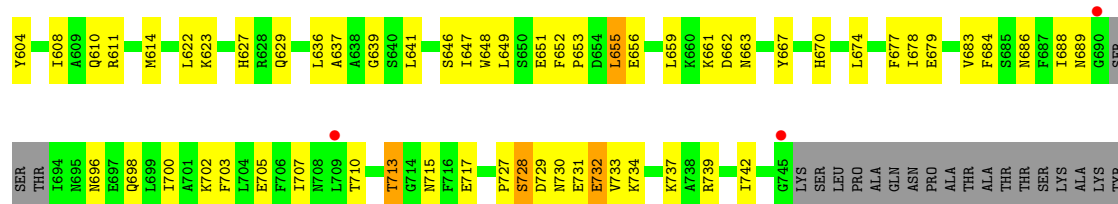
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Protein transport protein SEC31

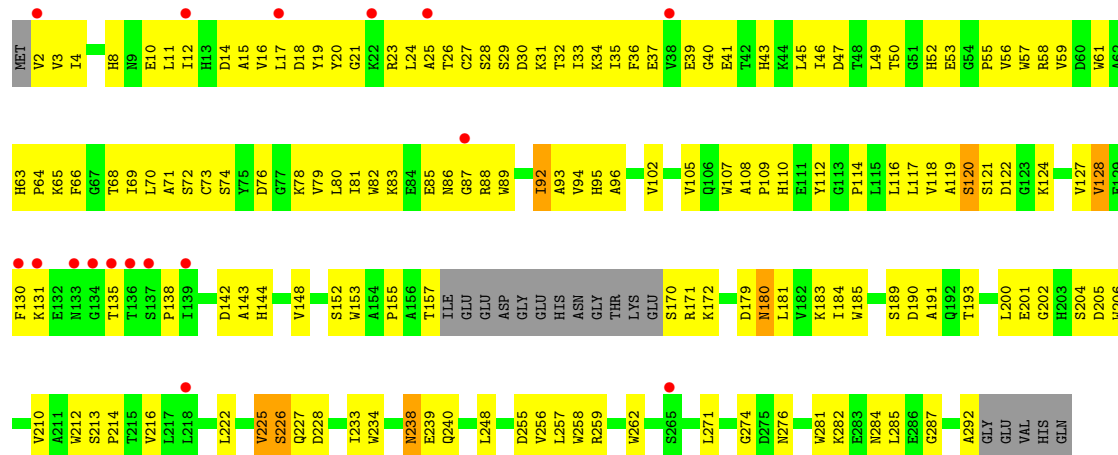


• Molecule 1: Protein transport protein SEC31

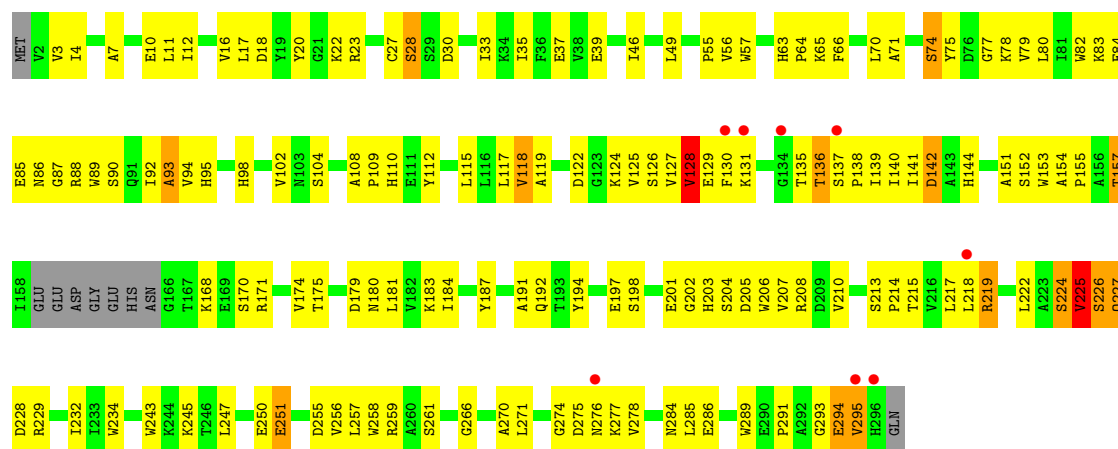




• Molecule 2: Protein transport protein SEC13



• Molecule 2: Protein transport protein SEC13



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.39Å 52.34Å 133.13Å 90.00° 108.62° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 30.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	88.0 (30.00-2.45) 88.0 (30.00-2.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.44Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.301 0.256 , 0.249	Depositor DCC
R_{free} test set	2997 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.39	0/2773	0.91	13/3744 (0.3%)
1	C	0.46	1/2790 (0.0%)	0.93	10/3767 (0.3%)
2	B	0.47	0/2256	0.99	6/3079 (0.2%)
2	D	0.56	0/2324	1.08	22/3170 (0.7%)
All	All	0.47	1/10143 (0.0%)	0.98	51/13760 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	ALA	CA-CB	-5.04	1.45	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	226	SER	N-CA-C	7.98	121.29	109.24
1	C	377	TYR	N-CA-C	7.33	120.55	109.41
1	C	713	THR	N-CA-C	-7.12	104.58	113.20
2	B	128	VAL	N-CA-C	7.05	118.27	108.12
2	D	138	PRO	N-CA-C	6.97	121.86	111.41
2	D	225	VAL	N-CA-C	-6.94	98.77	108.27
2	D	207	VAL	N-CA-C	-6.81	99.94	109.21
1	C	533	ASN	N-CA-C	-6.74	99.23	109.95
2	B	120	SER	N-CA-C	6.58	119.89	109.50
2	D	179	ASP	N-CA-C	-6.51	104.49	112.88
1	C	386	TRP	N-CA-C	-6.44	101.25	110.59
1	A	608	ILE	N-CA-C	6.42	117.16	110.62
1	A	377	TYR	N-CA-C	6.26	118.46	109.14
2	B	143	ALA	N-CA-C	6.12	121.67	113.72
1	C	406	ASN	CA-C-N	6.08	127.44	119.84
1	C	406	ASN	C-N-CA	6.08	127.44	119.84
2	D	224	SER	N-CA-C	-6.03	101.08	110.42
1	A	378	GLY	N-CA-C	5.98	123.32	115.36
2	D	57	TRP	N-CA-C	5.92	118.62	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	137	SER	CA-C-N	5.88	125.86	120.03
2	D	137	SER	C-N-CA	5.88	125.86	120.03
2	B	179	ASP	N-CA-C	-5.85	105.72	112.92
2	D	16	VAL	N-CA-C	5.80	116.23	108.11
2	D	227	GLN	N-CA-C	-5.76	105.14	111.82
2	D	250	GLU	N-CA-C	5.76	118.50	111.82
2	D	118	VAL	N-CA-C	5.76	116.17	108.11
2	D	110	HIS	N-CA-C	5.66	117.44	111.28
1	C	441	ASP	N-CA-C	5.64	117.43	111.28
2	D	154	ALA	N-CA-C	-5.57	103.11	110.40
2	D	219	ARG	N-CA-C	5.54	117.88	110.35
1	C	732	GLU	N-CA-C	-5.53	104.07	112.04
1	C	536	LEU	N-CA-C	5.53	117.00	110.97
2	D	136	THR	N-CA-C	5.51	117.45	109.07
1	A	376	TRP	N-CA-C	5.51	116.97	111.07
2	D	142	ASP	N-CA-C	-5.47	100.88	109.25
1	A	533	ASN	N-CA-C	-5.46	100.63	108.60
2	B	287	GLY	N-CA-C	-5.37	107.61	115.72
1	A	384	ALA	N-CA-C	5.36	117.21	110.24
1	A	600	ILE	N-CA-C	-5.35	107.20	111.81
2	D	289	TRP	N-CA-C	5.34	118.18	109.59
1	A	547	ASN	N-CA-C	-5.27	107.40	113.88
2	D	128	VAL	N-CA-C	5.26	115.70	108.12
2	D	226	SER	N-CA-C	5.11	117.18	109.41
1	A	453	LEU	N-CA-C	-5.10	105.85	111.71
2	D	275	ASP	N-CA-C	-5.10	106.33	113.37
1	A	406	ASN	CA-C-N	5.07	125.06	119.89
1	A	406	ASN	C-N-CA	5.07	125.06	119.89
1	C	648	TRP	N-CA-C	5.06	116.87	111.36
1	A	396	THR	CA-C-N	5.04	124.82	119.28
1	A	396	THR	C-N-CA	5.04	124.82	119.28
2	D	213	SER	N-CA-C	5.01	116.80	109.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2729	0	2706	219	0
1	C	2746	0	2725	190	0
2	B	2196	0	2138	174	0
2	D	2263	0	2203	123	0
3	A	28	0	0	15	1
3	B	61	0	0	24	0
3	C	51	0	0	8	0
3	D	121	0	0	15	1
All	All	10195	0	9772	648	1

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 33.

All (648) 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)
2:D:129:GLU:HG2	2:D:130:PHE:H	1.14	1.08
1:C:425:LYS:HE2	1:C:686:ASN:HD21	1.21	1.06
1:C:408:LYS:HD3	1:C:408:LYS:H	1.22	1.04
1:C:688:ILE:HG13	1:C:689:ASN:H	1.21	1.04
2:D:55:PRO:HA	3:D:416:HOH:O	1.55	1.04
1:A:431:ILE:HD11	1:A:683:VAL:HG11	1.42	1.01
2:B:11:LEU:O	2:B:28:SER:HB2	1.61	1.00
2:B:128:VAL:HG22	2:B:138:PRO:HB3	1.43	0.98
1:A:720:THR:HA	1:A:723:LEU:HD12	1.46	0.98
1:A:438:VAL:HG23	1:A:443:ASN:HD22	1.28	0.96
1:C:623:LYS:HE3	1:C:647:ILE:HD12	1.44	0.95
1:C:535:LEU:HB3	1:C:538:GLU:HG3	1.48	0.95
2:D:83:LYS:HB2	2:D:92:ILE:HD13	1.49	0.94
1:C:407:PRO:HD2	3:C:214:HOH:O	1.67	0.94
2:D:124:LYS:HG3	3:D:408:HOH:O	1.69	0.91
1:A:639:GLY:HA2	1:A:688:ILE:HD11	1.51	0.90
1:C:420:GLU:O	1:C:423:LYS:HG2	1.71	0.90
1:A:496:THR:HG23	1:C:557:ASN:HB3	1.54	0.89
2:B:81:ILE:HB	3:B:320:HOH:O	1.73	0.88
1:A:428:LYS:HB2	1:A:429:PRO:HD3	1.54	0.88
2:B:81:ILE:HD13	2:B:93:ALA:HB3	1.54	0.87
1:A:536:LEU:HD23	1:C:537:MET:HE1	1.54	0.87
1:A:412:LEU:HD21	1:A:713:THR:HG22	1.57	0.86
1:C:649:LEU:HD22	1:C:698:GLN:HG2	1.55	0.86
1:C:425:LYS:O	1:C:425:LYS:HD3	1.75	0.86
3:A:245:HOH:O	1:C:602:ASN:HB3	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:GLN:HE21	1:C:506:LEU:HD12	1.40	0.85
2:D:129:GLU:HG2	2:D:130:PHE:N	1.88	0.85
1:C:408:LYS:HE3	2:D:294:GLU:HG2	1.59	0.84
2:B:257:LEU:HD13	2:B:271:LEU:HD21	1.59	0.84
2:B:83:LYS:O	2:B:89:TRP:HA	1.76	0.84
1:C:524:LYS:HG3	1:C:525:SER:H	1.43	0.84
1:C:703:PHE:O	1:C:707:ILE:HG12	1.78	0.84
1:C:494:ILE:HG13	1:C:495:GLU:H	1.42	0.84
2:B:12:ILE:HA	2:B:28:SER:HB3	1.59	0.83
1:A:505:SER:HB3	1:C:589:ASP:HB2	1.62	0.81
1:C:439:ILE:HG21	1:C:659:LEU:HD21	1.63	0.80
1:A:420:GLU:HA	1:A:423:LYS:HE2	1.63	0.80
1:A:518:LEU:HB3	1:C:576:ILE:HD13	1.63	0.80
1:C:427:PHE:O	1:C:431:ILE:HG12	1.81	0.79
2:D:152:SER:HB2	3:D:407:HOH:O	1.80	0.79
1:C:408:LYS:HD3	1:C:408:LYS:N	1.97	0.78
1:A:590:VAL:HG13	1:A:622:LEU:HD23	1.65	0.78
1:C:652:PHE:HB3	1:C:653:PRO:HD3	1.64	0.78
1:C:688:ILE:HG13	1:C:689:ASN:N	1.98	0.78
1:C:393:VAL:HG21	2:D:17:LEU:HG	1.66	0.77
1:A:589:ASP:HB2	1:C:505:SER:HB3	1.67	0.77
2:D:95:HIS:CD2	2:D:128:VAL:HG21	2.20	0.76
1:A:393:VAL:HG22	1:A:404:ILE:HG13	1.67	0.76
2:D:144:HIS:CE1	2:D:183:LYS:HD2	2.19	0.76
1:C:513:THR:HB	3:C:202:HOH:O	1.84	0.75
1:C:524:LYS:HG3	1:C:525:SER:N	2.01	0.75
1:A:719:ALA:O	1:A:723:LEU:HG	1.87	0.75
1:A:723:LEU:HD11	1:A:740:VAL:HG21	1.69	0.75
2:B:10:GLU:HB2	3:B:336:HOH:O	1.86	0.75
1:C:408:LYS:HE3	2:D:294:GLU:CG	2.17	0.74
1:A:652:PHE:HB3	1:A:653:PRO:HD3	1.69	0.74
2:B:117:LEU:HA	3:B:340:HOH:O	1.86	0.73
1:A:578:LYS:O	1:A:580:GLU:HG3	1.88	0.73
1:A:393:VAL:HG21	2:B:17:LEU:HG	1.69	0.73
1:A:496:THR:O	1:A:497:ASN:HB2	1.89	0.73
1:C:592:GLN:HG3	1:C:595:PHE:HB3	1.69	0.72
1:C:428:LYS:HB2	1:C:429:PRO:HD3	1.69	0.72
1:C:510:ILE:HD12	1:C:510:ILE:H	1.55	0.72
2:D:259:ARG:HB2	3:D:413:HOH:O	1.90	0.72
2:B:255:ASP:OD2	2:B:274:GLY:HA3	1.89	0.72
1:C:548:ASN:O	1:C:552:LYS:HB2	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ILE:HD13	1:A:447:TRP:HZ3	1.55	0.71
2:B:105:VAL:HG23	2:B:118:VAL:HG22	1.73	0.71
1:A:518:LEU:HD13	1:C:576:ILE:HD12	1.73	0.71
1:A:388:PHE:HB2	1:A:739:ARG:HH21	1.56	0.70
1:A:428:LYS:NZ	1:A:455:MET:HG2	2.06	0.70
1:C:567:SER:HB3	1:C:570:SER:HB2	1.73	0.70
1:A:665:THR:OG1	1:A:668:GLU:HG3	1.91	0.70
1:A:420:GLU:HG3	1:A:423:LYS:HE2	1.72	0.70
2:B:74:SER:HB3	2:B:76:ASP:OD1	1.91	0.70
1:A:595:PHE:CZ	1:C:515:SER:HB2	2.28	0.69
2:D:78:LYS:HD2	3:D:378:HOH:O	1.91	0.69
2:D:95:HIS:NE2	2:D:128:VAL:HG21	2.08	0.69
2:B:24:LEU:HB3	2:B:36:PHE:HB2	1.76	0.68
1:C:444:GLU:HG2	1:C:448:ASN:ND2	2.08	0.68
2:B:144:HIS:CE1	2:B:183:LYS:HD2	2.28	0.68
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.76	0.68
2:B:274:GLY:C	2:B:276:ASN:H	2.00	0.68
1:A:528:LYS:HG3	1:C:493:GLN:HE22	1.58	0.67
1:A:736:GLU:O	1:A:740:VAL:HG23	1.93	0.67
1:C:425:LYS:HE2	1:C:686:ASN:ND2	2.02	0.67
2:B:53:GLU:HG3	3:B:337:HOH:O	1.93	0.67
1:A:427:PHE:O	1:A:431:ILE:HG12	1.94	0.67
1:A:727:PRO:C	1:A:729:ASP:H	2.01	0.67
1:C:519:VAL:C	1:C:521:GLY:H	2.02	0.67
1:A:590:VAL:HG13	1:A:622:LEU:CD2	2.23	0.67
1:A:402:VAL:HG11	2:B:24:LEU:HD21	1.76	0.67
1:C:509:ASN:N	1:C:509:ASN:HD22	1.92	0.67
2:B:3:VAL:C	2:B:4:ILE:HD12	2.21	0.66
2:D:129:GLU:O	2:D:136:THR:HG22	1.94	0.66
1:A:536:LEU:O	1:A:540:MET:HG3	1.96	0.66
1:A:498:PHE:HB2	1:C:561:ALA:HA	1.77	0.66
1:A:639:GLY:CA	1:A:688:ILE:HD11	2.25	0.66
1:C:439:ILE:HG13	1:C:440:ASP:H	1.60	0.66
1:C:535:LEU:HB3	1:C:538:GLU:CG	2.23	0.66
1:A:557:ASN:HB3	1:C:496:THR:HG23	1.77	0.65
1:C:590:VAL:HG13	1:C:622:LEU:CD2	2.25	0.65
2:D:184:ILE:HD11	2:D:222:LEU:HD11	1.78	0.65
2:B:157:THR:OG1	2:B:170:SER:HB2	1.95	0.65
1:A:414:SER:OG	1:A:715:ASN:HB2	1.96	0.65
1:C:416:THR:HG22	1:C:420:GLU:OE2	1.96	0.65
1:C:647:ILE:O	1:C:651:GLU:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:ILE:CD1	2:D:56:VAL:HG11	2.27	0.65
1:A:519:VAL:C	1:A:521:GLY:H	2.05	0.65
2:D:225:VAL:HG22	2:D:257:LEU:HB3	1.77	0.65
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.79	0.65
2:D:49:LEU:HB3	2:D:82:TRP:CZ3	2.32	0.65
1:A:427:PHE:CD2	1:A:683:VAL:HG22	2.31	0.65
2:D:274:GLY:C	2:D:276:ASN:H	2.05	0.64
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.62	0.64
1:C:408:LYS:H	1:C:408:LYS:CD	2.05	0.64
1:A:557:ASN:HB3	1:C:496:THR:CG2	2.27	0.64
2:B:40:GLY:N	3:B:335:HOH:O	2.30	0.64
2:B:33:ILE:HD11	2:B:56:VAL:HG11	1.80	0.64
2:D:225:VAL:HG22	2:D:257:LEU:CB	2.27	0.64
2:B:18:ASP:HB2	3:B:317:HOH:O	1.97	0.63
2:B:102:VAL:CG2	3:B:353:HOH:O	2.45	0.63
2:B:68:THR:C	2:B:69:ILE:HD12	2.23	0.63
1:C:727:PRO:C	1:C:729:ASP:H	2.06	0.63
1:A:608:ILE:HD13	1:A:611:ARG:HH11	1.62	0.63
2:B:238:ASN:HD22	2:B:240:GLN:H	1.44	0.63
2:D:3:VAL:C	2:D:4:ILE:HD12	2.23	0.63
1:A:458:THR:HG23	1:A:459:GLU:N	2.14	0.63
1:A:537:MET:HE1	1:C:536:LEU:HD23	1.78	0.63
1:C:661:LYS:C	1:C:663:ASN:H	2.06	0.63
1:A:592:GLN:HG3	1:A:595:PHE:HB3	1.80	0.63
2:D:174:VAL:HG23	2:D:183:LYS:O	1.99	0.63
2:B:23:ARG:NH1	2:B:68:THR:HG21	2.14	0.63
1:A:438:VAL:HG23	1:A:443:ASN:ND2	2.07	0.62
1:C:641:LEU:HD13	1:C:688:ILE:HG21	1.82	0.62
1:C:510:ILE:HA	3:C:202:HOH:O	1.99	0.62
2:B:12:ILE:HA	2:B:28:SER:CB	2.30	0.62
1:A:596:ILE:O	1:A:600:ILE:HG12	2.00	0.62
1:A:703:PHE:HA	3:A:200:HOH:O	2.00	0.62
2:B:66:PHE:HE2	2:B:114:PRO:HD3	1.65	0.62
1:A:514:ILE:HA	1:A:517:ASN:HD22	1.65	0.62
1:C:639:GLY:HA2	1:C:688:ILE:HD11	1.81	0.62
1:A:517:ASN:ND2	1:A:529:ASN:HD22	1.98	0.61
1:A:592:GLN:HG3	1:A:592:GLN:O	1.99	0.61
2:B:102:VAL:HG23	3:B:353:HOH:O	2.00	0.61
2:B:157:THR:HG22	2:B:157:THR:O	2.00	0.61
1:A:392:LEU:HD13	3:A:219:HOH:O	2.00	0.61
1:A:458:THR:HG23	1:A:459:GLU:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:TYR:CE2	1:C:610:GLN:HG2	2.36	0.61
1:C:742:ILE:HD12	2:D:20:TYR:CE2	2.35	0.61
2:B:37:GLU:HG2	2:B:46:ILE:HG13	1.82	0.61
2:B:257:LEU:CD1	2:B:271:LEU:HD21	2.30	0.61
2:B:30:ASP:OD1	2:B:32:THR:N	2.34	0.61
1:A:742:ILE:HB	2:B:20:TYR:CD2	2.36	0.61
2:B:189:SER:C	2:B:191:ALA:H	2.09	0.61
1:A:518:LEU:HB3	1:C:576:ILE:CD1	2.31	0.60
1:A:608:ILE:CD1	1:A:611:ARG:HH11	2.14	0.60
2:B:155:PRO:HG3	2:B:214:PRO:HA	1.83	0.60
1:A:675:THR:O	1:A:679:GLU:HG3	2.01	0.60
2:B:4:ILE:HG13	2:B:43:HIS:ND1	2.16	0.60
1:C:553:GLU:HG2	1:C:557:ASN:HD21	1.66	0.60
1:A:559:TYR:CD2	1:C:541:VAL:HG21	2.35	0.60
1:C:458:THR:HG23	1:C:459:GLU:H	1.65	0.60
2:B:200:LEU:HB3	2:B:234:TRP:CZ3	2.36	0.60
1:A:537:MET:O	1:A:541:VAL:HG23	2.02	0.60
1:A:396:THR:HG23	3:A:251:HOH:O	2.01	0.60
2:B:29:SER:HA	2:B:55:PRO:HB3	1.84	0.59
1:C:377:TYR:HB3	3:C:113:HOH:O	2.02	0.59
1:C:663:ASN:C	2:D:285:LEU:HD11	2.26	0.59
2:D:291:PRO:CB	2:D:295:VAL:HG22	2.32	0.59
2:B:180:ASN:N	2:B:180:ASN:HD22	2.00	0.59
1:C:670:HIS:HE1	1:C:705:GLU:OE1	1.86	0.59
1:A:709:LEU:O	1:A:713:THR:HG23	2.02	0.59
2:B:52:HIS:HA	3:B:337:HOH:O	2.01	0.59
2:B:216:VAL:HG12	2:B:216:VAL:O	2.03	0.59
1:A:386:TRP:HA	3:A:219:HOH:O	2.01	0.59
2:D:49:LEU:HD13	2:D:82:TRP:CD2	2.37	0.59
1:A:496:THR:O	1:A:497:ASN:CB	2.51	0.59
1:A:388:PHE:CD1	1:A:739:ARG:CZ	2.86	0.59
2:B:120:SER:HB3	2:B:122:ASP:OD1	2.03	0.59
1:A:674:LEU:O	1:A:678:ILE:HG12	2.03	0.59
1:A:730:ASN:O	1:A:733:VAL:HB	2.03	0.59
1:C:663:ASN:O	2:D:285:LEU:HD11	2.03	0.59
2:B:19:TYR:CD2	2:B:64:PRO:HG2	2.38	0.59
1:A:584:LEU:HD12	1:A:584:LEU:N	2.18	0.58
1:C:592:GLN:HG3	1:C:595:PHE:CB	2.33	0.58
1:A:496:THR:HG23	1:C:557:ASN:CB	2.31	0.58
1:A:511:GLU:HG3	3:A:107:HOH:O	2.03	0.58
2:B:83:LYS:HB2	2:B:92:ILE:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ASN:N	1:A:509:ASN:HD22	2.01	0.58
2:B:225:VAL:HG13	2:B:257:LEU:HB2	1.84	0.58
1:C:438:VAL:HG23	1:C:443:ASN:HD22	1.68	0.58
1:A:612:ASN:O	1:A:616:ILE:HG12	2.03	0.58
2:B:24:LEU:HG	2:B:25:ALA:N	2.19	0.58
2:B:108:ALA:HB1	2:B:109:PRO:CD	2.34	0.57
1:A:731:GLU:O	1:A:734:LYS:HB3	2.04	0.57
1:C:656:GLU:OE2	1:C:670:HIS:HA	2.04	0.57
2:D:255:ASP:OD1	2:D:256:VAL:N	2.35	0.57
1:A:438:VAL:HG22	1:A:439:ILE:N	2.20	0.57
1:A:531:LEU:C	1:A:533:ASN:H	2.13	0.57
2:B:222:LEU:HB2	2:B:234:TRP:HB2	1.85	0.57
1:A:423:LYS:HG3	1:A:424:THR:HG23	1.86	0.57
1:A:593:TRP:C	1:A:595:PHE:H	2.13	0.57
2:D:175:THR:C	3:D:369:HOH:O	2.47	0.57
1:A:468:PHE:CE1	1:A:598:LYS:HE3	2.40	0.57
2:D:79:VAL:HB	2:D:95:HIS:HB3	1.86	0.57
1:A:418:LEU:HG	1:A:718:LEU:HD11	1.87	0.57
1:A:647:ILE:O	1:A:651:GLU:HG3	2.04	0.57
1:C:430:LEU:HD11	1:C:679:GLU:HG2	1.86	0.56
1:C:535:LEU:CB	1:C:538:GLU:HG3	2.31	0.56
2:B:4:ILE:HG13	2:B:43:HIS:CG	2.40	0.56
1:A:551:LEU:C	1:A:553:GLU:H	2.11	0.56
1:C:462:LEU:HD22	1:C:637:ALA:HB2	1.87	0.56
1:A:616:ILE:HD11	1:A:640:SER:HB2	1.88	0.56
1:A:584:LEU:HD12	1:A:584:LEU:H	1.71	0.56
1:C:509:ASN:N	1:C:509:ASN:ND2	2.51	0.56
2:B:4:ILE:HD12	2:B:4:ILE:N	2.20	0.56
1:C:431:ILE:HD11	1:C:683:VAL:HG11	1.88	0.56
2:D:155:PRO:HG3	2:D:214:PRO:HA	1.88	0.56
2:B:69:ILE:HD12	2:B:69:ILE:N	2.21	0.56
1:A:509:ASN:N	1:A:509:ASN:ND2	2.54	0.55
1:A:537:MET:HE1	1:C:536:LEU:CD2	2.36	0.55
1:A:730:ASN:HB3	1:A:733:VAL:CG2	2.36	0.55
2:B:180:ASN:N	2:B:180:ASN:ND2	2.53	0.55
1:A:434:ARG:HG3	1:A:447:TRP:CZ2	2.41	0.55
1:A:528:LYS:HG3	1:C:493:GLN:NE2	2.22	0.55
2:B:66:PHE:CE2	2:B:114:PRO:HD3	2.41	0.55
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.39	0.55
2:B:56:VAL:HA	2:B:74:SER:HB2	1.88	0.55
2:D:210:VAL:HG23	2:D:210:VAL:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:HG3	1:A:423:LYS:CE	2.37	0.55
1:C:519:VAL:C	1:C:521:GLY:N	2.63	0.55
2:B:255:ASP:CG	2:B:256:VAL:H	2.14	0.55
1:C:444:GLU:HG2	1:C:448:ASN:HD21	1.71	0.55
2:B:73:CYS:HB2	2:B:102:VAL:CG1	2.37	0.55
2:D:4:ILE:HD12	2:D:4:ILE:N	2.22	0.55
2:D:33:ILE:HD11	2:D:56:VAL:HG11	1.87	0.54
1:C:535:LEU:HD22	1:C:538:GLU:HG3	1.88	0.54
1:C:733:VAL:O	1:C:737:LYS:HG3	2.07	0.54
2:D:226:SER:HB3	2:D:228:ASP:OD1	2.07	0.54
1:A:510:ILE:HB	3:A:107:HOH:O	2.06	0.54
1:A:623:LYS:HE3	1:A:647:ILE:HD12	1.89	0.54
1:A:517:ASN:HD21	1:A:529:ASN:ND2	2.04	0.54
1:C:519:VAL:HG23	1:C:520:SER:N	2.21	0.54
1:C:551:LEU:HD23	1:C:551:LEU:C	2.33	0.54
1:C:590:VAL:HG13	1:C:622:LEU:HD23	1.90	0.54
2:D:271:LEU:O	2:D:278:VAL:HA	2.08	0.54
1:A:723:LEU:HA	3:A:255:HOH:O	2.08	0.54
2:B:45:LEU:O	2:B:46:ILE:HD13	2.08	0.54
1:C:423:LYS:CG	1:C:424:THR:N	2.71	0.54
2:D:86:ASN:O	2:D:88:ARG:N	2.40	0.54
1:A:418:LEU:HD23	1:A:718:LEU:HD21	1.89	0.53
2:D:28:SER:O	3:D:416:HOH:O	2.19	0.53
2:D:56:VAL:HA	2:D:74:SER:HB2	1.91	0.53
1:C:604:TYR:CZ	1:C:610:GLN:HG2	2.43	0.53
1:C:510:ILE:HG21	1:C:533:ASN:ND2	2.23	0.53
1:C:696:ASN:O	1:C:700:ILE:HG13	2.08	0.53
1:A:742:ILE:H	1:A:742:ILE:HD12	1.73	0.53
1:C:614:MET:HA	1:C:614:MET:HE2	1.90	0.53
2:D:104:SER:OG	2:D:119:ALA:HB3	2.08	0.53
2:B:49:LEU:HB3	2:B:82:TRP:CZ3	2.44	0.53
2:B:80:LEU:CD2	2:B:94:VAL:HG23	2.38	0.53
1:C:707:ILE:O	1:C:710:THR:HB	2.09	0.53
2:D:10:GLU:HG3	2:D:30:ASP:HB3	1.90	0.53
1:A:439:ILE:HG21	1:A:659:LEU:HD21	1.90	0.53
2:B:39:GLU:HB2	3:B:335:HOH:O	2.08	0.53
1:A:388:PHE:CD1	1:A:739:ARG:NH2	2.77	0.53
1:A:593:TRP:C	1:A:595:PHE:N	2.66	0.53
2:D:227:GLN:HA	2:D:256:VAL:HG13	1.90	0.53
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.09	0.53
2:D:225:VAL:CG2	2:D:271:LEU:HD11	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:232:ILE:HD13	2:D:247:LEU:HD23	1.91	0.53
2:B:25:ALA:HB2	2:B:61:TRP:CZ2	2.44	0.52
1:C:494:ILE:HG13	1:C:495:GLU:N	2.18	0.52
2:D:83:LYS:HB3	2:D:92:ILE:HG21	1.90	0.52
2:D:22:LYS:HE2	2:D:39:GLU:OE1	2.09	0.52
2:D:294:GLU:O	2:D:294:GLU:HG3	2.09	0.52
2:B:128:VAL:CG2	2:B:138:PRO:HB3	2.27	0.52
1:A:412:LEU:C	1:A:412:LEU:HD23	2.35	0.52
1:A:608:ILE:HD13	1:A:611:ARG:NH1	2.24	0.52
1:A:505:SER:CB	1:C:589:ASP:HB2	2.37	0.52
1:A:584:LEU:H	1:A:584:LEU:CD1	2.22	0.52
2:B:29:SER:C	2:B:31:LYS:H	2.16	0.52
2:B:80:LEU:HD23	2:B:94:VAL:HG23	1.90	0.52
1:A:451:GLU:O	1:A:454:SER:HB3	2.09	0.52
2:D:232:ILE:HG21	2:D:234:TRP:CE2	2.44	0.52
2:B:33:ILE:CD1	2:B:56:VAL:HG11	2.39	0.52
2:B:117:LEU:HD12	3:B:340:HOH:O	2.08	0.52
1:C:674:LEU:HD21	1:C:705:GLU:HB3	1.91	0.52
1:A:420:GLU:CA	1:A:423:LYS:HE2	2.38	0.52
1:A:540:MET:HE1	1:C:541:VAL:HG23	1.91	0.52
2:B:69:ILE:HG22	2:B:70:LEU:N	2.25	0.52
1:A:688:ILE:HD13	1:A:689:ASN:N	2.25	0.51
1:C:377:TYR:HA	3:C:113:HOH:O	2.11	0.51
2:B:95:HIS:CE1	2:B:128:VAL:HG21	2.46	0.51
1:C:430:LEU:HD23	1:C:430:LEU:O	2.11	0.51
1:A:431:ILE:HD13	1:A:447:TRP:CZ3	2.40	0.51
1:C:727:PRO:C	1:C:729:ASP:N	2.67	0.51
1:A:519:VAL:CG1	1:C:599:ALA:HA	2.40	0.51
2:D:84:GLU:HB2	2:D:89:TRP:CE2	2.46	0.51
2:D:126:SER:HA	2:D:139:ILE:O	2.11	0.51
2:D:274:GLY:C	2:D:276:ASN:N	2.69	0.51
2:D:217:LEU:O	2:D:219:ARG:N	2.44	0.51
1:C:677:PHE:CD2	1:C:678:ILE:HD12	2.46	0.51
1:A:524:LYS:HG3	1:A:525:SER:N	2.26	0.50
2:B:238:ASN:HD22	2:B:240:GLN:N	2.07	0.50
2:D:115:LEU:HD11	2:D:127:VAL:HG12	1.93	0.50
1:C:494:ILE:HG23	1:C:495:GLU:N	2.26	0.50
1:C:636:LEU:HD12	1:C:688:ILE:HD12	1.93	0.50
2:D:11:LEU:O	2:D:28:SER:HB2	2.12	0.50
2:D:55:PRO:HD2	2:D:75:TYR:HB3	1.92	0.50
1:A:567:SER:HB3	1:A:570:SER:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ILE:O	2:B:4:ILE:HG22	2.11	0.50
2:B:33:ILE:HB	2:B:49:LEU:HB2	1.92	0.50
1:A:664:LYS:HA	1:A:668:GLU:OE1	2.11	0.50
2:B:30:ASP:OD1	2:B:30:ASP:C	2.55	0.50
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.77	0.50
1:C:397:PRO:HA	2:D:276:ASN:HD21	1.77	0.50
1:A:608:ILE:HB	1:A:611:ARG:NH1	2.27	0.50
2:B:26:THR:O	2:B:33:ILE:HG23	2.12	0.50
2:D:215:THR:HG23	2:D:215:THR:O	2.11	0.50
1:A:540:MET:HE1	1:C:541:VAL:CG2	2.42	0.50
1:A:727:PRO:C	1:A:729:ASP:N	2.69	0.50
2:B:112:TYR:CZ	2:B:171:ARG:HG2	2.47	0.50
1:A:543:ALA:C	1:A:545:ASP:H	2.19	0.50
1:C:601:GLN:HE22	1:C:611:ARG:HD3	1.77	0.50
1:A:402:VAL:HG11	2:B:24:LEU:CD2	2.42	0.49
2:B:105:VAL:CG2	2:B:116:LEU:HD21	2.41	0.49
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.47	0.49
2:D:33:ILE:HB	2:D:49:LEU:HB2	1.94	0.49
2:D:30:ASP:OD1	2:D:30:ASP:C	2.54	0.49
1:A:432:ASN:O	1:A:436:VAL:HG23	2.11	0.49
1:A:663:ASN:HA	2:B:285:LEU:HD11	1.94	0.49
2:B:95:HIS:HE1	2:B:138:PRO:HG3	1.77	0.49
2:D:10:GLU:CG	2:D:30:ASP:HB3	2.42	0.49
2:D:203:HIS:CE1	2:D:232:ILE:HG12	2.48	0.49
2:B:63:HIS:CD2	3:B:334:HOH:O	2.65	0.49
2:B:148:VAL:O	3:B:338:HOH:O	2.20	0.49
2:D:261:SER:HA	3:D:351:HOH:O	2.13	0.49
1:A:537:MET:HE2	1:C:540:MET:SD	2.51	0.49
1:C:530:SER:O	1:C:533:ASN:O	2.31	0.49
1:A:585:VAL:HA	1:A:596:ILE:HG21	1.95	0.49
2:D:222:LEU:HG	2:D:243:TRP:CZ3	2.48	0.49
1:A:430:LEU:O	1:A:430:LEU:HD23	2.13	0.49
1:A:731:GLU:HA	1:A:734:LYS:HB3	1.93	0.49
2:B:29:SER:C	2:B:31:LYS:N	2.70	0.49
1:A:555:VAL:O	1:A:558:ALA:HB3	2.12	0.49
1:A:568:SER:HB2	1:C:511:GLU:OE1	2.13	0.49
1:A:496:THR:HG22	1:A:497:ASN:N	2.27	0.49
2:B:184:ILE:N	2:B:184:ILE:HD12	2.28	0.49
2:B:57:TRP:O	2:B:58:ARG:HG2	2.14	0.48
1:A:466:LEU:O	1:A:598:LYS:HE2	2.13	0.48
1:A:644:VAL:HG11	1:A:684:PHE:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:VAL:O	2:D:94:VAL:HG13	2.11	0.48
1:A:551:LEU:C	1:A:553:GLU:N	2.71	0.48
2:D:70:LEU:HG	2:D:71:ALA:N	2.28	0.48
2:B:108:ALA:HA	2:B:153:TRP:CD1	2.49	0.48
2:B:225:VAL:HG13	2:B:257:LEU:CB	2.43	0.48
2:D:27:CYS:HB2	2:D:56:VAL:HB	1.94	0.48
1:C:388:PHE:CE1	1:C:739:ARG:HD3	2.49	0.48
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.29	0.48
1:C:733:VAL:HG12	1:C:737:LYS:HE3	1.95	0.48
2:D:10:GLU:HB2	2:D:28:SER:OG	2.14	0.48
2:B:59:VAL:HA	2:B:71:ALA:O	2.14	0.48
2:B:212:TRP:CD2	2:B:222:LEU:HD21	2.49	0.48
1:C:514:ILE:HA	1:C:517:ASN:HD22	1.79	0.48
2:D:227:GLN:HG2	3:D:409:HOH:O	2.13	0.48
2:D:90:SER:O	2:D:92:ILE:HG23	2.14	0.48
1:A:519:VAL:C	1:A:521:GLY:N	2.71	0.48
2:B:69:ILE:CG2	2:B:70:LEU:N	2.77	0.48
2:B:274:GLY:C	2:B:276:ASN:N	2.69	0.48
1:C:439:ILE:HG13	1:C:440:ASP:N	2.27	0.48
1:C:661:LYS:C	1:C:663:ASN:N	2.72	0.48
1:A:514:ILE:HA	1:A:517:ASN:ND2	2.28	0.48
2:B:8:HIS:CE1	2:B:34:LYS:HE2	2.48	0.47
2:B:15:ALA:HA	2:B:25:ALA:O	2.14	0.47
2:B:87:GLY:C	2:B:88:ARG:HG3	2.39	0.47
1:C:456:ASP:O	1:C:460:GLU:HB2	2.14	0.47
1:A:664:LYS:HB3	1:A:668:GLU:HB2	1.95	0.47
2:B:74:SER:C	2:B:76:ASP:N	2.71	0.47
2:B:74:SER:CB	2:B:76:ASP:OD1	2.61	0.47
2:B:93:ALA:HB1	3:B:344:HOH:O	2.14	0.47
2:B:255:ASP:CG	2:B:256:VAL:N	2.72	0.47
2:B:72:SER:O	2:B:79:VAL:HG13	2.14	0.47
2:B:172:LYS:HA	2:B:185:TRP:O	2.14	0.47
2:B:119:ALA:HB1	2:B:148:VAL:HG12	1.96	0.47
1:C:408:LYS:CE	2:D:294:GLU:HG2	2.36	0.47
1:A:426:ASP:OD1	1:A:429:PRO:HD3	2.14	0.47
2:B:27:CYS:HB2	2:B:56:VAL:CG1	2.45	0.47
1:C:424:THR:O	1:C:425:LYS:CB	2.62	0.47
2:B:34:LYS:HB3	2:B:36:PHE:HE1	1.80	0.47
1:C:438:VAL:HG21	1:C:444:GLU:HA	1.97	0.47
2:D:276:ASN:ND2	3:D:310:HOH:O	2.47	0.47
1:A:536:LEU:CD2	1:C:537:MET:HE1	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ASP:CG	2:B:23:ARG:HB3	2.39	0.47
2:B:109:PRO:HD2	2:B:112:TYR:CD1	2.50	0.47
2:B:119:ALA:HB1	2:B:148:VAL:CG1	2.45	0.47
1:C:386:TRP:NE1	2:D:270:ALA:HB2	2.30	0.47
1:C:536:LEU:O	1:C:537:MET:C	2.57	0.47
1:A:593:TRP:O	1:A:595:PHE:N	2.48	0.47
2:B:29:SER:O	2:B:31:LYS:HG3	2.14	0.47
2:D:92:ILE:O	2:D:93:ALA:HB2	2.15	0.47
1:A:392:LEU:CD1	3:A:219:HOH:O	2.61	0.47
1:A:652:PHE:HB3	1:A:653:PRO:CD	2.44	0.47
1:C:589:ASP:C	1:C:591:SER:H	2.23	0.47
1:A:572:ILE:CD1	1:C:504:PHE:HE1	2.28	0.47
1:A:608:ILE:CD1	1:A:611:ARG:NH1	2.78	0.47
2:B:18:ASP:OD2	2:B:23:ARG:HB3	2.14	0.47
2:B:233:ILE:CD1	2:B:248:LEU:HD13	2.43	0.47
1:C:412:LEU:CD2	1:C:713:THR:HG22	2.45	0.47
1:C:641:LEU:HD12	1:C:684:PHE:HE2	1.80	0.47
1:C:731:GLU:HA	1:C:734:LYS:HB3	1.97	0.47
2:D:35:ILE:HG13	2:D:89:TRP:CE2	2.50	0.47
2:D:108:ALA:HB2	2:D:153:TRP:CE2	2.50	0.47
1:C:553:GLU:HG2	1:C:557:ASN:ND2	2.28	0.46
2:D:225:VAL:HG21	2:D:271:LEU:HD11	1.97	0.46
2:D:277:LYS:HG3	2:D:278:VAL:N	2.30	0.46
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.46
2:D:222:LEU:HB2	2:D:234:TRP:HB2	1.97	0.46
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.97	0.46
1:A:542:ILE:HD11	1:C:573:LEU:CD2	2.44	0.46
1:A:542:ILE:HD11	1:C:573:LEU:HD21	1.96	0.46
1:C:438:VAL:HG23	1:C:443:ASN:ND2	2.30	0.46
2:D:141:ILE:HG22	3:D:322:HOH:O	2.14	0.46
2:B:37:GLU:HG2	2:B:46:ILE:CG1	2.44	0.46
2:D:245:LYS:NZ	3:D:335:HOH:O	2.44	0.46
1:A:441:ASP:HA	3:A:212:HOH:O	2.15	0.46
2:B:124:LYS:HE2	2:B:142:ASP:OD1	2.15	0.46
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.50	0.46
1:C:386:TRP:HZ3	3:C:214:HOH:O	1.98	0.46
2:D:98:HIS:ND1	2:D:122:ASP:OD2	2.49	0.46
1:A:739:ARG:HD2	2:B:19:TYR:CZ	2.50	0.46
2:D:65:LYS:HE2	2:D:66:PHE:CZ	2.50	0.46
1:A:718:LEU:O	1:A:722:PHE:HD1	1.98	0.46
2:B:31:LYS:O	3:B:321:HOH:O	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:LEU:HD12	1:C:684:PHE:CE2	2.51	0.46
1:A:436:VAL:O	1:A:436:VAL:HG12	2.16	0.46
1:A:551:LEU:C	1:A:551:LEU:HD23	2.41	0.46
1:A:663:ASN:CA	2:B:285:LEU:HD11	2.46	0.46
2:B:25:ALA:HB2	2:B:61:TRP:HZ2	1.81	0.46
2:B:117:LEU:HB2	2:B:153:TRP:NE1	2.31	0.46
2:D:284:ASN:OD1	2:D:286:GLU:N	2.49	0.46
2:B:127:VAL:HA	3:B:340:HOH:O	2.15	0.46
1:A:392:LEU:HA	3:A:219:HOH:O	2.16	0.45
1:A:412:LEU:CD2	1:A:713:THR:HG22	2.38	0.45
2:B:121:SER:HA	3:B:338:HOH:O	2.15	0.45
1:C:458:THR:HG23	1:C:459:GLU:N	2.30	0.45
1:C:497:ASN:CG	1:C:497:ASN:O	2.59	0.45
2:D:77:GLY:HA2	2:D:102:VAL:HG23	1.98	0.45
1:A:581:VAL:HG11	1:A:600:ILE:HD13	1.98	0.45
1:C:457:GLY:O	1:C:458:THR:C	2.59	0.45
2:D:80:LEU:HD23	2:D:94:VAL:HG23	1.98	0.45
1:C:596:ILE:O	1:C:600:ILE:HG13	2.16	0.45
1:A:414:SER:HG	1:A:715:ASN:HD22	1.64	0.45
1:A:563:TYR:C	1:A:565:SER:H	2.24	0.45
1:A:601:GLN:HE22	1:A:611:ARG:HD3	1.82	0.45
2:B:284:ASN:HB2	3:B:352:HOH:O	2.16	0.45
1:C:431:ILE:HD13	1:C:447:TRP:HZ3	1.82	0.45
1:C:639:GLY:HA2	1:C:688:ILE:CD1	2.47	0.45
2:D:37:GLU:HB2	2:D:46:ILE:HD11	1.98	0.45
1:A:559:TYR:CE2	1:C:541:VAL:HG21	2.52	0.45
1:C:524:LYS:CG	1:C:525:SER:H	2.24	0.45
2:B:66:PHE:CD2	2:B:114:PRO:HB3	2.51	0.45
2:B:191:ALA:HB1	2:B:193:THR:HG22	1.99	0.45
1:C:590:VAL:O	1:C:590:VAL:CG1	2.64	0.45
1:C:674:LEU:O	1:C:678:ILE:HD13	2.15	0.45
1:A:564:GLY:HA2	1:A:570:SER:OG	2.16	0.45
2:B:239:GLU:HG3	3:B:327:HOH:O	2.16	0.45
1:C:727:PRO:O	1:C:729:ASP:N	2.50	0.45
2:D:83:LYS:CB	2:D:92:ILE:HG21	2.47	0.45
2:D:139:ILE:O	2:D:140:ILE:HD13	2.16	0.45
2:B:30:ASP:OD1	2:B:32:THR:HG23	2.17	0.45
2:B:35:ILE:HG13	2:B:89:TRP:CE2	2.51	0.45
1:C:399:GLY:O	2:D:11:LEU:HD12	2.17	0.45
1:C:432:ASN:O	1:C:436:VAL:HG23	2.16	0.45
2:B:4:ILE:HG21	2:B:36:PHE:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:LEU:CD2	2:B:201:GLU:HG2	2.47	0.45
1:C:412:LEU:C	1:C:412:LEU:HD23	2.42	0.45
1:A:399:GLY:O	2:B:11:LEU:HD12	2.17	0.44
1:A:449:LEU:O	1:A:453:LEU:HB2	2.17	0.44
2:B:74:SER:C	2:B:76:ASP:H	2.26	0.44
1:C:377:TYR:CA	3:C:113:HOH:O	2.64	0.44
1:C:622:LEU:O	1:C:627:HIS:HB2	2.16	0.44
2:D:108:ALA:HB1	2:D:109:PRO:HD2	2.00	0.44
1:A:595:PHE:C	1:A:597:SER:N	2.72	0.44
1:A:604:TYR:N	1:A:605:PRO:CD	2.81	0.44
1:A:573:LEU:HD23	1:C:518:LEU:CD1	2.47	0.44
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.58	0.44
1:C:652:PHE:HB3	1:C:653:PRO:CD	2.42	0.44
1:A:379:GLU:HG2	2:B:258:TRP:CZ2	2.53	0.44
1:A:504:PHE:CZ	1:C:588:LEU:HD13	2.52	0.44
1:A:688:ILE:HG12	1:A:689:ASN:H	1.82	0.44
2:B:30:ASP:OD1	2:B:32:THR:OG1	2.36	0.44
2:B:105:VAL:HG22	2:B:116:LEU:HD11	1.99	0.44
1:C:543:ALA:C	1:C:545:ASP:H	2.25	0.44
2:D:108:ALA:O	2:D:109:PRO:C	2.59	0.44
2:D:142:ASP:HB3	3:D:366:HOH:O	2.17	0.44
2:D:187:TYR:HB2	2:D:194:TYR:CE2	2.53	0.44
1:A:688:ILE:CG1	1:A:689:ASN:H	2.31	0.44
1:C:608:ILE:HD13	1:C:611:ARG:NH1	2.33	0.44
2:D:112:TYR:CZ	2:D:171:ARG:HG2	2.53	0.44
1:A:706:PHE:CB	3:A:200:HOH:O	2.66	0.44
2:B:85:GLU:O	2:B:86:ASN:HB2	2.18	0.44
2:D:184:ILE:O	2:D:197:GLU:HB2	2.17	0.44
2:B:102:VAL:HG22	3:B:353:HOH:O	2.13	0.44
2:B:213:SER:HB2	2:B:262:TRP:CE2	2.53	0.44
2:D:227:GLN:C	2:D:229:ARG:H	2.26	0.44
1:A:538:GLU:O	1:A:539:ALA:C	2.60	0.43
2:D:63:HIS:ND1	2:D:64:PRO:HD2	2.32	0.43
2:D:108:ALA:HB1	2:D:109:PRO:CD	2.48	0.43
1:A:639:GLY:HA2	1:A:688:ILE:CD1	2.35	0.43
2:B:63:HIS:CE1	2:B:65:LYS:HB3	2.53	0.43
2:B:112:TYR:N	2:B:112:TYR:CD2	2.86	0.43
1:C:571:ARG:O	1:C:574:TYR:HB3	2.18	0.43
1:A:423:LYS:HG3	1:A:424:THR:N	2.33	0.43
1:C:384:ALA:N	3:D:413:HOH:O	2.50	0.43
1:C:420:GLU:HA	1:C:423:LYS:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:ASN:HD22	2:B:238:ASN:C	2.26	0.43
1:A:537:MET:CE	1:C:536:LEU:HD23	2.48	0.43
1:C:636:LEU:HD12	1:C:688:ILE:CD1	2.48	0.43
2:D:251:GLU:H	2:D:251:GLU:CD	2.25	0.43
1:A:422:LEU:CD2	1:A:721:GLU:HG2	2.49	0.43
2:B:227:GLN:HA	2:B:256:VAL:HG13	2.01	0.43
2:D:208:ARG:CZ	2:D:258:TRP:HZ3	2.32	0.43
2:B:238:ASN:ND2	2:B:240:GLN:H	2.14	0.43
1:C:439:ILE:CG2	1:C:659:LEU:HD21	2.39	0.43
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	0.43
1:A:496:THR:CG2	1:A:497:ASN:N	2.81	0.43
1:A:504:PHE:CE1	1:C:588:LEU:HD13	2.53	0.43
1:A:537:MET:HE1	1:C:536:LEU:CG	2.48	0.43
2:B:107:TRP:CH2	2:B:130:PHE:HE1	2.37	0.43
1:C:412:LEU:HD21	1:C:713:THR:HG22	2.01	0.43
1:C:468:PHE:O	1:C:469:ASP:C	2.62	0.43
1:C:551:LEU:C	1:C:553:GLU:N	2.76	0.43
2:B:46:ILE:HG22	2:B:46:ILE:O	2.19	0.43
2:B:64:PRO:HD2	3:B:334:HOH:O	2.18	0.43
1:A:608:ILE:HA	1:A:611:ARG:NH1	2.34	0.42
1:C:519:VAL:O	1:C:521:GLY:N	2.51	0.42
1:C:551:LEU:C	1:C:553:GLU:H	2.27	0.42
1:C:590:VAL:HG13	1:C:622:LEU:HD22	1.99	0.42
1:A:438:VAL:CG2	1:A:439:ILE:N	2.81	0.42
1:A:511:GLU:HG2	1:C:569:LEU:HB2	1.99	0.42
1:A:639:GLY:C	1:A:688:ILE:HD11	2.44	0.42
2:B:225:VAL:CG2	2:B:271:LEU:HD11	2.50	0.42
2:B:226:SER:HB3	2:B:228:ASP:OD1	2.19	0.42
1:A:399:GLY:HA3	2:B:11:LEU:CD1	2.49	0.42
1:A:610:GLN:HA	1:A:610:GLN:OE1	2.20	0.42
1:A:706:PHE:HB2	3:A:200:HOH:O	2.19	0.42
2:D:124:LYS:HE3	2:D:142:ASP:OD1	2.19	0.42
2:D:224:SER:OG	2:D:232:ILE:HB	2.19	0.42
1:A:404:ILE:N	1:A:404:ILE:HD12	2.35	0.42
1:A:563:TYR:C	1:A:565:SER:N	2.77	0.42
2:B:16:VAL:HG12	2:B:61:TRP:HD1	1.84	0.42
1:C:646:SER:O	1:C:647:ILE:C	2.62	0.42
1:A:584:LEU:N	1:A:584:LEU:CD1	2.81	0.42
1:A:733:VAL:HG13	3:A:255:HOH:O	2.20	0.42
2:B:49:LEU:HA	3:B:355:HOH:O	2.20	0.42
2:B:155:PRO:CG	2:B:214:PRO:HA	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:GLU:HA	1:C:423:LYS:CD	2.50	0.42
2:D:157:THR:HG21	2:D:170:SER:HB2	2.00	0.42
2:D:225:VAL:HG22	2:D:257:LEU:HB2	2.00	0.42
1:A:428:LYS:HB2	1:A:429:PRO:CD	2.38	0.42
1:A:497:ASN:OD1	1:A:498:PHE:N	2.53	0.42
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.42
2:D:86:ASN:C	2:D:88:ARG:H	2.28	0.42
2:D:180:ASN:ND2	2:D:205:ASP:C	2.78	0.42
1:A:500:PRO:O	1:A:501:GLU:HG2	2.20	0.42
2:B:63:HIS:CD2	2:B:110:HIS:HB3	2.54	0.42
2:B:281:TRP:CD1	2:B:281:TRP:N	2.87	0.42
1:C:655:LEU:HD12	1:C:655:LEU:HA	1.78	0.42
1:A:431:ILE:HG21	1:A:451:GLU:HA	2.02	0.42
1:A:429:PRO:HD2	3:A:159:HOH:O	2.18	0.42
1:A:447:TRP:O	1:A:451:GLU:N	2.53	0.42
1:A:458:THR:CG2	1:A:459:GLU:N	2.81	0.42
1:C:408:LYS:HG3	2:D:294:GLU:OE1	2.19	0.42
1:C:493:GLN:HG3	1:C:494:ILE:N	2.35	0.42
1:A:549:GLU:HA	1:A:552:LYS:HB3	2.01	0.42
2:B:233:ILE:HD12	2:B:233:ILE:N	2.35	0.42
2:D:118:VAL:O	2:D:125:VAL:HA	2.20	0.42
2:D:118:VAL:HB	2:D:126:SER:OG	2.20	0.42
1:A:644:VAL:HG21	1:A:684:PHE:CZ	2.55	0.41
1:C:531:LEU:C	1:C:533:ASN:N	2.77	0.41
1:A:517:ASN:HD21	1:A:529:ASN:HD22	1.60	0.41
2:B:121:SER:CA	3:B:338:HOH:O	2.68	0.41
2:B:205:ASP:O	2:B:206:TRP:C	2.62	0.41
2:B:225:VAL:CG1	2:B:257:LEU:O	2.68	0.41
2:B:282:LYS:HB3	2:B:292:ALA:HB2	2.02	0.41
1:C:667:TYR:CD1	2:D:266:GLY:HA2	2.55	0.41
2:D:86:ASN:C	2:D:88:ARG:N	2.77	0.41
1:A:412:LEU:HD23	1:A:413:GLU:N	2.36	0.41
1:A:430:LEU:C	1:A:430:LEU:CD2	2.94	0.41
2:B:213:SER:HB2	2:B:262:TRP:CD2	2.55	0.41
1:C:424:THR:O	1:C:425:LYS:HB3	2.19	0.41
1:C:510:ILE:O	1:C:511:GLU:C	2.63	0.41
2:D:7:ALA:HB3	2:D:12:ILE:HD11	2.01	0.41
2:D:277:LYS:HG3	2:D:278:VAL:H	1.86	0.41
1:A:517:ASN:ND2	1:A:529:ASN:ND2	2.63	0.41
1:A:653:PRO:O	1:A:654:ASP:C	2.64	0.41
1:A:653:PRO:O	1:A:656:GLU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:VAL:HG13	2:B:41:GLU:HA	2.03	0.41
2:B:17:LEU:HB3	2:B:21:GLY:HA2	2.03	0.41
2:B:152:SER:OG	2:B:210:VAL:O	2.33	0.41
2:B:238:ASN:HB2	3:B:327:HOH:O	2.20	0.41
1:C:447:TRP:CE3	1:C:450:LEU:HD12	2.55	0.41
1:C:596:ILE:O	1:C:597:SER:C	2.63	0.41
2:D:191:ALA:O	2:D:192:GLN:HB2	2.20	0.41
1:A:420:GLU:O	1:A:423:LYS:HG2	2.20	0.41
1:A:434:ARG:HG3	1:A:447:TRP:CH2	2.55	0.41
2:B:212:TRP:HA	2:B:222:LEU:HD23	2.03	0.41
1:A:578:LYS:HD3	1:A:580:GLU:OE2	2.21	0.41
2:D:181:LEU:CD2	2:D:201:GLU:HG2	2.50	0.41
2:D:203:HIS:NE2	2:D:232:ILE:HG12	2.35	0.41
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.02	0.41
1:C:438:VAL:HG21	1:C:444:GLU:CA	2.50	0.41
1:A:396:THR:HB	1:A:398:ASP:OD1	2.21	0.41
1:A:421:ALA:O	1:A:425:LYS:HA	2.21	0.41
1:A:444:GLU:HG2	1:A:448:ASN:ND2	2.36	0.41
1:A:581:VAL:O	1:A:582:ASP:C	2.63	0.41
1:A:704:LEU:O	1:A:707:ILE:HB	2.21	0.41
2:B:120:SER:C	2:B:122:ASP:H	2.29	0.41
2:D:18:ASP:CG	2:D:23:ARG:H	2.29	0.41
1:A:388:PHE:HB2	1:A:739:ARG:NH2	2.30	0.41
1:A:556:LYS:C	1:A:558:ALA:N	2.78	0.41
2:B:46:ILE:O	2:B:47:ASP:HB2	2.21	0.41
1:C:730:ASN:C	1:C:732:GLU:N	2.79	0.41
1:A:497:ASN:O	1:A:498:PHE:HB3	2.20	0.40
1:A:519:VAL:O	1:A:521:GLY:N	2.52	0.40
2:B:23:ARG:NH1	2:B:68:THR:CG2	2.83	0.40
2:B:78:LYS:HG2	2:B:96:ALA:CB	2.52	0.40
1:C:649:LEU:CD2	1:C:698:GLN:HG2	2.38	0.40
2:D:33:ILE:HB	2:D:49:LEU:HD12	2.03	0.40
2:D:122:ASP:C	3:D:408:HOH:O	2.64	0.40
1:A:439:ILE:HG13	1:A:440:ASP:H	1.85	0.40
1:A:598:LYS:O	1:A:602:ASN:HB2	2.20	0.40
1:C:551:LEU:O	1:C:553:GLU:N	2.54	0.40
1:C:677:PHE:HD2	1:C:678:ILE:HD12	1.83	0.40
2:D:64:PRO:C	2:D:66:PHE:N	2.79	0.40
2:D:117:LEU:HD21	2:D:151:ALA:HB1	2.03	0.40
1:A:456:ASP:O	1:A:460:GLU:HB2	2.22	0.40
1:C:572:ILE:HG22	1:C:573:LEU:N	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:PHE:CE2	1:C:702:LYS:HE2	2.56	0.40
1:C:730:ASN:C	1:C:732:GLU:H	2.29	0.40
2:B:24:LEU:HG	2:B:25:ALA:H	1.85	0.40
1:C:409:ILE:HB	1:C:412:LEU:HB3	2.04	0.40
1:C:535:LEU:CD2	1:C:538:GLU:HG3	2.52	0.40
1:C:717:GLU:N	3:C:127:HOH:O	2.55	0.40
2:D:293:GLY:O	2:D:294:GLU:C	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:118:HOH:O	3:D:311:HOH:O[1_644]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/399 (85%)	285 (84%)	43 (13%)	11 (3%)	3	1
1	C	341/399 (86%)	298 (87%)	34 (10%)	9 (3%)	4	2
2	B	275/297 (93%)	241 (88%)	30 (11%)	4 (2%)	8	7
2	D	284/297 (96%)	255 (90%)	20 (7%)	9 (3%)	3	1
All	All	1239/1392 (89%)	1079 (87%)	127 (10%)	33 (3%)	4	2

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	ASN
2	B	131	LYS
1	C	715	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	131	LYS
2	D	218	LEU
2	D	294	GLU
1	A	388	PHE
1	A	425	LYS
1	A	518	LEU
2	B	135	THR
1	C	425	LYS
2	D	87	GLY
2	D	135	THR
1	A	520	SER
1	A	728	SER
2	B	190	ASP
1	C	439	ILE
1	C	552	LYS
1	C	728	SER
1	A	439	ILE
1	A	498	PHE
1	A	561	ALA
2	B	202	GLY
1	C	407	PRO
2	D	168	LYS
2	D	206	TRP
1	A	548	ASN
1	A	653	PRO
1	C	520	SER
1	C	662	ASP
2	D	202	GLY
2	D	93	ALA
1	C	494	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	306/350 (87%)	298 (97%)	8 (3%)	40 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	308/350 (88%)	294 (96%)	14 (4%)	24	37
2	B	237/252 (94%)	231 (98%)	6 (2%)	42	56
2	D	244/252 (97%)	234 (96%)	10 (4%)	27	40
All	All	1095/1204 (91%)	1057 (96%)	38 (4%)	32	46

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	LEU
1	A	509	ASN
1	A	537	MET
1	A	545	ASP
1	A	572	ILE
1	A	688	ILE
1	A	703	PHE
1	A	720	THR
2	B	50	THR
2	B	92	ILE
2	B	180	ASN
2	B	204	SER
2	B	225	VAL
2	B	238	ASN
1	C	377	TYR
1	C	381	SER
1	C	407	PRO
1	C	408	LYS
1	C	413	GLU
1	C	432	ASN
1	C	509	ASN
1	C	510	ILE
1	C	538	GLU
1	C	545	ASP
1	C	572	ILE
1	C	590	VAL
1	C	629	GLN
1	C	655	LEU
2	D	28	SER
2	D	74	SER
2	D	85	GLU
2	D	128	VAL
2	D	157	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	198	SER
2	D	204	SER
2	D	225	VAL
2	D	251	GLU
2	D	295	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	GLN
1	A	443	ASN
1	A	448	ASN
1	A	509	ASN
1	A	512	GLN
1	A	517	ASN
1	A	529	ASN
1	A	592	GLN
1	A	601	GLN
1	A	612	ASN
2	B	91	GLN
2	B	95	HIS
2	B	149	ASN
2	B	180	ASN
2	B	238	ASN
2	B	240	GLN
1	C	443	ASN
1	C	448	ASN
1	C	493	GLN
1	C	509	ASN
1	C	512	GLN
1	C	517	ASN
1	C	547	ASN
1	C	557	ASN
1	C	601	GLN
1	C	602	ASN
1	C	606	ASN
1	C	612	ASN
1	C	670	HIS
1	C	686	ASN
2	D	110	HIS
2	D	149	ASN
2	D	180	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	227	GLN
2	D	240	GLN
2	D	276	ASN

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 oligosaccharides 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	345/399 (86%)	0.77	23 (6%) 24 21	49, 83, 114, 130	0
1	C	347/399 (86%)	0.33	14 (4%) 42 41	30, 66, 103, 130	0
2	B	279/297 (93%)	0.47	17 (6%) 27 24	15, 62, 110, 142	0
2	D	288/297 (96%)	-0.03	8 (2%) 55 56	16, 47, 96, 135	0
All	All	1259/1392 (90%)	0.40	62 (4%) 35 33	15, 68, 109, 142	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	595	PHE	5.8
1	C	519	VAL	5.6
2	B	130	PHE	4.8
2	B	134	GLY	4.2
2	D	130	PHE	4.1
1	C	745	GLY	4.0
2	B	136	THR	3.5
1	A	738	ALA	3.5
2	B	265	SER	3.4
2	D	276	ASN	3.2
2	B	135	THR	3.2
1	C	494	ILE	3.2
2	B	12	ILE	3.2
2	D	295	VAL	3.1
2	D	137	SER	3.1
1	A	592	GLN	3.1
1	C	709	LEU	3.1
1	A	741	LEU	2.9
1	A	551	LEU	2.9
1	A	552	LYS	2.8
2	B	38	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	436	VAL	2.7
1	A	694	ILE	2.7
2	B	22	LYS	2.6
1	A	496	THR	2.5
1	A	439	ILE	2.5
2	D	296	HIS	2.5
2	D	134	GLY	2.5
2	B	137	SER	2.5
2	B	218	LEU	2.4
1	A	464	GLU	2.4
2	B	139	ILE	2.4
2	B	133	ASN	2.4
1	C	526	ALA	2.3
2	B	87	GLY	2.3
1	A	674	LEU	2.3
2	B	17	LEU	2.3
1	A	683	VAL	2.3
2	B	25	ALA	2.3
2	B	2	VAL	2.3
2	B	131	LYS	2.2
2	D	131	LYS	2.2
1	A	543	ALA	2.2
1	A	397	PRO	2.2
1	A	690	GLY	2.2
1	C	500	PRO	2.2
1	A	508	GLY	2.1
1	A	667	TYR	2.1
1	A	440	ASP	2.1
1	C	515	SER	2.1
1	C	493	GLN	2.1
1	C	690	GLY	2.1
1	C	545	ASP	2.1
1	C	595	PHE	2.1
2	D	218	LEU	2.1
1	A	528	LYS	2.1
1	A	745	GLY	2.0
1	C	532	GLU	2.0
1	C	438	VAL	2.0
1	A	452	LYS	2.0
1	C	439	ILE	2.0
1	A	520	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.