Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 06:55 PM JST

PDB ID	:	5GTY
Title	:	Crystal structure of EGFR 696-1022 T790M in complex with LXX-6-26
Authors	:	Yan, X.E.; Yun, C.H.
Deposited on	:	2016-08-23
Resolution	:	3.14 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

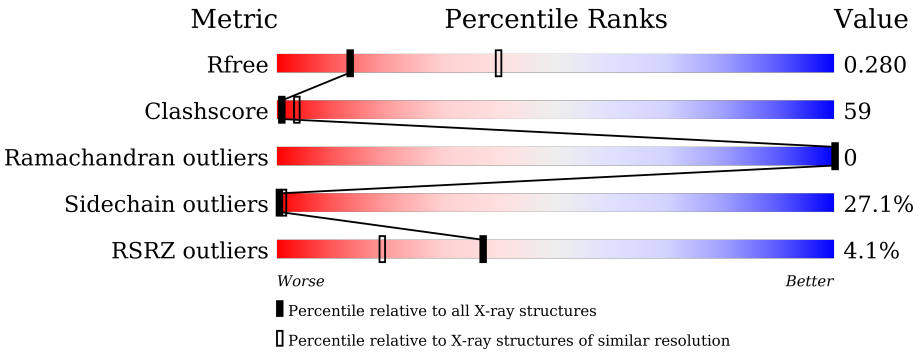
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.14 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	2% 31% 47% 13% 9%
1	B	331	4% 32% 46% 12% 10%
1	C	331	5% 25% 46% 18% 11%
1	D	331	4% 26% 51% 13% 10%
1	E	331	7% 34% 43% 13% 10%
1	F	331	2% 31% 44% 15% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	331	5% 32% 44% 14% 10%
1	H	331	2% 33% 43% 14% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	H	1104	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19277 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	2	0
			2377	1529	397	432	19			
1	B	299	Total	C	N	O	S	0	0	0
			2333	1499	389	426	19			
1	D	297	Total	C	N	O	S	0	0	0
			2281	1468	377	418	18			
1	E	297	Total	C	N	O	S	0	0	0
			2297	1482	386	411	18			
1	F	297	Total	C	N	O	S	0	0	0
			2328	1499	393	417	19			
1	G	299	Total	C	N	O	S	0	1	0
			2367	1519	397	432	19			
1	H	300	Total	C	N	O	S	0	0	0
			2362	1521	392	430	19			
1	C	295	Total	C	N	O	S	0	0	0
			2325	1492	395	419	19			

There are 40 discrepancies between the modelled and reference sequences:

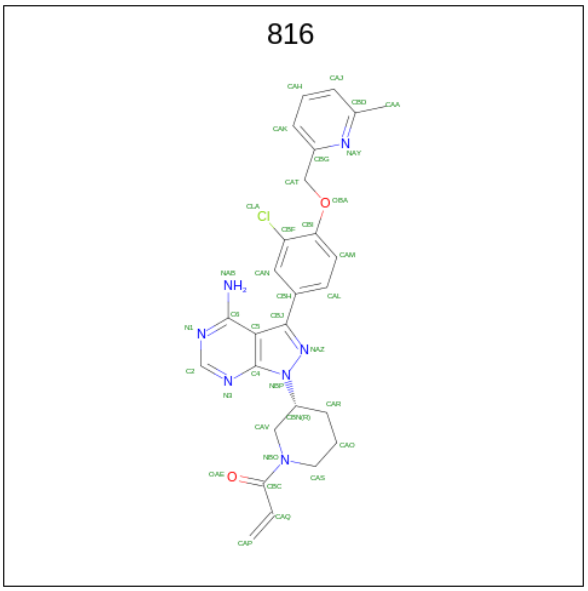
Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	ALA	-	expression tag	UNP P00533
A	694	MET	-	expression tag	UNP P00533
A	695	GLY	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	ALA	-	expression tag	UNP P00533
B	694	MET	-	expression tag	UNP P00533
B	695	GLY	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	ALA	-	expression tag	UNP P00533
D	694	MET	-	expression tag	UNP P00533

Continued on next page...

Continued from previous page...

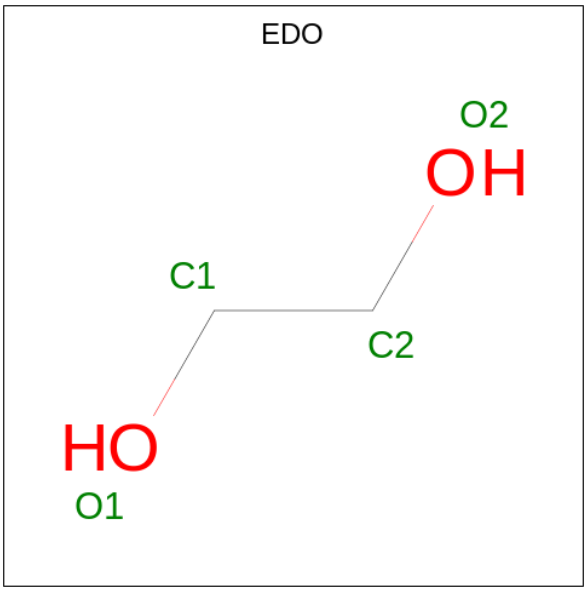
Chain	Residue	Modelled	Actual	Comment	Reference
D	695	GLY	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
E	692	GLY	-	expression tag	UNP P00533
E	693	ALA	-	expression tag	UNP P00533
E	694	MET	-	expression tag	UNP P00533
E	695	GLY	-	expression tag	UNP P00533
E	790	MET	THR	engineered mutation	UNP P00533
F	692	GLY	-	expression tag	UNP P00533
F	693	ALA	-	expression tag	UNP P00533
F	694	MET	-	expression tag	UNP P00533
F	695	GLY	-	expression tag	UNP P00533
F	790	MET	THR	engineered mutation	UNP P00533
G	692	GLY	-	expression tag	UNP P00533
G	693	ALA	-	expression tag	UNP P00533
G	694	MET	-	expression tag	UNP P00533
G	695	GLY	-	expression tag	UNP P00533
G	790	MET	THR	engineered mutation	UNP P00533
H	692	GLY	-	expression tag	UNP P00533
H	693	ALA	-	expression tag	UNP P00533
H	694	MET	-	expression tag	UNP P00533
H	695	GLY	-	expression tag	UNP P00533
H	790	MET	THR	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	ALA	-	expression tag	UNP P00533
C	694	MET	-	expression tag	UNP P00533
C	695	GLY	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533

- Molecule 2 is 1-[(3R)-3-[4-azanyl-3-[3-chloranyl-4-[(6-methylpyridin-2-yl)methoxy]phenyl]pyrazolo[3,4-d]pyrimidin-1-yl]piperidin-1-yl]prop-2-en-1-one (three-letter code: 816) (formula: $C_{26}H_{26}ClN_7O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		
2	B	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		
2	D	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		
2	E	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		
2	F	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		
2	G	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		
2	H	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		
2	C	1	Total	C	Cl	N	O	0	0
			36	26	1	7	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

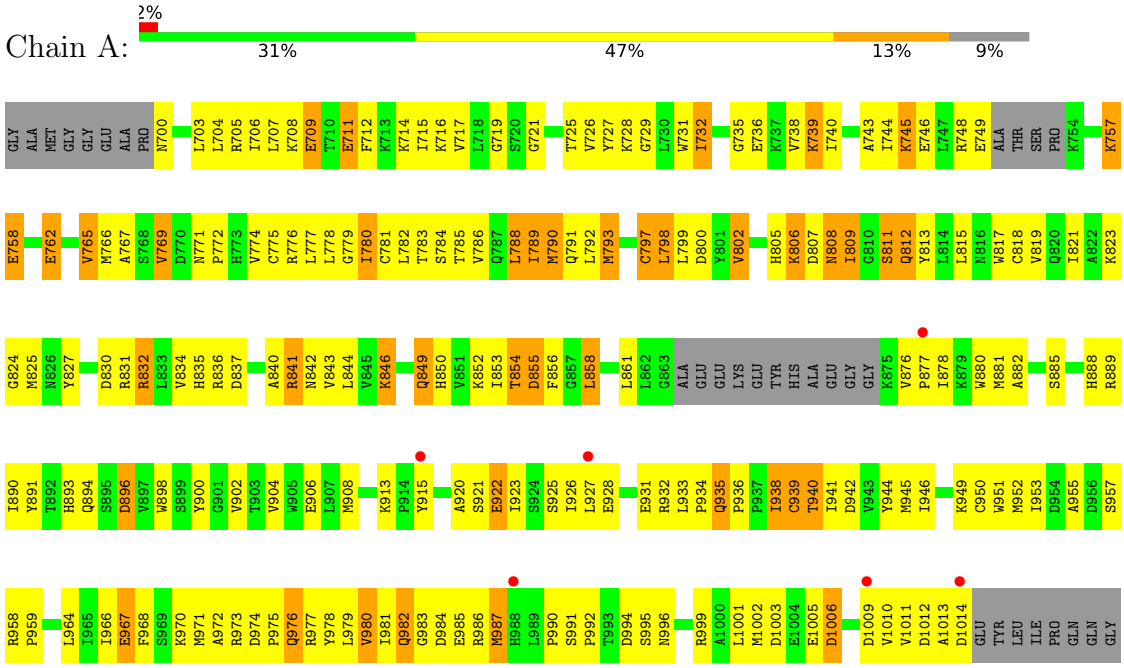
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	45	Total O 45 45	0	0
4	B	37	Total O 37 37	0	0
4	D	19	Total O 19 19	0	0
4	E	42	Total O 42 42	0	0
4	F	50	Total O 50 50	0	0
4	G	48	Total O 48 48	0	0
4	H	27	Total O 27 27	0	0
4	C	35	Total O 35 35	0	0

3 Residue-property plots (i)

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

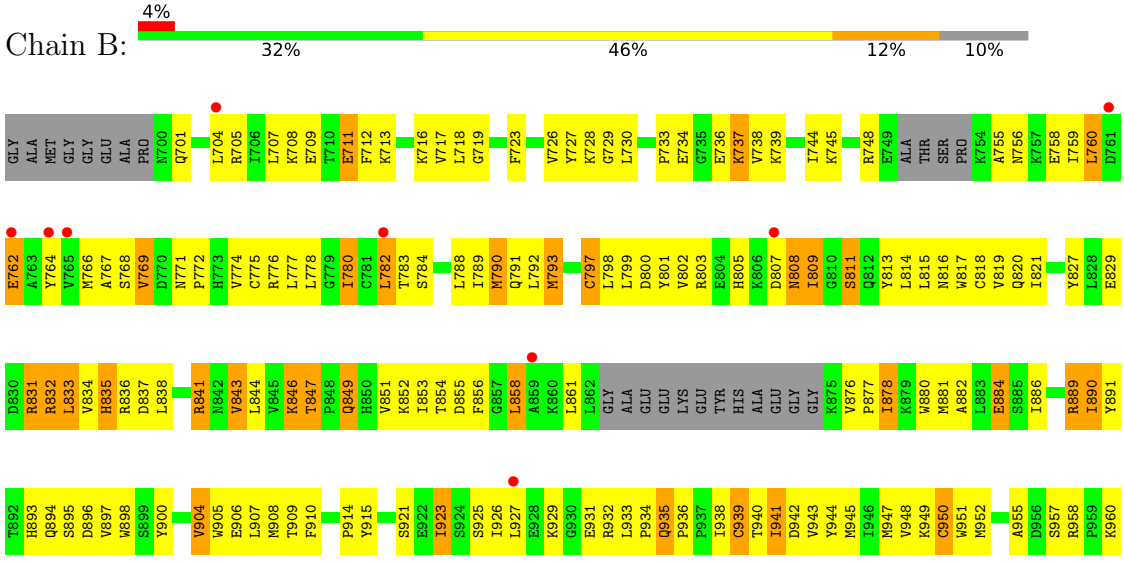
• Molecule 1: Epidermal growth factor receptor

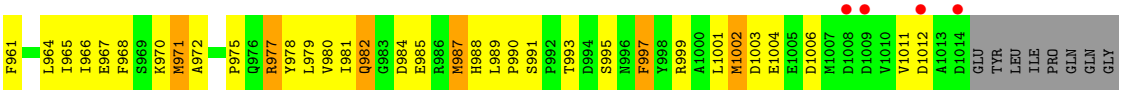
Chain A:



• Molecule 1: Epidermal growth factor receptor

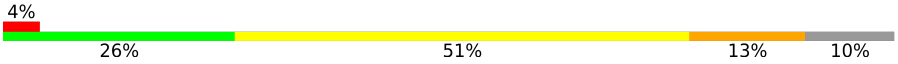
Chain B:

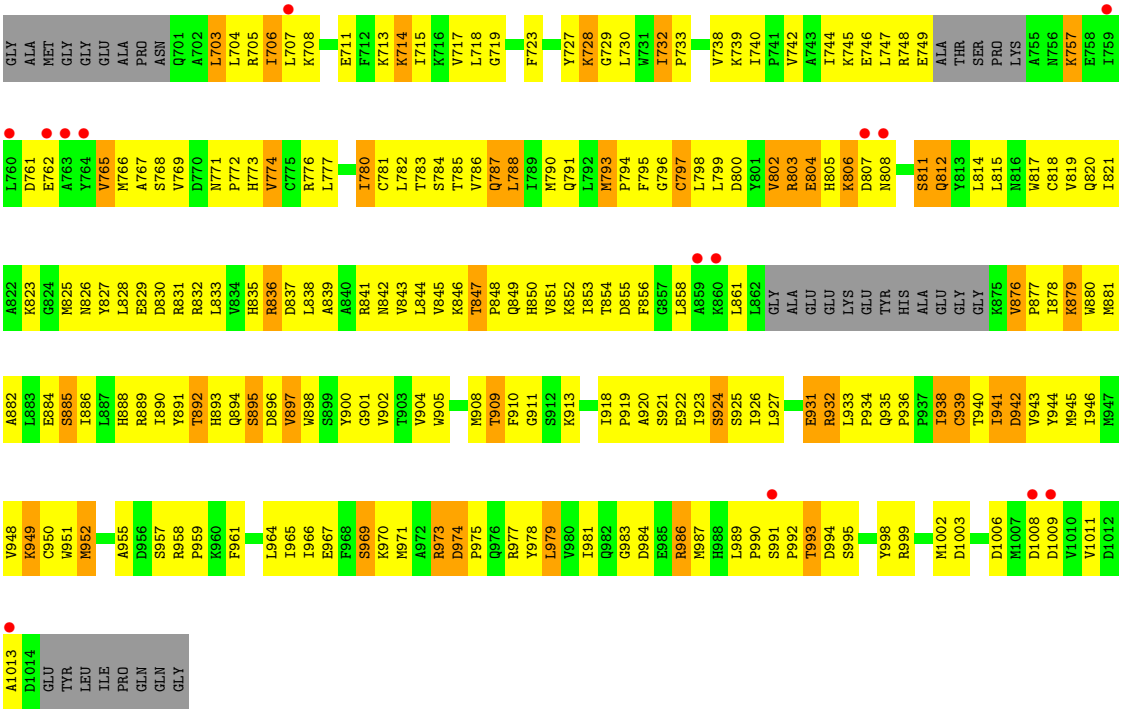




• Molecule 1: Epidermal growth factor receptor

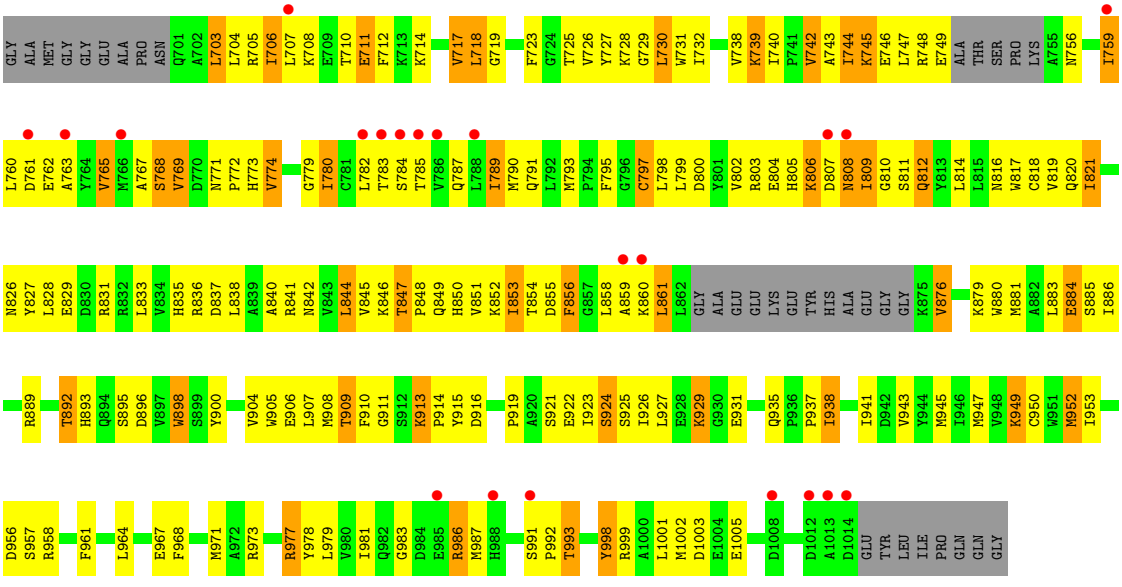
Chain D:





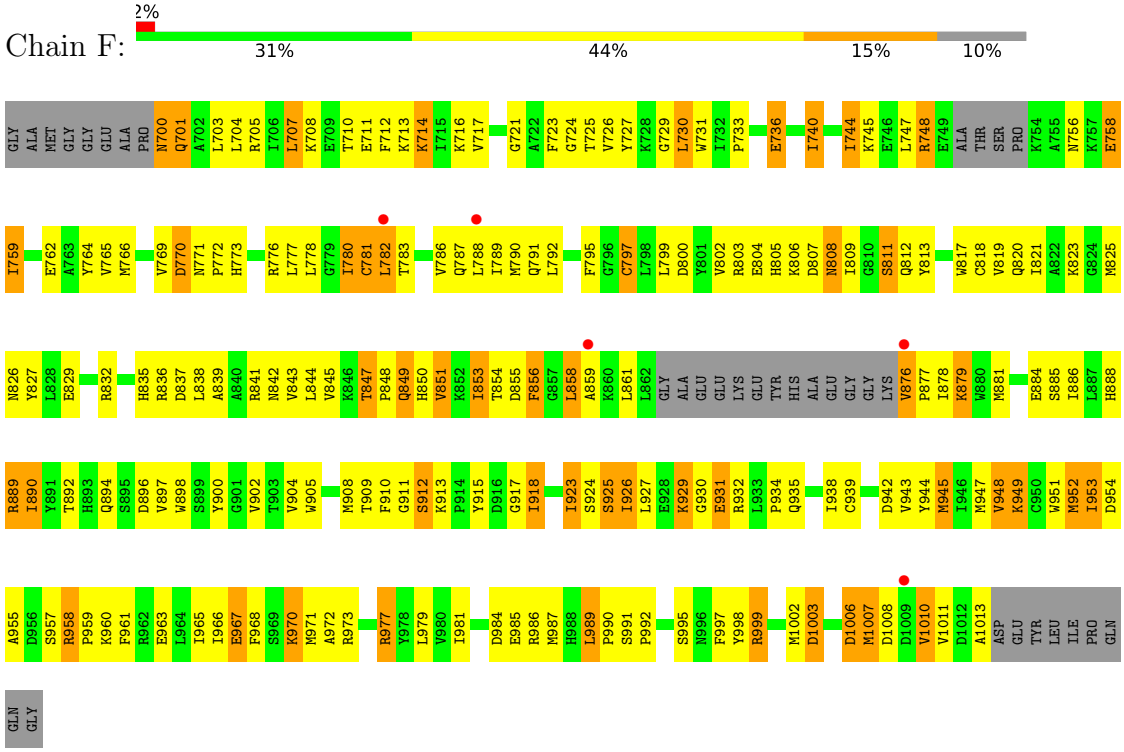
• Molecule 1: Epidermal growth factor receptor

Chain E:



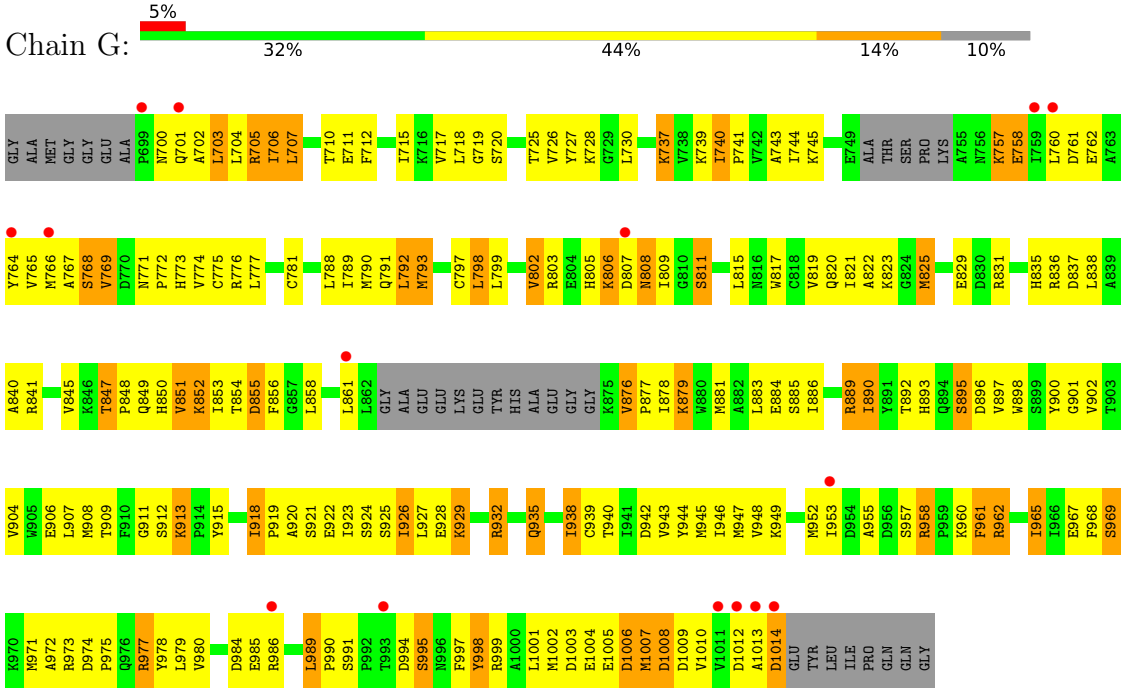
• Molecule 1: Epidermal growth factor receptor

Chain F:



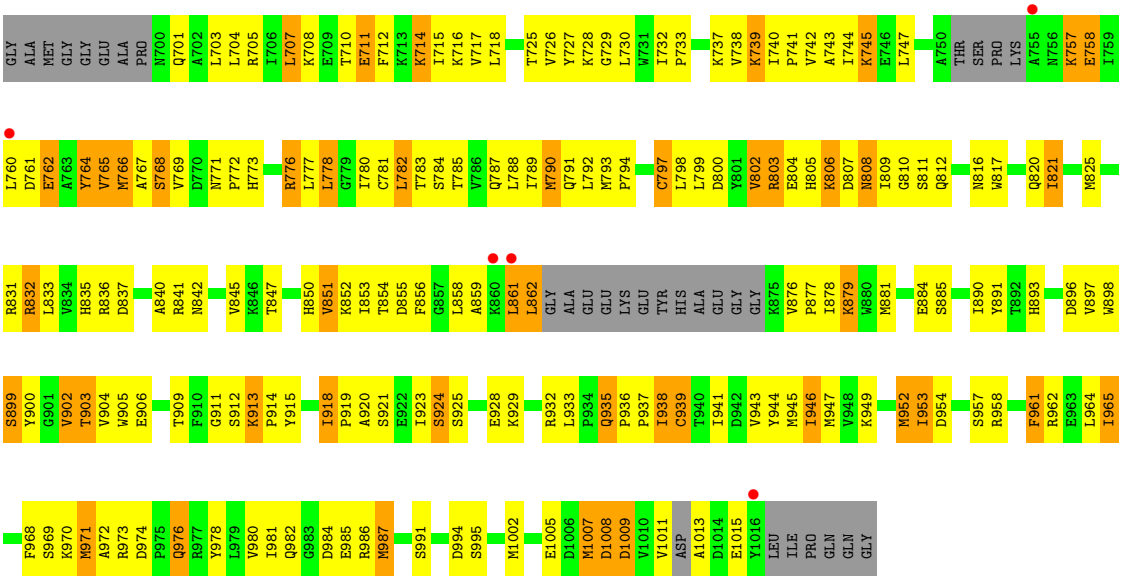
• Molecule 1: Epidermal growth factor receptor

Chain G:



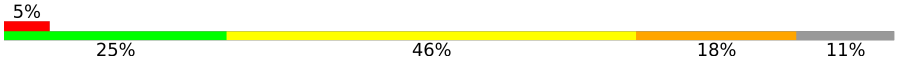
• Molecule 1: Epidermal growth factor receptor

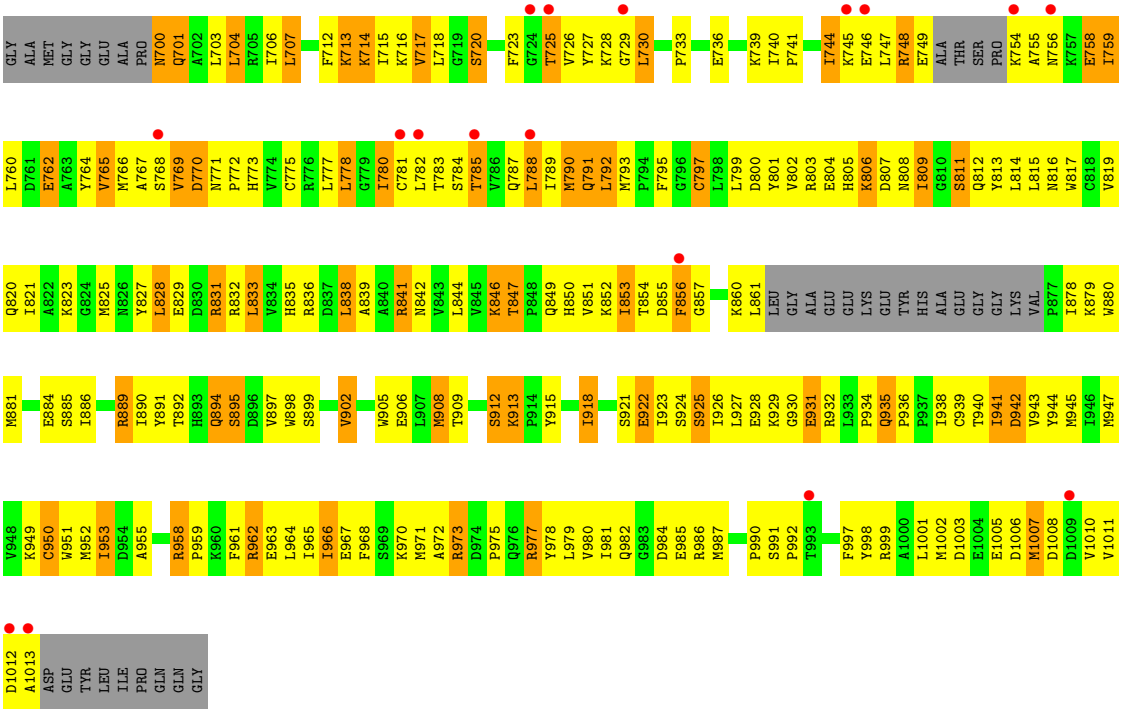
Chain H:



• Molecule 1: Epidermal growth factor receptor

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.43Å 71.80Å 152.53Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	49.81 – 3.14 49.81 – 3.14	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.81-3.14) 95.7 (49.81-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 3.12Å)	Xtriage
Refinement program	PHENIX (dev_2400)	Depositor
R, R_{free}	0.257 , 0.280 0.256 , 0.280	Depositor DCC
R_{free} test set	2103 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 83.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19277	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5445e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 816, EDO

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	0.45	0/2429	0.55	0/3291
1	B	0.44	0/2382	0.55	0/3231
1	C	0.44	0/2373	0.55	0/3213
1	D	0.45	0/2330	0.54	0/3164
1	E	0.45	0/2346	0.55	0/3184
1	F	0.46	0/2376	0.57	0/3219
1	G	0.45	0/2420	0.56	0/3278
1	H	0.44	0/2409	0.55	0/3260
All	All	0.45	0/19065	0.55	0/25840

There are no bond length outliers.

There are no bond angle outliers.

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	2377	0	2361	276	0
1	B	2333	0	2286	277	0
1	C	2325	0	2316	350	0
1	D	2281	0	2200	246	0
1	E	2297	0	2247	270	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2328	0	2317	273	0
1	G	2367	0	2355	277	0
1	H	2362	0	2353	255	0
2	A	36	0	0	4	0
2	B	36	0	0	6	0
2	C	36	0	0	9	0
2	D	36	0	0	11	0
2	E	36	0	0	8	0
2	F	36	0	0	9	0
2	G	36	0	0	14	0
2	H	36	0	0	11	0
3	G	4	0	6	2	0
3	H	12	0	18	4	0
4	A	45	0	0	14	0
4	B	37	0	0	3	0
4	C	35	0	0	4	0
4	D	19	0	0	3	0
4	E	42	0	0	5	0
4	F	50	0	0	15	0
4	G	48	0	0	10	0
4	H	27	0	0	4	0
All	All	19277	0	18459	2198	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 59.

All (2198) 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:H:707:LEU:CD1	1:H:789:ILE:HD13	1.41	1.50
1:H:707:LEU:HD13	1:H:789:ILE:CD1	1.50	1.42
1:G:989:LEU:HD22	1:G:990:PRO:CD	1.52	1.39
1:H:812:GLN:NE2	1:H:1013:ALA:HB2	1.43	1.29
1:C:835:HIS:CD2	1:C:856:PHE:HA	1.67	1.28
1:B:941:ILE:O	1:B:941:ILE:HD12	1.34	1.24
1:C:961:PHE:O	1:C:965:ILE:HD12	1.34	1.24
1:C:941:ILE:HD12	1:C:941:ILE:O	1.34	1.23
1:A:798:LEU:HD12	1:A:798:LEU:O	1.34	1.23
1:F:989:LEU:HD23	1:F:989:LEU:C	1.55	1.22
1:G:995:SER:O	1:G:999[B]:ARG:HD2	1.40	1.21
1:H:905:TRP:O	1:H:909:THR:HG23	1.40	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:825:MET:SD	1:C:838:LEU:CD2	2.30	1.20
1:B:835:HIS:CB	1:B:856:PHE:HB2	1.73	1.19
1:D:730:LEU:HD22	1:D:739:LYS:HB3	1.20	1.18
1:G:806:LYS:HD3	1:G:807:ASP:N	1.58	1.18
1:G:806:LYS:HD3	1:G:806:LYS:C	1.61	1.17
1:H:778:LEU:N	1:H:778:LEU:HD23	1.54	1.17
1:B:771:ASN:ND2	1:B:772:PRO:HD2	1.59	1.17
1:C:805:HIS:O	1:C:809:ILE:HG22	1.41	1.17
1:C:894:GLN:HG3	1:C:955:ALA:O	1.45	1.17
1:B:835:HIS:HB3	1:B:856:PHE:HB2	1.24	1.16
1:C:778:LEU:HD23	1:C:778:LEU:H	1.09	1.16
1:F:977:ARG:HD2	1:F:977:ARG:O	1.42	1.16
1:F:842:ASN:O	1:F:854:THR:HG22	1.44	1.15
1:E:759:ILE:HD11	1:E:780:ILE:HD11	1.21	1.15
1:G:940:THR:HG22	1:G:943:VAL:HG23	1.24	1.15
1:B:977:ARG:HG3	1:B:977:ARG:HH21	1.02	1.14
1:B:982:GLN:NE2	1:B:982:GLN:H	1.46	1.14
1:D:815:LEU:CD2	1:D:979:LEU:HD11	1.77	1.13
1:F:773:HIS:O	1:F:853:ILE:HD13	1.48	1.13
1:H:715:ILE:HD11	1:H:728:LYS:HE2	1.28	1.11
1:C:778:LEU:HD23	1:C:778:LEU:N	1.63	1.11
1:B:977:ARG:HH21	1:B:977:ARG:CG	1.65	1.10
1:D:815:LEU:HD21	1:D:979:LEU:HD11	1.19	1.10
1:C:835:HIS:HD2	1:C:856:PHE:HB2	1.06	1.10
1:C:856:PHE:HD1	1:C:857:GLY:N	1.49	1.10
1:H:799:LEU:O	1:H:803:ARG:HG3	1.50	1.10
1:C:760:LEU:CD1	1:C:782:LEU:HD11	1.80	1.10
1:D:815:LEU:HD21	1:D:979:LEU:CD1	1.81	1.09
1:B:755:ALA:O	1:B:759:ILE:HD12	1.52	1.09
1:G:811:SER:HB3	1:G:984:ASP:OD1	1.50	1.09
1:G:989:LEU:CD2	1:G:990:PRO:CD	2.30	1.09
1:C:825:MET:SD	1:C:838:LEU:HD22	1.91	1.09
1:D:981:ILE:HB	1:D:984:ASP:HB2	1.35	1.08
1:D:771:ASN:HB3	1:D:774:VAL:HG23	1.22	1.08
1:G:849:GLN:HE21	1:G:990:PRO:HG3	1.12	1.08
1:B:831:ARG:HG2	1:B:831:ARG:HH11	1.19	1.08
1:F:771:ASN:ND2	1:F:772:PRO:HD2	1.67	1.08
1:E:937:PRO:HD2	4:E:1211:HOH:O	1.50	1.08
1:C:835:HIS:CD2	1:C:856:PHE:CA	2.36	1.08
1:F:876:VAL:HB	1:F:877:PRO:HD2	1.34	1.07
1:H:986:ARG:HB3	1:H:986:ARG:HH11	1.12	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:729:GLY:C	1:F:730:LEU:HD23	1.72	1.07
1:E:759:ILE:CD1	1:E:780:ILE:HD11	1.83	1.06
1:F:707:LEU:H	1:F:707:LEU:HD12	1.13	1.06
1:H:832:ARG:HH11	1:H:832:ARG:HG2	1.01	1.06
1:E:743:ALA:C	1:E:744:ILE:HD13	1.76	1.05
1:B:809:ILE:O	1:B:987:MET:CE	2.04	1.05
1:D:941:ILE:O	1:D:945:MET:HG3	1.56	1.05
1:G:989:LEU:CD2	1:G:990:PRO:HD2	1.86	1.05
1:C:760:LEU:HD13	1:C:782:LEU:CD1	1.86	1.05
1:E:945:MET:HE1	1:C:934:PRO:HG2	1.10	1.05
1:D:730:LEU:CD2	1:D:739:LYS:HB3	1.85	1.05
1:C:913:LYS:H	1:C:913:LYS:CD	1.66	1.05
1:G:845:VAL:HG13	1:G:847:THR:O	1.57	1.04
1:E:945:MET:HE1	1:C:934:PRO:CG	1.86	1.04
1:C:760:LEU:HD13	1:C:782:LEU:HD11	1.05	1.04
1:D:790:MET:HE2	2:D:1101:816:CAA	1.88	1.03
1:C:908:MET:CG	1:C:939:CYS:SG	2.46	1.03
1:C:878:ILE:HG23	1:C:886:ILE:HD11	1.41	1.03
1:G:811:SER:HB3	1:G:984:ASP:CG	1.79	1.03
1:H:953:ILE:CD1	1:H:953:ILE:H	1.72	1.03
1:C:835:HIS:HD2	1:C:856:PHE:CB	1.72	1.03
1:C:909:THR:HB	1:C:912:SER:HB2	1.38	1.03
1:H:845:VAL:HG13	1:H:847:THR:O	1.57	1.02
1:E:845:VAL:HG13	1:E:847:THR:O	1.58	1.02
1:C:908:MET:HG3	1:C:939:CYS:SG	1.98	1.02
1:C:940:THR:HB	1:C:978:TYR:O	1.57	1.02
1:D:815:LEU:HD11	1:D:979:LEU:HD12	1.39	1.02
1:E:707:LEU:CD1	1:E:789:ILE:HG12	1.89	1.02
1:B:809:ILE:C	1:B:987:MET:HE3	1.81	1.01
1:H:899:SER:HA	1:H:902:VAL:CG2	1.90	1.01
1:E:790:MET:HE1	2:E:1101:816:NAB	1.76	1.01
1:F:853:ILE:HD12	1:F:853:ILE:N	1.71	1.01
1:C:908:MET:CE	1:C:979:LEU:HD21	1.90	1.01
1:A:841:ARG:HH21	1:A:841:ARG:HG2	1.20	1.01
1:C:700:ASN:N	1:C:703:LEU:HD12	1.76	1.01
1:A:717:VAL:O	1:A:717:VAL:HG12	1.61	1.00
1:G:881:MET:HE3	1:G:885:SER:HB3	1.43	1.00
1:C:717:VAL:HG23	1:C:727:TYR:CE2	1.96	1.00
1:F:989:LEU:C	1:F:989:LEU:CD2	2.30	1.00
1:C:894:GLN:HA	1:C:894:GLN:OE1	1.58	1.00
1:D:783:THR:HG22	1:D:784:SER:H	1.24	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:989:LEU:CD2	1:G:990:PRO:HD3	1.92	0.99
1:C:715:ILE:HD11	1:C:728:LYS:NZ	1.76	0.99
1:E:842:ASN:O	1:E:854:THR:HG22	1.61	0.99
1:E:795:PHE:HE2	1:E:1002:MET:HE1	1.27	0.99
1:D:1013:ALA:HB2	4:D:1210:HOH:O	1.61	0.99
1:H:799:LEU:HD13	1:H:840:ALA:HB3	1.41	0.99
1:A:777:LEU:HD21	1:A:788:LEU:HD23	1.44	0.99
1:F:708:LYS:N	1:F:711:GLU:HG3	1.77	0.99
1:C:835:HIS:CD2	1:C:856:PHE:HB2	1.97	0.99
1:G:989:LEU:HD22	1:G:990:PRO:HD2	1.01	0.98
1:F:990:PRO:HG3	4:F:1215:HOH:O	1.63	0.98
1:C:856:PHE:CD1	1:C:857:GLY:N	2.30	0.98
1:E:795:PHE:HE2	1:E:1002:MET:CE	1.76	0.98
1:C:913:LYS:H	1:C:913:LYS:HD3	1.25	0.98
1:C:835:HIS:CD2	1:C:856:PHE:CB	2.46	0.98
1:G:730:LEU:HD13	1:G:739:LYS:HB3	1.46	0.97
1:G:806:LYS:C	1:G:806:LYS:CD	2.30	0.97
1:E:730:LEU:HD13	1:E:739:LYS:HB3	1.46	0.97
1:E:707:LEU:HD11	1:E:789:ILE:HG12	1.45	0.97
1:B:972:ALA:HB3	1:B:1011:VAL:HG11	1.43	0.97
1:H:757:LYS:HD2	1:H:757:LYS:C	1.85	0.97
1:H:832:ARG:HG2	1:H:832:ARG:NH1	1.70	0.97
1:B:972:ALA:CB	1:B:1011:VAL:HG11	1.94	0.97
1:B:988:HIS:CB	1:B:989:LEU:C	2.33	0.97
1:H:772:PRO:O	1:H:852:LYS:HE3	1.63	0.97
1:B:790:MET:HE2	2:B:1101:816:NAB	1.80	0.97
1:D:815:LEU:CD2	1:D:979:LEU:CD1	2.42	0.96
1:H:762:GLU:O	1:H:765:VAL:HG23	1.63	0.96
1:H:953:ILE:HD12	1:H:953:ILE:N	1.77	0.96
1:G:854:THR:HG22	1:G:855:ASP:N	1.79	0.96
1:F:707:LEU:HD12	1:F:707:LEU:N	1.81	0.95
1:G:974:ASP:OD2	3:G:1102:EDO:H21	1.67	0.95
1:D:717:VAL:HG13	1:D:727:TYR:HE2	1.29	0.95
1:C:972:ALA:O	1:C:975:PRO:HD3	1.66	0.95
1:E:847:THR:HG23	1:E:850:HIS:HB3	1.45	0.95
1:F:769:VAL:O	1:F:769:VAL:HG23	1.65	0.95
1:F:853:ILE:CD1	1:F:853:ILE:H	1.80	0.95
1:B:769:VAL:HG12	1:B:827:TYR:HE2	1.29	0.95
1:E:759:ILE:CD1	1:E:780:ILE:CD1	2.45	0.94
1:F:853:ILE:N	1:F:853:ILE:CD1	2.30	0.94
1:B:988:HIS:HA	1:B:989:LEU:CB	1.98	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:VAL:CG2	1:C:727:TYR:CE2	2.49	0.94
1:H:778:LEU:N	1:H:778:LEU:CD2	2.30	0.94
1:C:1007:MET:HG2	1:C:1008:ASP:N	1.82	0.94
1:A:946:ILE:CD1	1:A:971:MET:CE	2.46	0.94
1:D:790:MET:CE	2:D:1101:816:CAA	2.46	0.94
1:B:790:MET:CE	2:B:1101:816:NAB	2.30	0.94
1:E:945:MET:CE	1:C:934:PRO:HG2	1.97	0.94
1:H:986:ARG:HH11	1:H:986:ARG:CB	1.82	0.93
1:C:707:LEU:HD11	1:C:789:ILE:HD13	1.50	0.93
1:F:977:ARG:HD2	1:F:977:ARG:C	1.79	0.93
1:F:989:LEU:HD23	1:F:990:PRO:N	1.81	0.93
1:H:986:ARG:CB	1:H:986:ARG:NH1	2.30	0.93
1:E:840:ALA:HB3	1:E:906:GLU:OE2	1.67	0.93
1:B:940:THR:HB	1:B:978:TYR:O	1.67	0.93
1:D:790:MET:CE	2:D:1101:816:NAY	2.32	0.93
1:D:815:LEU:CD1	1:D:979:LEU:HD12	1.99	0.93
1:H:986:ARG:HB3	1:H:986:ARG:NH1	1.84	0.93
1:B:809:ILE:O	1:B:987:MET:HE2	1.68	0.93
1:D:839:ALA:O	1:D:843:VAL:HG23	1.68	0.93
1:C:717:VAL:CG2	1:C:727:TYR:HE2	1.82	0.93
1:D:717:VAL:HG13	1:D:727:TYR:CE2	2.02	0.92
1:A:977:ARG:HE	1:E:926:ILE:HD12	1.33	0.92
1:B:977:ARG:HG3	1:B:977:ARG:NH2	1.83	0.92
1:E:718:LEU:HB2	1:E:726:VAL:O	1.68	0.92
1:G:989:LEU:HD22	1:G:990:PRO:HD3	1.47	0.92
1:B:736:GLU:HA	1:B:736:GLU:OE2	1.70	0.91
1:H:812:GLN:CD	1:H:1013:ALA:HB2	1.90	0.91
1:C:717:VAL:HG23	1:C:727:TYR:HE2	1.32	0.91
1:H:953:ILE:CD1	1:H:953:ILE:N	2.30	0.91
1:B:894:GLN:NE2	1:B:960:LYS:HE2	1.85	0.91
1:H:778:LEU:HD23	1:H:778:LEU:H	1.32	0.91
1:H:854:THR:HG22	1:H:855:ASP:N	1.83	0.91
1:D:815:LEU:CG	1:D:979:LEU:CD1	2.48	0.91
1:A:946:ILE:CD1	1:A:971:MET:HE1	2.01	0.90
1:E:793:MET:HG3	1:E:844:LEU:CD1	2.02	0.90
1:F:756:ASN:ND2	1:F:782:LEU:HD13	1.86	0.90
1:E:998:TYR:O	1:E:1002:MET:HB2	1.72	0.90
1:F:778:LEU:HD23	1:F:790:MET:HA	1.52	0.90
1:E:762:GLU:O	1:E:765:VAL:HG23	1.70	0.90
1:H:899:SER:HA	1:H:902:VAL:HG23	1.53	0.90
1:A:946:ILE:HD11	1:A:971:MET:HE1	1.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:CYS:SG	2:G:1101:816:OAE	2.30	0.90
1:C:704:LEU:HD12	1:C:764:TYR:HE1	1.37	0.90
1:B:935:GLN:HG3	1:B:944:TYR:CD2	2.06	0.90
1:D:900:TYR:O	1:D:904:VAL:HG23	1.72	0.90
1:H:898:TRP:O	1:H:902:VAL:HG22	1.72	0.90
1:C:897:VAL:HG13	1:C:950:CYS:SG	2.11	0.90
1:H:812:GLN:NE2	1:H:1013:ALA:CB	2.33	0.89
1:C:913:LYS:CD	1:C:913:LYS:N	2.30	0.89
1:A:777:LEU:CD2	1:A:788:LEU:HD23	2.01	0.89
1:C:715:ILE:CD1	1:C:728:LYS:NZ	2.36	0.89
1:A:830:ASP:HB3	1:C:717:VAL:HG11	1.55	0.89
1:E:771:ASN:HB3	1:E:774:VAL:HG23	1.52	0.89
1:H:812:GLN:HE22	1:H:1013:ALA:HB2	1.30	0.89
1:B:934:PRO:O	1:B:936:PRO:HD3	1.73	0.89
1:A:923:ILE:HA	1:A:926:ILE:HG12	1.54	0.89
1:B:737:LYS:HD3	1:B:738:VAL:CG1	2.03	0.89
1:A:705:ARG:NE	1:A:707:LEU:HD21	1.88	0.88
1:B:982:GLN:H	1:B:982:GLN:HE21	1.17	0.88
1:H:832:ARG:HH11	1:H:832:ARG:CG	1.86	0.88
1:F:708:LYS:N	1:F:711:GLU:CG	2.36	0.88
1:F:811:SER:HB3	1:F:984:ASP:OD2	1.72	0.88
1:G:919:PRO:HD2	1:G:922:GLU:OE1	1.72	0.88
1:A:806:LYS:O	1:A:806:LYS:HD2	1.73	0.88
1:E:790:MET:CE	2:E:1101:816:NAB	2.36	0.88
1:H:899:SER:CA	1:H:902:VAL:HG23	2.04	0.88
1:B:818:CYS:SG	1:B:904:VAL:HG22	2.12	0.88
1:E:795:PHE:CE2	1:E:1002:MET:CE	2.56	0.88
1:B:809:ILE:C	1:B:987:MET:CE	2.40	0.88
1:E:856:PHE:CD1	1:E:856:PHE:C	2.46	0.88
1:F:955:ALA:O	1:F:958:ARG:HG3	1.73	0.88
1:A:834:VAL:HB	4:A:1209:HOH:O	1.74	0.87
1:G:775:CYS:SG	1:G:854:THR:OG1	2.32	0.87
1:H:817:TRP:O	1:H:821:ILE:HG13	1.74	0.87
1:D:717:VAL:HA	1:D:727:TYR:HD2	1.37	0.87
1:D:800:ASP:O	1:D:804:GLU:HG2	1.74	0.87
1:D:878:ILE:HA	1:D:881:MET:HE3	1.54	0.87
1:B:778:LEU:HD11	1:B:791:GLN:HG2	1.55	0.87
1:G:798:LEU:O	1:G:802:VAL:HG22	1.75	0.87
1:C:856:PHE:CD1	1:C:856:PHE:C	2.48	0.87
1:C:908:MET:HG2	1:C:939:CYS:SG	2.13	0.87
1:D:932:ARG:HG2	1:D:932:ARG:HH11	1.39	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:798:LEU:O	1:E:802:VAL:HG22	1.75	0.87
1:C:717:VAL:O	1:C:717:VAL:HG12	1.72	0.87
1:A:878:ILE:HD12	4:A:1214:HOH:O	1.73	0.87
1:C:773:HIS:O	1:C:853:ILE:HG23	1.73	0.87
1:B:816:ASN:HA	1:B:819:VAL:HG23	1.54	0.87
1:B:941:ILE:HD12	1:B:941:ILE:C	1.93	0.87
1:C:897:VAL:CG1	1:C:950:CYS:SG	2.62	0.87
1:C:908:MET:HE3	1:C:979:LEU:HD21	1.54	0.87
1:A:798:LEU:HD12	1:A:798:LEU:C	1.92	0.86
1:F:876:VAL:HB	1:F:877:PRO:CD	2.04	0.86
1:A:783:THR:HB	1:A:785:THR:O	1.76	0.86
1:C:955:ALA:O	1:C:958:ARG:HG3	1.76	0.86
1:B:835:HIS:HB2	1:B:856:PHE:CA	2.05	0.86
1:H:798:LEU:O	1:H:802:VAL:HG22	1.76	0.86
1:D:717:VAL:HA	1:D:727:TYR:CD2	2.10	0.86
1:D:940:THR:HG22	1:D:943:VAL:HG23	1.58	0.86
1:G:919:PRO:HG2	1:G:922:GLU:OE1	1.76	0.86
1:A:786:VAL:HG23	4:A:1228:HOH:O	1.76	0.85
1:B:737:LYS:HD3	1:B:738:VAL:HG13	1.57	0.85
1:C:908:MET:HE1	1:C:979:LEU:HD21	1.58	0.85
1:E:986:ARG:HG2	1:E:987:MET:N	1.89	0.85
1:C:801:TYR:HE2	1:C:817:TRP:HH2	1.24	0.85
1:D:719:GLY:HA3	2:D:1101:816:CAS	2.07	0.85
1:H:718:LEU:HD11	1:H:792:LEU:HD11	1.56	0.85
1:A:950:CYS:O	1:A:958:ARG:HD3	1.75	0.85
1:A:977:ARG:HG2	1:E:931:GLU:OE2	1.75	0.85
1:D:815:LEU:CG	1:D:979:LEU:HD12	2.05	0.85
1:E:723:PHE:CE2	1:E:859:ALA:HA	2.09	0.85
1:H:747:LEU:HD13	1:H:862:LEU:HD21	1.59	0.85
1:B:831:ARG:HG2	1:B:831:ARG:NH1	1.83	0.85
1:G:854:THR:HG22	1:G:855:ASP:H	1.37	0.85
1:G:940:THR:CG2	1:G:943:VAL:HG23	2.07	0.85
1:C:940:THR:HG22	1:C:943:VAL:HG23	1.56	0.85
1:B:797:CYS:SG	1:B:800:ASP:OD2	2.35	0.85
1:B:834:VAL:HG22	1:B:893:HIS:CD2	2.12	0.85
1:G:825:MET:HE1	1:G:853:ILE:HD13	1.59	0.85
1:E:950:CYS:O	1:E:958:ARG:HD2	1.76	0.85
1:C:714:LYS:CE	1:C:787:GLN:HE22	1.89	0.85
1:F:730:LEU:HD23	1:F:730:LEU:N	1.89	0.84
1:C:953:ILE:HD13	1:C:953:ILE:N	1.91	0.84
1:B:771:ASN:ND2	1:B:772:PRO:CD	2.39	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:877:PRO:O	1:D:881:MET:HG3	1.75	0.84
1:H:935:GLN:OE1	1:H:944:TYR:CD2	2.30	0.84
1:C:790:MET:HE1	2:C:1101:816:NAB	1.91	0.84
1:F:836:ARG:HB2	1:F:859:ALA:HB3	1.58	0.84
1:E:756:ASN:O	1:E:759:ILE:HG22	1.77	0.84
1:G:823:LYS:HE2	1:G:1008:ASP:OD2	1.77	0.84
1:C:941:ILE:HD12	1:C:941:ILE:C	1.96	0.84
1:A:856:PHE:O	1:A:856:PHE:CD1	2.30	0.84
1:A:881:MET:HE3	1:A:885:SER:HB2	1.59	0.84
1:E:945:MET:CE	1:C:934:PRO:CG	2.54	0.84
1:G:773:HIS:ND1	1:G:820:GLN:HB3	1.91	0.84
1:G:849:GLN:HE21	1:G:990:PRO:CG	1.89	0.84
1:B:905:TRP:O	1:B:909:THR:HG23	1.77	0.84
1:D:707:LEU:HD22	1:D:711:GLU:HB2	1.58	0.84
1:A:806:LYS:CD	1:A:806:LYS:C	2.46	0.84
1:A:881:MET:HE3	1:A:885:SER:CB	2.07	0.84
1:B:835:HIS:CB	1:B:856:PHE:CB	2.54	0.84
1:F:848:PRO:HB2	1:F:849:GLN:OE1	1.77	0.84
1:H:715:ILE:HD11	1:H:728:LYS:CE	2.05	0.84
1:B:817:TRP:O	1:B:821:ILE:HG13	1.78	0.83
1:E:808:ASN:O	1:E:809:ILE:HG12	1.77	0.83
1:H:762:GLU:HB3	1:H:861:LEU:HD21	1.60	0.83
1:B:945:MET:CE	1:D:909:THR:HG22	2.08	0.83
1:G:878:ILE:HG23	1:G:886:ILE:HD13	1.60	0.83
1:D:878:ILE:HG13	1:D:881:MET:CE	2.09	0.83
1:E:836:ARG:HD2	1:E:860:LYS:CB	2.08	0.83
1:A:841:ARG:HG2	1:A:841:ARG:NH2	1.91	0.83
1:H:715:ILE:CD1	1:H:728:LYS:HE2	2.07	0.83
1:H:835:HIS:CE1	1:H:837:ASP:O	2.30	0.83
1:E:793:MET:HE1	1:E:846:LYS:HB2	1.60	0.83
1:D:815:LEU:HG	1:D:979:LEU:CD1	2.08	0.83
1:D:799:LEU:O	1:D:803:ARG:HG3	1.79	0.83
1:D:941:ILE:HD11	1:D:945:MET:HE2	1.60	0.83
1:A:806:LYS:HD2	1:A:806:LYS:C	1.99	0.83
1:B:798:LEU:HB2	1:B:843:VAL:HG12	1.61	0.83
1:H:899:SER:C	1:H:902:VAL:HG23	1.99	0.83
1:C:905:TRP:O	1:C:909:THR:HG23	1.78	0.83
1:D:798:LEU:O	1:D:802:VAL:HG22	1.79	0.82
1:G:704:LEU:CD1	1:G:767:ALA:HB2	2.09	0.82
1:A:777:LEU:CD2	1:A:788:LEU:CD2	2.57	0.82
1:D:845:VAL:HG22	1:D:851:VAL:HG12	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:989:LEU:HD23	1:F:989:LEU:O	1.77	0.82
1:C:878:ILE:HG23	1:C:886:ILE:CD1	2.09	0.82
1:G:769:VAL:HG11	1:G:856:PHE:HZ	1.44	0.82
1:E:759:ILE:HD11	1:E:780:ILE:CD1	2.05	0.82
1:A:762:GLU:O	1:A:765:VAL:HG12	1.79	0.82
1:C:790:MET:CE	2:C:1101:816:NAB	2.42	0.82
1:E:744:ILE:HD13	1:E:744:ILE:N	1.84	0.82
1:F:747:LEU:HG	1:F:788:LEU:HD11	1.62	0.82
1:F:818:CYS:SG	1:F:904:VAL:HG13	2.19	0.82
1:D:936:PRO:HB2	1:D:939:CYS:HB2	1.62	0.81
1:B:777:LEU:HD21	1:B:788:LEU:HD22	1.61	0.81
1:F:989:LEU:HD21	1:F:990:PRO:O	1.79	0.81
1:F:723:PHE:O	1:F:748:ARG:HG2	1.79	0.81
1:F:729:GLY:HA3	1:F:744:ILE:HD11	1.62	0.81
1:F:876:VAL:CB	1:F:877:PRO:HD2	2.10	0.81
1:H:935:GLN:HB3	1:H:944:TYR:CE2	2.15	0.81
1:H:953:ILE:H	1:H:953:ILE:HD13	1.45	0.81
1:A:705:ARG:HE	1:A:707:LEU:CD2	1.94	0.81
1:G:932:ARG:HB3	1:G:932:ARG:HH11	1.45	0.81
1:F:908:MET:HG3	1:F:939:CYS:SG	2.20	0.81
1:A:936:PRO:HB2	1:A:939:CYS:HB2	1.62	0.81
1:A:946:ILE:HD11	1:A:971:MET:CE	2.09	0.81
1:B:999:ARG:HH11	1:B:999:ARG:HG3	1.45	0.81
1:E:803:ARG:HG2	1:E:911:GLY:HA3	1.62	0.81
1:G:889:ARG:HH11	1:G:889:ARG:CG	1.94	0.81
1:C:879:LYS:HD3	1:C:915:TYR:HB2	1.61	0.81
1:B:997:PHE:O	1:B:997:PHE:HD1	1.63	0.80
1:E:723:PHE:HE2	1:E:859:ALA:CA	1.95	0.80
1:G:924:SER:O	1:G:928:GLU:HG3	1.81	0.80
1:H:799:LEU:HD13	1:H:840:ALA:CB	2.10	0.80
1:H:962:ARG:HA	1:H:965:ILE:HG13	1.63	0.80
1:B:977:ARG:CG	1:B:977:ARG:NH2	2.36	0.80
1:B:835:HIS:HB2	1:B:856:PHE:HA	1.62	0.80
1:G:806:LYS:O	1:G:806:LYS:CE	2.30	0.80
1:B:769:VAL:HG12	1:B:827:TYR:CE2	2.17	0.80
1:D:707:LEU:HD22	1:D:711:GLU:CB	2.11	0.80
1:A:806:LYS:O	1:A:806:LYS:CD	2.30	0.80
1:B:935:GLN:HG3	1:B:944:TYR:CG	2.16	0.80
1:F:721:GLY:CA	1:F:724:GLY:O	2.30	0.80
1:F:729:GLY:C	1:F:730:LEU:CD2	2.49	0.80
1:G:1007:MET:CE	1:G:1008:ASP:O	2.30	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:991:SER:HB2	1:F:992:PRO:CD	2.11	0.80
1:C:816:ASN:O	1:C:820:GLN:HG3	1.80	0.80
1:D:797:CYS:HB3	1:D:800:ASP:HB2	1.62	0.80
1:E:723:PHE:HE2	1:E:859:ALA:HA	1.43	0.80
1:F:823:LYS:NZ	1:F:1008:ASP:CG	2.35	0.80
1:B:755:ALA:O	1:B:759:ILE:CD1	2.30	0.80
1:F:944:TYR:O	1:F:948:VAL:HG22	1.81	0.80
1:G:790:MET:HG2	2:G:1101:816:CLA	2.19	0.80
1:H:743:ALA:HB2	1:H:792:LEU:HD12	1.64	0.80
1:C:913:LYS:N	1:C:913:LYS:HD2	1.96	0.80
1:A:783:THR:HG22	1:A:784:SER:H	1.47	0.79
1:D:878:ILE:HD13	1:D:920:ALA:HB1	1.63	0.79
1:F:771:ASN:ND2	1:F:772:PRO:CD	2.45	0.79
1:F:989:LEU:CD2	1:F:990:PRO:O	2.30	0.79
1:C:780:ILE:CD1	1:C:787:GLN:O	2.30	0.79
1:E:967:GLU:O	1:E:971:MET:HG3	1.82	0.79
1:E:704:LEU:HB2	1:E:767:ALA:CB	2.12	0.79
1:G:845:VAL:CG1	1:G:847:THR:O	2.30	0.79
1:E:845:VAL:CG1	1:E:847:THR:O	2.30	0.79
1:C:842:ASN:O	1:C:854:THR:HG22	1.81	0.79
1:C:894:GLN:OE1	1:C:894:GLN:CA	2.30	0.79
1:A:717:VAL:HG23	1:A:727:TYR:CE2	2.17	0.79
1:G:919:PRO:CD	1:G:922:GLU:OE1	2.30	0.79
1:A:849:GLN:OE1	1:A:995:SER:HB2	1.83	0.79
1:H:899:SER:HA	1:H:902:VAL:HG21	1.63	0.79
1:C:701:GLN:OE1	1:C:701:GLN:HA	1.81	0.79
1:H:762:GLU:O	1:H:765:VAL:CG2	2.30	0.79
1:C:894:GLN:HB3	1:C:955:ALA:HB1	1.65	0.79
1:F:769:VAL:O	1:F:769:VAL:CG2	2.30	0.79
1:A:900:TYR:O	1:A:904:VAL:HG23	1.83	0.78
1:B:717:VAL:O	1:B:717:VAL:HG12	1.82	0.78
1:E:844:LEU:CD2	1:E:854:THR:HG21	2.14	0.78
1:G:915:TYR:HE1	1:G:926:ILE:HD11	1.47	0.78
1:G:915:TYR:CE1	1:G:926:ILE:HD11	2.19	0.78
1:D:704:LEU:HB2	1:D:767:ALA:CB	2.12	0.78
1:C:701:GLN:OE1	1:C:701:GLN:CA	2.30	0.78
1:B:931:GLU:O	1:B:932:ARG:HD2	1.83	0.78
1:D:757:LYS:HD2	1:D:761:ASP:OD2	1.83	0.78
1:C:805:HIS:O	1:C:809:ILE:CG2	2.30	0.78
1:E:718:LEU:CB	1:E:726:VAL:O	2.32	0.78
1:E:841:ARG:HD2	4:E:1218:HOH:O	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:LEU:N	1:C:778:LEU:CD2	2.40	0.78
1:F:977:ARG:O	1:F:977:ARG:CD	2.30	0.78
1:G:919:PRO:CG	1:G:922:GLU:OE1	2.32	0.78
1:H:817:TRP:CD1	1:H:851:VAL:HG11	2.19	0.78
1:A:935:GLN:HG3	1:A:944:TYR:CG	2.19	0.78
1:H:835:HIS:CD2	1:H:856:PHE:HB3	2.19	0.78
1:C:736:GLU:HA	1:C:736:GLU:OE2	1.83	0.78
1:B:780:ILE:HD13	1:B:782:LEU:HD22	1.66	0.78
1:D:819:VAL:O	1:D:823:LYS:HG3	1.84	0.78
1:C:817:TRP:O	1:C:821:ILE:HG13	1.84	0.78
1:C:839:ALA:CB	1:C:841:ARG:HG3	2.14	0.78
1:G:854:THR:CG2	1:G:855:ASP:H	1.97	0.78
1:G:940:THR:HG22	1:G:943:VAL:CG2	2.10	0.77
1:B:783:THR:HG22	1:B:784:SER:N	2.00	0.77
1:H:845:VAL:CG1	1:H:847:THR:O	2.30	0.77
1:C:811:SER:HB3	1:C:984:ASP:OD1	1.85	0.77
1:D:746:GLU:HG3	1:D:787:GLN:HG2	1.65	0.77
1:F:991:SER:HB2	1:F:992:PRO:HD2	1.66	0.77
1:E:730:LEU:HD13	1:E:739:LYS:CB	2.14	0.77
1:H:800:ASP:O	1:H:804:GLU:HG3	1.84	0.77
1:H:899:SER:O	1:H:902:VAL:HG23	1.84	0.77
1:C:825:MET:SD	1:C:838:LEU:HD21	2.24	0.77
1:C:881:MET:HE2	1:C:886:ILE:CG1	2.15	0.77
1:C:955:ALA:O	1:C:958:ARG:CG	2.32	0.77
1:E:835:HIS:CE1	1:E:856:PHE:HA	2.18	0.77
1:F:836:ARG:HB2	1:F:859:ALA:CB	2.15	0.77
1:E:719:GLY:HA3	2:E:1101:816:CAS	2.14	0.77
1:C:707:LEU:CD1	1:C:789:ILE:HD13	2.14	0.77
1:H:935:GLN:HB3	1:H:944:TYR:CD2	2.19	0.77
1:A:705:ARG:NE	1:A:707:LEU:CD2	2.48	0.76
1:G:817:TRP:CD1	1:G:851:VAL:HG11	2.20	0.76
1:G:1007:MET:HE2	1:G:1008:ASP:O	1.85	0.76
1:C:715:ILE:CD1	1:C:728:LYS:HZ1	1.98	0.76
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.20	0.76
1:D:923:ILE:O	1:D:926:ILE:HG12	1.85	0.76
1:E:898:TRP:HE3	1:E:958:ARG:NH1	1.83	0.76
1:E:706:ILE:HG22	1:E:706:ILE:O	1.86	0.76
1:F:944:TYR:O	1:F:948:VAL:CG2	2.32	0.76
1:G:854:THR:CG2	1:G:855:ASP:N	2.48	0.76
1:G:889:ARG:HH11	1:G:889:ARG:HG2	1.51	0.76
1:G:1006:ASP:CB	4:G:1220:HOH:O	2.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ASN:N	1:A:703:LEU:HD12	2.00	0.76
1:A:966:ILE:CD1	1:C:804:GLU:OE2	2.33	0.76
1:D:762:GLU:OE1	1:D:861:LEU:CB	2.33	0.76
1:G:717:VAL:HG22	1:G:727:TYR:CE2	2.20	0.76
1:C:801:TYR:HE2	1:C:817:TRP:CH2	2.03	0.76
1:C:973:ARG:HG2	1:C:973:ARG:NH1	2.01	0.76
1:G:703:LEU:HD23	1:G:703:LEU:N	2.01	0.76
1:H:905:TRP:O	1:H:909:THR:CG2	2.30	0.76
1:A:777:LEU:HD22	1:A:788:LEU:CD2	2.16	0.76
1:B:816:ASN:HA	1:B:819:VAL:CG2	2.14	0.76
1:D:771:ASN:HB3	1:D:774:VAL:CG2	2.10	0.76
1:A:819:VAL:HG12	1:A:823:LYS:HE3	1.66	0.76
1:C:835:HIS:NE2	1:C:856:PHE:HA	2.01	0.76
1:C:940:THR:CB	1:C:978:TYR:O	2.31	0.76
1:D:878:ILE:HA	1:D:881:MET:CE	2.16	0.76
1:H:845:VAL:CG1	1:H:847:THR:C	2.54	0.76
1:A:717:VAL:O	1:A:717:VAL:CG1	2.30	0.75
1:A:793:MET:HE2	1:A:844:LEU:HD12	1.68	0.75
1:E:743:ALA:C	1:E:744:ILE:CD1	2.54	0.75
1:G:704:LEU:HD13	1:G:767:ALA:HB2	1.67	0.75
1:G:825:MET:CE	1:G:853:ILE:HD13	2.16	0.75
1:G:932:ARG:HB3	1:G:932:ARG:NH1	2.00	0.75
1:D:793:MET:O	2:D:1101:816:C2	2.35	0.75
1:D:932:ARG:HG2	1:D:932:ARG:NH1	1.97	0.75
1:C:909:THR:CB	1:C:912:SER:HB2	2.14	0.75
1:A:815[B]:LEU:HD22	1:A:979:LEU:HD12	1.68	0.75
1:G:849:GLN:NE2	1:G:990:PRO:HG3	1.96	0.75
1:H:986:ARG:NH1	1:H:986:ARG:HB2	2.00	0.75
1:C:839:ALA:HB3	1:C:841:ARG:HG3	1.68	0.75
1:B:737:LYS:CD	1:B:738:VAL:HG13	2.16	0.75
1:G:825:MET:HG2	1:G:961:PHE:CE2	2.21	0.75
1:G:949:LYS:O	1:G:952:MET:HG2	1.87	0.75
1:A:881:MET:CE	1:A:885:SER:HB2	2.17	0.75
1:E:748:ARG:HH11	1:E:748:ARG:HG3	1.52	0.75
1:A:949:LYS:O	1:A:952:MET:HG3	1.87	0.75
1:B:705:ARG:HD3	1:B:707:LEU:HD21	1.69	0.75
1:B:894:GLN:HE22	1:B:960:LYS:HE2	1.51	0.75
1:E:748:ARG:O	1:E:749:GLU:CB	2.33	0.75
1:G:1007:MET:HE3	1:G:1010:VAL:HG12	1.69	0.75
1:H:879:LYS:HD2	1:H:915:TYR:HB2	1.68	0.75
1:C:728:LYS:HZ3	1:C:730:LEU:HD21	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:VAL:CG2	1:B:727:TYR:CE2	2.69	0.74
1:E:833:LEU:HD13	1:E:856:PHE:CE1	2.22	0.74
1:G:743:ALA:CB	2:G:1101:816:NAB	2.50	0.74
1:G:923:ILE:HA	1:G:926:ILE:CG2	2.17	0.74
1:C:728:LYS:NZ	1:C:730:LEU:HD21	2.02	0.74
1:A:946:ILE:HD12	1:A:971:MET:CE	2.16	0.74
1:B:982:GLN:NE2	1:B:982:GLN:N	2.30	0.74
1:B:943:VAL:HG21	1:B:979:LEU:HD21	1.69	0.74
1:E:977:ARG:HG2	1:C:918:ILE:HD11	1.69	0.74
1:A:844:LEU:N	1:A:844:LEU:HD23	2.01	0.74
1:E:821:ILE:CG2	1:E:900:TYR:HE1	2.01	0.74
1:A:726:VAL:CG2	1:A:745:LYS:HG3	2.17	0.74
1:H:793:MET:H	2:H:1101:816:C2	2.00	0.74
1:C:1007:MET:HG2	1:C:1008:ASP:O	1.87	0.74
1:E:744:ILE:N	1:E:744:ILE:CD1	2.51	0.74
1:F:729:GLY:O	1:F:730:LEU:CD2	2.35	0.74
1:H:854:THR:CG2	1:H:855:ASP:N	2.49	0.74
1:H:781:CYS:HB3	1:H:787:GLN:HB2	1.68	0.74
1:C:704:LEU:HD12	1:C:764:TYR:CE1	2.22	0.74
1:A:783:THR:HG22	1:A:784:SER:N	2.03	0.73
1:B:759:ILE:HD12	1:B:759:ILE:H	1.52	0.73
1:C:760:LEU:CD1	1:C:782:LEU:CD1	2.55	0.73
1:D:795:PHE:HB2	1:D:845:VAL:HG12	1.69	0.73
1:A:757:LYS:HD3	1:A:757:LYS:N	2.03	0.73
1:F:842:ASN:O	1:F:854:THR:CG2	2.32	0.73
1:H:893:HIS:O	1:H:896:ASP:HB2	1.89	0.73
1:B:982:GLN:HE21	1:B:982:GLN:N	1.86	0.73
1:G:743:ALA:HB3	2:G:1101:816:NAB	2.03	0.73
1:F:825:MET:CE	1:F:835:HIS:HB3	2.19	0.73
1:G:825:MET:CE	1:G:853:ILE:CD1	2.66	0.73
1:H:825:MET:HE2	1:H:961:PHE:HZ	1.54	0.73
1:H:798:LEU:O	1:H:802:VAL:CG2	2.36	0.73
1:D:783:THR:HG22	1:D:784:SER:N	2.02	0.73
1:D:844:LEU:HD11	2:D:1101:816:CAL	2.19	0.73
1:E:806:LYS:HE2	4:E:1207:HOH:O	1.88	0.73
1:F:967:GLU:O	1:F:971:MET:HG3	1.88	0.73
1:F:972:ALA:HB3	1:F:1011:VAL:HG11	1.71	0.73
1:B:771:ASN:HD22	1:B:772:PRO:HD2	1.49	0.73
1:C:973:ARG:HG2	1:C:973:ARG:HH11	1.52	0.73
1:D:878:ILE:HG23	1:D:886:ILE:HD11	1.69	0.73
1:F:717:VAL:HG22	1:F:727:TYR:CE2	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:754:LYS:HG2	1:C:755:ALA:H	1.54	0.72
1:D:983:GLY:O	1:D:986:ARG:HG3	1.89	0.72
1:H:945:MET:HE1	3:H:1103:EDO:C2	2.18	0.72
1:D:900:TYR:CE2	1:D:904:VAL:HG21	2.23	0.72
1:F:1007:MET:HG2	1:F:1008:ASP:O	1.89	0.72
1:G:798:LEU:O	1:G:798:LEU:HD12	1.88	0.72
1:D:790:MET:HE3	2:D:1101:816:NAY	2.04	0.72
1:G:974:ASP:OD2	3:G:1102:EDO:C2	2.36	0.72
1:H:898:TRP:O	1:H:902:VAL:CG2	2.37	0.72
1:C:769:VAL:CG2	1:C:769:VAL:O	2.38	0.72
1:C:769:VAL:HG11	1:C:856:PHE:HE2	1.54	0.72
1:A:934:PRO:O	1:A:936:PRO:HD3	1.90	0.72
1:D:815:LEU:O	1:D:819:VAL:HG23	1.90	0.72
1:H:935:GLN:OE1	1:H:944:TYR:HD2	1.71	0.72
1:A:704:LEU:HD12	1:A:779:GLY:HA2	1.71	0.72
1:H:938:ILE:HG13	1:H:939:CYS:N	2.04	0.72
1:C:744:ILE:HG23	1:C:789:ILE:HG13	1.71	0.72
1:B:748:ARG:CB	4:B:1219:HOH:O	2.37	0.72
1:B:854:THR:O	1:B:855:ASP:HB2	1.89	0.72
1:A:837:ASP:HB2	4:A:1204:HOH:O	1.90	0.72
1:C:723:PHE:O	1:C:748:ARG:CG	2.37	0.72
1:C:778:LEU:H	1:C:778:LEU:CD2	1.84	0.72
1:B:790:MET:HE1	2:B:1101:816:NAB	2.04	0.71
1:D:940:THR:CG2	1:D:978:TYR:O	2.38	0.71
1:D:820:GLN:OE1	1:D:851:VAL:HG22	1.89	0.71
1:F:881:MET:CE	1:F:886:ILE:HG12	2.20	0.71
1:F:825:MET:HE3	1:F:835:HIS:CB	2.20	0.71
1:F:825:MET:SD	1:F:838:LEU:HD22	2.31	0.71
1:H:935:GLN:HB2	1:H:944:TYR:CG	2.25	0.71
1:C:715:ILE:CD1	1:C:728:LYS:HZ2	2.02	0.71
1:F:832:ARG:HG2	1:F:832:ARG:O	1.90	0.71
1:B:733:PRO:HB2	1:B:736:GLU:HB2	1.72	0.71
1:E:818:CYS:SG	1:E:904:VAL:HG22	2.30	0.71
1:F:823:LYS:HG2	1:F:965:ILE:HD13	1.71	0.71
1:G:995:SER:O	1:G:999[B]:ARG:CD	2.31	0.71
1:H:799:LEU:O	1:H:803:ARG:CG	2.34	0.71
1:H:812:GLN:HE22	1:H:1013:ALA:CB	1.95	0.71
1:A:726:VAL:HG22	1:A:745:LYS:HG3	1.71	0.71
1:G:955:ALA:O	1:G:958:ARG:HG3	1.90	0.71
1:F:708:LYS:H	1:F:711:GLU:CG	2.02	0.71
1:G:945:MET:O	1:G:949:LYS:HG3	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1006:ASP:HB3	4:G:1220:HOH:O	1.89	0.71
1:H:817:TRP:CD1	1:H:851:VAL:CG1	2.74	0.71
1:H:949:LYS:O	1:H:952:MET:HG3	1.90	0.71
1:C:913:LYS:H	1:C:913:LYS:HD2	1.53	0.71
1:G:1007:MET:HG2	1:G:1008:ASP:N	2.04	0.71
1:H:854:THR:HG22	1:H:855:ASP:H	1.56	0.71
1:C:715:ILE:HD11	1:C:728:LYS:HZ2	1.53	0.71
1:B:835:HIS:HB2	1:B:856:PHE:HB2	1.70	0.71
1:F:730:LEU:N	1:F:730:LEU:CD2	2.54	0.71
1:A:967[B]:GLU:OE2	1:A:970:LYS:HD2	1.89	0.70
1:B:707:LEU:HD22	1:B:711:GLU:OE2	1.90	0.70
1:E:821:ILE:HG22	1:E:900:TYR:CE1	2.25	0.70
1:C:780:ILE:HD13	1:C:787:GLN:O	1.90	0.70
1:B:726:VAL:HG23	1:B:745:LYS:HE2	1.73	0.70
1:A:729:GLY:HA3	1:A:744:ILE:CD1	2.21	0.70
1:A:738:VAL:HG23	4:A:1232:HOH:O	1.91	0.70
1:A:758:GLU:OE2	1:A:758:GLU:C	2.30	0.70
1:D:790:MET:HE1	2:D:1101:816:NAY	2.06	0.70
1:F:758:GLU:OE2	1:F:758:GLU:C	2.30	0.70
1:G:1013:ALA:C	1:G:1014:ASP:OD1	2.30	0.70
1:C:758:GLU:OE2	1:C:758:GLU:C	2.30	0.70
1:B:881:MET:CE	1:B:891:TYR:OH	2.39	0.70
1:E:884:GLU:HG2	1:E:885:SER:N	2.06	0.70
1:G:989:LEU:HD23	1:G:990:PRO:HD3	1.68	0.70
1:A:977:ARG:HD2	1:A:977:ARG:O	1.92	0.70
1:C:714:LYS:HE3	1:C:787:GLN:HE22	1.56	0.70
1:E:726:VAL:CG2	1:E:745:LYS:HD2	2.22	0.70
1:G:825:MET:HG2	1:G:961:PHE:CZ	2.26	0.70
1:C:975:PRO:HD2	1:C:1013:ALA:HB2	1.73	0.70
1:A:881:MET:CE	1:A:885:SER:CB	2.69	0.70
1:E:833:LEU:HD13	1:E:856:PHE:CZ	2.26	0.70
1:A:757:LYS:HD3	1:A:757:LYS:H	1.56	0.70
1:B:988:HIS:CB	1:B:989:LEU:O	2.39	0.70
1:D:811:SER:HB2	1:D:981:ILE:HG13	1.72	0.70
1:E:704:LEU:HB2	1:E:767:ALA:HB2	1.74	0.70
1:B:898:TRP:CZ2	1:B:927:LEU:HD13	2.26	0.70
1:D:704:LEU:HB2	1:D:767:ALA:HB2	1.73	0.70
1:A:898:TRP:CZ2	1:A:927:LEU:HD13	2.27	0.69
1:E:881:MET:HE2	1:E:886:ILE:HG13	1.73	0.69
1:H:758:GLU:O	1:H:758:GLU:CD	2.30	0.69
1:C:715:ILE:HG12	1:C:728:LYS:O	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LEU:HD12	1:A:789:ILE:O	1.92	0.69
1:F:856:PHE:C	1:F:856:PHE:CD1	2.64	0.69
1:G:935:GLN:HB2	1:G:944:TYR:CD1	2.27	0.69
1:H:962:ARG:CA	1:H:965:ILE:HG13	2.22	0.69
1:F:799:LEU:O	1:F:803:ARG:HG3	1.92	0.69
1:H:879:LYS:HD3	1:H:923:ILE:HD11	1.75	0.69
1:C:973:ARG:HH11	1:C:973:ARG:CG	2.03	0.69
1:E:821:ILE:HG22	1:E:900:TYR:HE1	1.57	0.69
1:E:856:PHE:CD1	1:E:856:PHE:O	2.45	0.69
1:F:825:MET:HE3	1:F:835:HIS:HB2	1.74	0.69
1:F:961:PHE:O	1:F:965:ILE:HG13	1.92	0.69
2:F:1101:816:CAP	2:F:1101:816:CAV	2.70	0.69
1:F:999:ARG:O	1:F:1003:ASP:C	2.30	0.69
1:G:935:GLN:HB2	1:G:944:TYR:CG	2.27	0.69
1:B:940:THR:HG23	1:B:943:VAL:H	1.56	0.69
1:D:806:LYS:HG2	1:D:807:ASP:N	2.06	0.69
1:C:985:GLU:H	1:C:985:GLU:CD	1.95	0.69
1:A:938:ILE:HD12	1:A:981:ILE:HG12	1.75	0.69
1:B:707:LEU:HD12	1:B:789:ILE:HD13	1.73	0.69
1:B:726:VAL:CG2	1:B:745:LYS:HE2	2.22	0.69
1:B:816:ASN:CA	1:B:819:VAL:HG23	2.23	0.69
1:D:805:HIS:CD2	4:D:1202:HOH:O	2.45	0.69
1:E:821:ILE:CG2	1:E:900:TYR:CE1	2.76	0.69
1:F:805:HIS:O	1:F:809:ILE:HG13	1.93	0.69
1:F:848:PRO:CB	1:F:849:GLN:OE1	2.40	0.69
1:C:881:MET:HE2	1:C:886:ILE:HG13	1.74	0.69
1:A:877:PRO:O	1:A:881:MET:HG3	1.93	0.69
1:E:798:LEU:HD23	1:E:907:LEU:HD21	1.75	0.69
1:F:723:PHE:O	1:F:748:ARG:CG	2.40	0.69
1:F:853:ILE:HD13	1:F:853:ILE:H	1.56	0.69
1:F:989:LEU:CD2	1:F:989:LEU:O	2.38	0.69
1:G:898:TRP:O	1:G:902:VAL:HG23	1.92	0.69
1:C:704:LEU:O	1:C:704:LEU:HD13	1.92	0.69
1:H:757:LYS:HD2	1:H:757:LYS:O	1.93	0.69
1:D:730:LEU:HD22	1:D:739:LYS:CB	2.13	0.68
1:H:800:ASP:O	1:H:804:GLU:CG	2.42	0.68
1:H:878:ILE:HD13	1:H:920:ALA:HB1	1.75	0.68
1:C:819:VAL:HG22	1:C:968:PHE:HB3	1.75	0.68
1:B:818:CYS:SG	1:B:904:VAL:CG2	2.80	0.68
1:E:856:PHE:O	1:E:856:PHE:CG	2.46	0.68
1:G:893:HIS:O	1:G:896:ASP:HB2	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:943:VAL:O	1:H:946:ILE:HG22	1.93	0.68
1:C:813:TYR:OH	1:C:990:PRO:HD3	1.93	0.68
1:F:708:LYS:O	1:F:711:GLU:CG	2.41	0.68
1:F:898:TRP:HE3	1:F:958:ARG:NH2	1.92	0.68
2:A:1101:816:CAP	2:A:1101:816:CAV	2.71	0.68
1:D:938:ILE:HD11	1:D:979:LEU:HD22	1.75	0.68
1:E:759:ILE:HD13	1:E:780:ILE:HD12	1.76	0.68
1:E:835:HIS:O	1:E:836:ARG:HB2	1.91	0.68
1:E:879:LYS:HE2	1:E:923:ILE:HD11	1.75	0.68
1:E:881:MET:HE2	1:E:886:ILE:CG1	2.24	0.68
1:G:825:MET:HE2	1:G:853:ILE:CD1	2.24	0.68
1:F:999:ARG:HA	1:F:1003:ASP:CB	2.24	0.68
1:H:762:GLU:HB3	1:H:861:LEU:CD2	2.24	0.68
1:A:705:ARG:CD	1:A:707:LEU:HD21	2.23	0.68
1:E:879:LYS:CE	1:E:923:ILE:HD11	2.23	0.68
1:G:923:ILE:O	1:G:927:LEU:HG	1.93	0.68
1:F:708:LYS:H	1:F:711:GLU:CD	1.96	0.68
1:F:724:GLY:HA2	1:F:748:ARG:HD2	1.76	0.68
1:B:835:HIS:HB2	1:B:856:PHE:CB	2.23	0.68
1:E:762:GLU:O	1:E:765:VAL:CG2	2.41	0.68
1:F:773:HIS:CE1	1:F:820:GLN:HG2	2.29	0.68
1:F:825:MET:CE	1:F:835:HIS:CB	2.72	0.68
1:E:837:ASP:C	1:E:837:ASP:OD1	2.30	0.67
1:C:715:ILE:HD11	1:C:728:LYS:HZ1	1.55	0.67
1:A:815[B]:LEU:HD22	1:A:979:LEU:CD1	2.22	0.67
1:D:765:VAL:HG12	1:D:766:MET:N	2.09	0.67
1:D:919:PRO:HB2	1:D:922:GLU:HG3	1.76	0.67
1:E:790:MET:HG2	2:E:1101:816:CLA	2.30	0.67
1:H:757:LYS:C	1:H:757:LYS:CD	2.58	0.67
1:D:832:ARG:CG	4:G:1202:HOH:O	2.42	0.67
1:F:990:PRO:CG	4:F:1215:HOH:O	2.32	0.67
1:A:705:ARG:HE	1:A:707:LEU:HD23	1.58	0.67
1:D:894:GLN:O	1:D:897:VAL:HG23	1.94	0.67
1:A:748:ARG:O	1:A:749:GLU:CB	2.41	0.67
1:B:972:ALA:HB1	1:B:1011:VAL:HG11	1.76	0.67
1:G:815:LEU:O	1:G:819:VAL:HG23	1.95	0.67
1:G:803:ARG:HG2	1:G:911:GLY:HA3	1.76	0.67
1:G:806:LYS:HD3	1:G:807:ASP:CA	2.25	0.67
1:A:854:THR:O	1:A:855:ASP:HB2	1.94	0.67
1:A:945:MET:CE	1:E:909:THR:HG22	2.24	0.67
1:E:706:ILE:O	1:E:706:ILE:CG2	2.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:708:LYS:O	1:F:711:GLU:HG3	1.93	0.67
1:A:777:LEU:HD21	1:A:788:LEU:CD2	2.17	0.67
1:F:721:GLY:HA3	1:F:724:GLY:O	1.95	0.67
1:F:707:LEU:HB2	1:F:711:GLU:CG	2.25	0.67
1:F:817:TRP:O	1:F:821:ILE:HG13	1.95	0.67
1:A:817:TRP:O	1:A:821:ILE:HG13	1.95	0.67
1:B:708:LYS:O	1:B:711:GLU:HG3	1.95	0.67
1:F:856:PHE:CD1	1:F:856:PHE:O	2.48	0.67
1:G:995:SER:C	1:G:999[B]:ARG:HD2	2.13	0.67
1:E:783:THR:HG22	1:E:784:SER:N	2.08	0.66
1:D:878:ILE:HG23	1:D:886:ILE:CD1	2.24	0.66
1:E:844:LEU:HD23	1:E:854:THR:HG21	1.76	0.66
1:F:823:LYS:HZ1	1:F:1008:ASP:CG	1.97	0.66
1:C:717:VAL:HG23	1:C:727:TYR:CD2	2.30	0.66
1:B:756:ASN:HA	1:B:759:ILE:HD13	1.77	0.66
1:D:941:ILE:HD11	1:D:945:MET:CE	2.25	0.66
1:D:950:CYS:O	1:D:958:ARG:CD	2.43	0.66
1:F:701:GLN:CA	1:F:701:GLN:OE1	2.44	0.66
1:F:797:CYS:HB3	1:F:800:ASP:HB2	1.76	0.66
1:E:938:ILE:HD11	1:E:979:LEU:HD13	1.77	0.66
1:E:950:CYS:O	1:E:958:ARG:CD	2.43	0.66
1:B:798:LEU:O	1:B:802:VAL:HG22	1.96	0.66
1:D:790:MET:CE	2:D:1101:816:CBD	2.72	0.66
1:D:854:THR:O	1:D:855:ASP:HB2	1.95	0.66
1:B:997:PHE:O	1:B:997:PHE:CD1	2.46	0.66
1:D:940:THR:CG2	1:D:943:VAL:HG23	2.24	0.66
1:G:1007:MET:CE	1:G:1010:VAL:HG12	2.25	0.66
1:A:945:MET:CE	1:E:909:THR:CG2	2.73	0.66
1:B:737:LYS:HD3	1:B:738:VAL:HG12	1.78	0.66
1:G:817:TRP:CD1	1:G:851:VAL:CG1	2.79	0.66
1:H:987:MET:CE	4:H:1214:HOH:O	2.42	0.66
1:A:940:THR:HB	1:A:978:TYR:O	1.94	0.66
1:B:910:PHE:CE2	1:B:938:ILE:HD11	2.31	0.66
1:F:990:PRO:HD3	4:F:1215:HOH:O	1.95	0.66
1:G:823:LYS:HA	1:G:965:ILE:HD11	1.76	0.66
1:A:797:CYS:CB	1:A:800:ASP:OD2	2.44	0.66
1:F:823:LYS:HZ2	1:F:1008:ASP:CG	1.98	0.66
1:E:793:MET:HG3	1:E:844:LEU:HD12	1.76	0.65
1:C:926:ILE:HB	1:C:931:GLU:HG3	1.76	0.65
1:B:802:VAL:HG11	1:B:907:LEU:HD22	1.78	0.65
1:A:711:GLU:O	1:A:732:ILE:HG22	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:MET:HE3	1:A:885:SER:HB3	1.79	0.65
1:B:831:ARG:HH11	1:B:831:ARG:CG	2.00	0.65
1:E:845:VAL:CG1	1:E:847:THR:C	2.64	0.65
1:B:808:ASN:N	1:B:808:ASN:OD1	2.30	0.65
1:C:835:HIS:O	1:C:836:ARG:HB2	1.96	0.65
1:C:961:PHE:C	1:C:965:ILE:HD12	2.13	0.65
1:F:707:LEU:H	1:F:707:LEU:CD1	2.01	0.65
1:F:756:ASN:CG	1:F:782:LEU:HD13	2.17	0.65
1:G:1014:ASP:OD1	1:G:1014:ASP:N	2.30	0.65
1:C:801:TYR:CE2	1:C:817:TRP:CH2	2.84	0.65
1:A:982:GLN:OE1	1:A:982:GLN:N	2.30	0.65
1:B:811:SER:OG	1:B:975:PRO:HB2	1.96	0.65
1:H:835:HIS:O	1:H:836:ARG:HB2	1.95	0.65
1:C:817:TRP:CD1	1:C:851:VAL:CG1	2.80	0.65
1:C:835:HIS:NE2	1:C:856:PHE:CA	2.57	0.65
1:E:835:HIS:ND1	1:E:837:ASP:O	2.30	0.65
1:F:849:GLN:OE1	1:F:849:GLN:N	2.30	0.65
1:F:878:ILE:HD13	1:F:881:MET:CE	2.27	0.65
1:G:704:LEU:HD12	1:G:767:ALA:HB2	1.79	0.65
1:G:835:HIS:ND1	1:G:837:ASP:O	2.30	0.65
1:C:881:MET:HE2	1:C:886:ILE:HG12	1.78	0.65
1:F:701:GLN:OE1	1:F:701:GLN:N	2.30	0.65
1:H:935:GLN:CB	1:H:944:TYR:CD2	2.79	0.65
1:G:703:LEU:N	1:G:703:LEU:CD2	2.59	0.65
1:G:889:ARG:CG	1:G:889:ARG:NH1	2.58	0.65
1:H:825:MET:HE2	1:H:961:PHE:CZ	2.31	0.65
1:A:922:GLU:OE2	1:A:926:ILE:CG2	2.46	0.64
1:A:949:LYS:O	1:A:952:MET:CG	2.45	0.64
1:B:783:THR:CG2	1:B:784:SER:N	2.61	0.64
1:B:940:THR:CB	1:B:978:TYR:O	2.43	0.64
1:F:900:TYR:O	1:F:904:VAL:HG23	1.97	0.64
1:G:878:ILE:HG23	1:G:886:ILE:CD1	2.28	0.64
1:H:757:LYS:O	1:H:757:LYS:CD	2.44	0.64
1:C:716:LYS:HG3	1:C:717:VAL:N	2.11	0.64
1:C:801:TYR:CE2	1:C:817:TRP:HH2	2.13	0.64
1:A:835:HIS:O	1:A:836:ARG:HB2	1.96	0.64
1:E:991:SER:OG	1:E:992:PRO:HD2	1.97	0.64
1:H:808:ASN:N	1:H:808:ASN:OD1	2.30	0.64
1:C:809:ILE:HD11	1:C:814:LEU:HG	1.79	0.64
1:G:923:ILE:HA	1:G:926:ILE:HG23	1.79	0.64
1:H:777:LEU:HB2	2:H:1101:816:CAA	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:GLU:O	1:C:766:MET:HG3	1.97	0.64
1:B:771:ASN:HB3	1:B:774:VAL:HG23	1.78	0.64
1:G:808:ASN:OD1	1:G:808:ASN:N	2.30	0.64
1:G:879:LYS:HG2	1:G:915:TYR:HB2	1.79	0.64
1:G:923:ILE:O	1:G:926:ILE:HG23	1.97	0.64
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.31	0.64
1:F:745:LYS:NZ	4:F:1201:HOH:O	2.30	0.64
1:B:831:ARG:O	1:B:832:ARG:HB2	1.96	0.64
1:E:880:TRP:NE1	1:E:906:GLU:OE1	2.31	0.64
1:F:905:TRP:O	1:F:909:THR:HG23	1.98	0.64
1:G:960:LYS:CD	4:G:1203:HOH:O	2.44	0.64
1:C:952:MET:O	1:C:958:ARG:NH1	2.30	0.64
1:A:717:VAL:HG23	1:A:727:TYR:CD2	2.33	0.64
1:A:856:PHE:CD1	1:A:856:PHE:C	2.71	0.64
1:F:808:ASN:OD1	1:F:808:ASN:N	2.30	0.64
1:F:898:TRP:CE3	1:F:958:ARG:NH2	2.64	0.64
1:G:985:GLU:HG2	1:G:986:ARG:N	2.12	0.64
1:F:729:GLY:O	1:F:730:LEU:HD22	1.98	0.64
1:F:758:GLU:OE2	1:F:759:ILE:N	2.30	0.64
1:B:910:PHE:HE2	1:B:938:ILE:HD11	1.62	0.64
1:B:988:HIS:CA	1:B:989:LEU:CB	2.75	0.64
1:G:740:ILE:HG22	1:G:741:PRO:HD2	1.79	0.64
1:G:1008:ASP:N	1:G:1008:ASP:OD1	2.31	0.64
1:B:704:LEU:HB2	1:B:767:ALA:CB	2.29	0.63
1:B:771:ASN:HD22	1:B:772:PRO:CD	2.06	0.63
1:G:944:TYR:O	1:G:947:MET:HB2	1.98	0.63
1:H:925:SER:OG	1:H:929:LYS:NZ	2.30	0.63
1:C:827:TYR:CZ	1:C:831:ARG:CD	2.81	0.63
1:F:977:ARG:C	1:F:977:ARG:CD	2.53	0.63
1:G:737:LYS:CG	1:G:737:LYS:O	2.46	0.63
1:H:790:MET:HG2	2:H:1101:816:NAB	2.13	0.63
1:D:707:LEU:CD2	1:D:711:GLU:CB	2.76	0.63
1:H:825:MET:HB3	1:H:961:PHE:CZ	2.33	0.63
1:H:985:GLU:HG2	1:H:986:ARG:N	2.12	0.63
1:C:717:VAL:O	1:C:717:VAL:CG1	2.43	0.63
1:C:758:GLU:OE2	1:C:759:ILE:N	2.30	0.63
1:C:815:LEU:O	1:C:819:VAL:HG23	1.99	0.63
1:A:806:LYS:NZ	4:A:1201:HOH:O	2.30	0.63
1:D:718:LEU:HD13	1:D:728:LYS:HB2	1.80	0.63
1:D:835:HIS:O	1:D:836:ARG:HB2	1.98	0.63
1:E:759:ILE:HD13	1:E:780:ILE:CD1	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:812:GLN:O	1:E:816:ASN:ND2	2.30	0.63
1:H:703:LEU:HD13	1:H:768:SER:HA	1.79	0.63
1:A:808:ASN:OD1	1:A:808:ASN:N	2.30	0.63
1:D:949:LYS:O	1:D:952:MET:HG3	1.99	0.63
1:F:721:GLY:N	1:F:724:GLY:O	2.32	0.63
1:G:835:HIS:NE2	1:G:856:PHE:HB3	2.13	0.63
1:D:745:LYS:NZ	1:D:855:ASP:OD1	2.31	0.63
1:E:844:LEU:HD21	1:E:854:THR:HG21	1.80	0.63
1:F:736:GLU:HA	1:F:736:GLU:OE2	1.98	0.63
1:G:775:CYS:HB2	1:G:854:THR:OG1	1.98	0.63
1:A:799:LEU:O	1:A:802:VAL:HG23	1.98	0.63
1:A:815[A]:LEU:HG	1:A:979:LEU:HD11	1.79	0.63
1:A:972:ALA:O	1:A:975:PRO:HD3	1.98	0.63
1:D:790:MET:HE3	2:D:1101:816:CAA	2.27	0.63
1:G:825:MET:SD	1:G:838:LEU:HD22	2.39	0.63
1:H:837:ASP:O	1:H:842:ASN:ND2	2.30	0.63
1:H:854:THR:CG2	1:H:855:ASP:H	2.08	0.63
1:C:728:LYS:HG3	1:C:792:LEU:HD11	1.81	0.63
1:C:894:GLN:CB	1:C:955:ALA:HB1	2.29	0.63
1:A:762:GLU:OE1	1:A:861:LEU:CD2	2.47	0.63
1:A:813:TYR:OH	1:A:990:PRO:HD3	1.99	0.63
1:C:723:PHE:O	1:C:748:ARG:HG2	1.99	0.63
1:B:999:ARG:HH11	1:B:999:ARG:CG	2.12	0.62
1:D:846:LYS:O	1:D:847:THR:HG22	1.98	0.62
1:C:961:PHE:HA	1:C:964:LEU:HD12	1.81	0.62
1:F:858:LEU:HD13	2:F:1101:816:CAK	2.28	0.62
1:H:961:PHE:O	1:H:965:ILE:HG12	1.99	0.62
1:C:799:LEU:O	1:C:802:VAL:HG22	1.99	0.62
1:D:774:VAL:HG21	1:D:827:TYR:CD2	2.34	0.62
1:F:881:MET:HE3	1:F:886:ILE:HG12	1.81	0.62
1:F:945:MET:O	1:F:948:VAL:HG23	1.99	0.62
1:G:773:HIS:HE1	1:G:820:GLN:HG2	1.64	0.62
1:G:835:HIS:CE1	1:G:837:ASP:O	2.52	0.62
1:H:757:LYS:NZ	1:H:761:ASP:OD2	2.30	0.62
1:A:977:ARG:NE	1:E:926:ILE:HD12	2.11	0.62
1:B:815:LEU:O	1:B:819:VAL:HG23	1.99	0.62
1:F:780:ILE:HD13	1:F:787:GLN:O	2.00	0.62
1:C:770:ASP:C	1:C:770:ASP:OD1	2.38	0.62
1:C:1007:MET:CG	1:C:1008:ASP:O	2.47	0.62
1:F:781:CYS:SG	1:F:783:THR:CG2	2.87	0.62
1:G:767:ALA:O	1:G:776:ARG:NH1	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:VAL:HG12	1:B:843:VAL:O	1.98	0.62
1:D:991:SER:OG	1:D:992:PRO:HD2	2.00	0.62
1:C:769:VAL:O	1:C:769:VAL:HG23	2.00	0.62
1:C:797:CYS:SG	1:C:800:ASP:OD2	2.58	0.62
1:C:849:GLN:OE1	1:C:849:GLN:N	2.30	0.62
1:B:945:MET:HE1	1:D:909:THR:HG22	1.82	0.62
1:E:949:LYS:O	1:E:958:ARG:HG3	1.98	0.62
1:B:717:VAL:HG22	1:B:727:TYR:CD2	2.35	0.62
1:F:878:ILE:HD13	1:F:881:MET:HE2	1.81	0.62
1:C:790:MET:HE2	2:C:1101:816:NAB	2.14	0.62
1:A:799:LEU:O	1:A:799:LEU:HD12	1.99	0.62
1:E:748:ARG:HG3	1:E:748:ARG:NH1	2.14	0.62
1:G:877:PRO:O	1:G:881:MET:HG3	1.99	0.62
1:H:924:SER:O	1:H:928:GLU:HG3	2.00	0.62
1:C:717:VAL:CG2	1:C:727:TYR:CD2	2.83	0.62
1:C:918:ILE:HG22	1:C:918:ILE:O	1.99	0.62
1:A:769:VAL:HG12	1:A:827:TYR:HE2	1.64	0.62
1:E:790:MET:HE3	1:E:791:GLN:O	2.00	0.62
1:F:832:ARG:HG2	4:F:1211:HOH:O	2.00	0.62
1:F:1007:MET:HG2	1:F:1008:ASP:N	2.15	0.62
1:G:881:MET:HE3	1:G:885:SER:CB	2.23	0.62
1:G:883:LEU:HD22	1:G:953:ILE:CD1	2.29	0.62
1:B:837:ASP:OD2	1:B:841:ARG:NH1	2.33	0.61
1:B:940:THR:CG2	1:B:943:VAL:H	2.13	0.61
1:D:837:ASP:CG	1:D:837:ASP:O	2.38	0.61
1:E:836:ARG:HD2	1:E:860:LYS:CA	2.29	0.61
1:F:733:PRO:HB2	1:F:736:GLU:HB2	1.81	0.61
1:E:840:ALA:CB	1:E:906:GLU:OE2	2.45	0.61
1:F:700:ASN:CB	1:F:703:LEU:HD12	2.28	0.61
1:G:705:ARG:NH2	1:G:711:GLU:OE1	2.31	0.61
1:G:772:PRO:O	1:G:852:LYS:HD2	1.99	0.61
1:G:805:HIS:O	1:G:809:ILE:HG13	2.00	0.61
1:C:1007:MET:CE	1:C:1008:ASP:O	2.48	0.61
1:A:983:GLY:O	1:A:987:MET:HG2	2.00	0.61
1:B:950:CYS:O	1:B:958:ARG:NE	2.33	0.61
1:D:967:GLU:O	1:D:971:MET:HG3	2.00	0.61
1:E:886:ILE:HG21	1:E:924:SER:HB2	1.82	0.61
1:F:925:SER:O	1:F:929:LYS:N	2.30	0.61
1:F:947:MET:HB3	1:F:951:TRP:CH2	2.34	0.61
1:C:880:TRP:NE1	1:C:906:GLU:OE2	2.32	0.61
1:G:845:VAL:CG1	1:G:847:THR:C	2.68	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:PHE:CB	1:D:845:VAL:HG12	2.30	0.61
1:D:799:LEU:O	1:D:802:VAL:HG23	2.00	0.61
1:G:766:MET:O	1:G:769:VAL:HG13	2.00	0.61
1:C:980:VAL:CG2	1:C:980:VAL:O	2.49	0.61
1:A:705:ARG:HD3	1:A:707:LEU:HD21	1.83	0.61
1:B:799:LEU:O	1:B:803:ARG:HG3	2.00	0.61
1:E:983:GLY:O	1:E:986:ARG:HD3	2.01	0.61
1:G:999[B]:ARG:HB3	1:G:1003:ASP:O	2.00	0.61
1:A:922:GLU:O	1:A:926:ILE:HG23	2.00	0.61
1:A:952:MET:O	1:A:958:ARG:NH2	2.30	0.61
1:F:707:LEU:HB2	1:F:711:GLU:HG3	1.83	0.61
2:F:1101:816:CAN	2:F:1101:816:NAB	2.63	0.61
1:G:940:THR:HB	1:G:978:TYR:O	2.00	0.61
1:G:969:SER:O	1:G:972:ALA:HB3	2.00	0.61
1:A:926:ILE:HG13	1:A:927:LEU:N	2.15	0.61
1:D:842:ASN:O	1:D:854:THR:HG22	2.00	0.61
1:G:835:HIS:CD2	1:G:856:PHE:HB3	2.36	0.61
1:H:771:ASN:OD1	1:H:773:HIS:N	2.30	0.61
1:C:942:ASP:OD1	1:C:977:ARG:NH2	2.34	0.61
1:A:946:ILE:HD12	1:A:971:MET:HE1	1.77	0.61
1:H:743:ALA:HB3	2:H:1101:816:NAB	2.16	0.61
1:H:962:ARG:O	1:H:965:ILE:HG13	2.00	0.61
1:C:981:ILE:HG21	1:C:987:MET:HE3	1.83	0.61
1:A:800:ASP:HB3	4:A:1218:HOH:O	2.01	0.61
1:B:881:MET:HE1	1:B:891:TYR:OH	1.99	0.61
1:E:797:CYS:HB2	1:E:800:ASP:H	1.65	0.61
1:G:799:LEU:O	1:G:803:ARG:HG3	2.00	0.61
1:C:898:TRP:HE3	1:C:958:ARG:NH1	1.98	0.61
1:C:953:ILE:N	1:C:953:ILE:CD1	2.62	0.61
1:D:703:LEU:HD12	1:D:768:SER:HA	1.82	0.60
1:E:769:VAL:HG12	1:E:827:TYR:HE2	1.66	0.60
1:E:783:THR:CG2	1:E:784:SER:N	2.64	0.60
1:E:795:PHE:CE2	1:E:1002:MET:HE3	2.36	0.60
1:D:739:LYS:O	1:D:740:ILE:HD13	2.02	0.60
1:E:898:TRP:CE3	1:E:958:ARG:NH1	2.66	0.60
1:H:835:HIS:HE1	1:H:837:ASP:O	1.81	0.60
1:H:1008:ASP:OD2	1:H:1008:ASP:N	2.30	0.60
1:C:701:GLN:OE1	1:C:701:GLN:N	2.34	0.60
1:C:898:TRP:CZ2	1:C:927:LEU:HD13	2.36	0.60
1:F:805:HIS:HB3	1:F:809:ILE:HG12	1.83	0.60
1:A:876:VAL:HG23	1:A:878:ILE:HG13	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:743:ALA:CB	2:G:1101:816:C6	2.79	0.60
1:H:758:GLU:CD	1:H:758:GLU:C	2.59	0.60
1:C:854:THR:O	1:C:855:ASP:HB2	2.00	0.60
1:C:905:TRP:CD2	1:C:909:THR:HG21	2.36	0.60
1:H:776:ARG:CG	1:H:776:ARG:HH11	2.13	0.60
1:A:774:VAL:HG23	1:A:824:GLY:CA	2.32	0.60
1:B:877:PRO:O	1:B:881:MET:HG3	2.02	0.60
1:F:856:PHE:O	1:F:856:PHE:CG	2.54	0.60
1:H:797:CYS:SG	2:H:1101:816:OAE	2.60	0.60
1:C:704:LEU:HD13	1:C:704:LEU:C	2.22	0.60
1:C:935:GLN:HB2	1:C:944:TYR:CG	2.37	0.60
1:C:940:THR:HG23	1:C:943:VAL:H	1.66	0.60
1:F:966:ILE:HG23	1:F:970:LYS:HE3	1.84	0.60
1:G:775:CYS:CB	1:G:854:THR:OG1	2.50	0.60
1:H:881:MET:CE	1:H:891:TYR:OH	2.50	0.60
1:A:708:LYS:O	1:A:711:GLU:HG3	2.01	0.60
1:B:737:LYS:H	1:B:737:LYS:HD2	1.67	0.60
1:E:719:GLY:HA3	2:E:1101:816:CAO	2.32	0.60
1:F:884:GLU:HG2	1:F:885:SER:N	2.16	0.60
1:G:962:ARG:NH2	4:G:1201:HOH:O	2.34	0.60
1:A:774:VAL:HG23	1:A:824:GLY:HA2	1.83	0.60
1:D:780:ILE:HG12	1:D:781:CYS:N	2.17	0.60
1:G:737:LYS:O	1:G:737:LYS:HG2	2.01	0.60
1:G:769:VAL:O	1:G:769:VAL:CG2	2.47	0.60
1:C:973:ARG:O	1:C:1013:ALA:HA	2.01	0.60
1:A:798:LEU:O	1:A:802:VAL:HG22	2.01	0.60
1:E:795:PHE:CE2	1:E:1002:MET:HE1	2.20	0.60
1:C:879:LYS:NZ	1:C:915:TYR:O	2.34	0.60
1:H:797:CYS:HB3	1:H:841:ARG:O	2.02	0.59
1:H:825:MET:HG2	1:H:853:ILE:CD1	2.31	0.59
1:C:926:ILE:O	1:C:930:GLY:N	2.36	0.59
1:A:966:ILE:HD11	1:C:804:GLU:OE2	2.01	0.59
1:F:945:MET:C	1:F:948:VAL:HG23	2.22	0.59
1:G:999[A]:ARG:NH1	1:G:1005:GLU:O	2.35	0.59
1:H:1009:ASP:N	1:H:1009:ASP:OD1	2.35	0.59
1:D:811:SER:CB	1:D:981:ILE:HG13	2.31	0.59
1:G:811:SER:CB	1:G:984:ASP:OD1	2.38	0.59
1:F:858:LEU:CD1	2:F:1101:816:CAK	2.79	0.59
1:C:800:ASP:O	1:C:804:GLU:HG3	2.02	0.59
1:C:972:ALA:O	1:C:975:PRO:CD	2.48	0.59
1:A:935:GLN:HG3	1:A:944:TYR:CD2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:893:HIS:O	1:B:897:VAL:HG23	2.02	0.59
1:G:825:MET:HE2	1:G:853:ILE:HD12	1.84	0.59
1:C:985:GLU:OE1	1:C:985:GLU:N	2.30	0.59
1:B:941:ILE:C	1:B:941:ILE:CD1	2.66	0.59
1:D:908:MET:SD	1:D:979:LEU:HD21	2.42	0.59
1:C:748:ARG:O	1:C:749:GLU:CB	2.51	0.59
1:A:704:LEU:HB2	1:A:767:ALA:CB	2.33	0.59
1:B:791:GLN:HG3	4:B:1211:HOH:O	2.02	0.59
1:H:776:ARG:O	1:H:778:LEU:CD2	2.50	0.59
1:D:820:GLN:NE2	1:D:849:GLN:O	2.30	0.59
1:F:826:ASN:ND2	4:F:1202:HOH:O	2.36	0.59
1:G:700:ASN:OD1	1:G:701:GLN:N	2.36	0.59
1:H:899:SER:CA	1:H:902:VAL:CG2	2.67	0.59
1:A:778:LEU:HD11	1:A:791:GLN:HG2	1.85	0.59
1:B:972:ALA:HB1	1:B:1011:VAL:CG1	2.32	0.59
1:D:815:LEU:CD2	1:D:979:LEU:HD12	2.30	0.59
1:E:771:ASN:HB3	1:E:774:VAL:CG2	2.29	0.59
1:F:876:VAL:CB	1:F:877:PRO:CD	2.74	0.59
1:G:769:VAL:HG11	1:G:856:PHE:CZ	2.33	0.59
1:H:877:PRO:O	1:H:881:MET:HG3	2.02	0.59
1:C:894:GLN:HG3	1:C:955:ALA:C	2.21	0.59
1:A:900:TYR:CE2	1:A:964:LEU:HD13	2.38	0.59
1:B:719:GLY:HA3	2:B:1101:816:CAO	2.33	0.59
1:F:707:LEU:N	1:F:707:LEU:CD1	2.56	0.59
1:F:817:TRP:CD1	1:F:851:VAL:HG22	2.38	0.59
1:H:730:LEU:HD13	1:H:739:LYS:HB2	1.85	0.59
1:B:851:VAL:O	1:B:851:VAL:HG23	2.01	0.58
1:D:714:LYS:O	1:D:714:LYS:HG2	2.01	0.58
2:A:1101:816:CAN	2:A:1101:816:NAB	2.66	0.58
1:F:790:MET:HE2	2:F:1101:816:NAB	2.17	0.58
2:H:1101:816:NAB	2:H:1101:816:CAN	2.66	0.58
1:D:955:ALA:O	1:D:958:ARG:HB2	2.03	0.58
1:E:842:ASN:O	1:E:854:THR:CG2	2.45	0.58
1:F:835:HIS:CD2	1:F:856:PHE:HB2	2.38	0.58
1:D:940:THR:HG22	1:D:978:TYR:O	2.01	0.58
1:E:833:LEU:CD1	1:E:856:PHE:CZ	2.86	0.58
1:F:942:ASP:OD1	1:F:977:ARG:NH1	2.32	0.58
1:H:949:LYS:O	1:H:952:MET:CG	2.51	0.58
1:C:715:ILE:HD11	1:C:728:LYS:CE	2.34	0.58
1:A:790:MET:HE3	1:A:791:GLN:O	2.03	0.58
1:D:769:VAL:HG23	1:D:769:VAL:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:940:THR:HB	1:D:978:TYR:O	2.02	0.58
1:E:814:LEU:HD23	1:E:817:TRP:CE3	2.39	0.58
1:H:790:MET:HG3	1:H:791:GLN:N	2.17	0.58
1:C:797:CYS:CB	1:C:800:ASP:OD2	2.52	0.58
1:C:849:GLN:HB3	1:C:1010:VAL:HG11	1.85	0.58
1:B:717:VAL:CG2	1:B:727:TYR:CD2	2.86	0.58
1:E:941:ILE:HG13	1:E:945:MET:HE2	1.85	0.58
2:G:1101:816:NAB	2:G:1101:816:CAN	2.67	0.58
1:H:776:ARG:NH1	1:H:776:ARG:HG2	2.17	0.58
1:C:745:LYS:HB3	1:C:788:LEU:HD13	1.86	0.58
1:A:815[B]:LEU:HD13	1:A:979:LEU:HD11	1.85	0.58
1:D:767:ALA:O	1:D:776:ARG:HG3	2.04	0.58
1:C:745:LYS:HB3	1:C:788:LEU:CD1	2.33	0.58
1:G:700:ASN:OD1	1:G:702:ALA:N	2.30	0.58
1:G:997:PHE:CE2	1:G:1001:LEU:HD11	2.39	0.58
1:C:712:PHE:HZ	1:C:787:GLN:OE1	1.87	0.58
1:B:790:MET:HE2	1:B:791:GLN:O	2.03	0.58
1:E:820:GLN:NE2	1:E:849:GLN:O	2.33	0.58
1:G:806:LYS:O	1:G:806:LYS:HE3	2.04	0.58
1:H:825:MET:CE	1:H:961:PHE:CZ	2.87	0.58
1:A:950:CYS:O	1:A:958:ARG:CD	2.50	0.57
1:B:736:GLU:OE2	1:B:736:GLU:CA	2.48	0.57
1:G:878:ILE:HD13	1:G:920:ALA:HB1	1.85	0.57
1:C:980:VAL:O	1:C:980:VAL:HG23	2.03	0.57
1:E:809:ILE:HG22	1:E:810:GLY:N	2.18	0.57
1:C:715:ILE:HD13	1:C:728:LYS:NZ	2.19	0.57
1:A:945:MET:HE1	1:E:909:THR:CG2	2.35	0.57
1:H:961:PHE:HA	1:H:964:LEU:HD12	1.86	0.57
1:C:827:TYR:CZ	1:C:831:ARG:HD3	2.39	0.57
1:C:836:ARG:HG2	1:C:891:TYR:CD1	2.39	0.57
1:A:819:VAL:O	1:A:823:LYS:HG3	2.04	0.57
1:B:809:ILE:N	1:B:987:MET:HE3	2.18	0.57
1:E:759:ILE:HG23	1:E:760:LEU:N	2.18	0.57
1:B:876:VAL:HG21	1:B:889:ARG:NH1	2.19	0.57
1:B:905:TRP:O	1:B:909:THR:CG2	2.50	0.57
1:F:923:ILE:HD12	1:F:926:ILE:HD11	1.86	0.57
1:G:757:LYS:C	1:G:757:LYS:CD	2.72	0.57
1:G:999[A]:ARG:HH12	1:G:1006:ASP:HA	1.68	0.57
1:C:716:LYS:O	1:C:728:LYS:N	2.34	0.57
1:C:828:LEU:HD11	1:C:856:PHE:HB2	1.86	0.57
1:C:839:ALA:HB1	1:C:841:ARG:CG	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:HIS:O	1:A:809:ILE:HG13	2.05	0.57
1:A:898:TRP:CH2	1:A:927:LEU:HD13	2.39	0.57
1:A:1006:ASP:OD1	1:A:1006:ASP:N	2.30	0.57
1:E:846:LYS:CE	1:E:1005:GLU:OE1	2.53	0.57
1:E:952:MET:O	1:E:958:ARG:NH1	2.35	0.57
1:H:769:VAL:HG11	1:H:856:PHE:HZ	1.70	0.57
1:H:986:ARG:HB2	1:H:986:ARG:CZ	2.34	0.57
1:D:739:LYS:C	1:D:740:ILE:HD13	2.24	0.57
1:D:900:TYR:CE2	1:D:904:VAL:CG2	2.87	0.57
1:E:885:SER:O	1:E:889:ARG:HA	2.04	0.57
1:G:836:ARG:HG3	4:G:1210:HOH:O	2.05	0.57
1:C:833:LEU:HD13	1:C:856:PHE:CZ	2.39	0.57
1:D:812:GLN:HG2	1:D:975:PRO:CG	2.34	0.57
1:F:832:ARG:CG	4:F:1211:HOH:O	2.51	0.57
1:G:790:MET:HE2	2:G:1101:816:NAB	2.19	0.57
1:G:823:LYS:HG2	1:G:965:ILE:CD1	2.35	0.57
1:G:856:PHE:CD1	1:G:856:PHE:O	2.57	0.57
1:H:718:LEU:HD11	1:H:792:LEU:CD1	2.31	0.57
1:H:961:PHE:O	1:H:965:ILE:CG1	2.53	0.57
1:C:815:LEU:CD1	1:C:975:PRO:HA	2.34	0.57
1:D:786:VAL:HG13	1:D:786:VAL:O	2.05	0.57
1:E:847:THR:HG23	1:E:850:HIS:CB	2.28	0.57
1:F:845:VAL:HG12	1:F:847:THR:O	2.04	0.57
1:F:897:VAL:HG21	4:F:1228:HOH:O	2.03	0.57
1:F:989:LEU:HD23	1:F:990:PRO:O	2.04	0.57
1:G:835:HIS:O	1:G:836:ARG:HB2	2.04	0.57
1:G:897:VAL:O	1:G:901:GLY:N	2.33	0.57
1:D:884:GLU:HG2	1:D:885:SER:N	2.18	0.57
1:E:745:LYS:HZ1	1:E:858:LEU:HD21	1.69	0.57
1:C:940:THR:CG2	1:C:978:TYR:O	2.53	0.57
1:A:830:ASP:HB3	1:C:717:VAL:CG1	2.32	0.56
1:B:704:LEU:HB2	1:B:767:ALA:HB2	1.86	0.56
1:B:809:ILE:CA	1:B:987:MET:HE3	2.35	0.56
1:F:819:VAL:HG23	1:F:968:PHE:HB3	1.86	0.56
1:G:823:LYS:HG2	1:G:965:ILE:HD13	1.86	0.56
1:G:997:PHE:CE2	1:G:1001:LEU:CD1	2.88	0.56
1:H:987:MET:HE3	4:H:1214:HOH:O	2.05	0.56
1:B:835:HIS:CG	1:B:856:PHE:HB2	2.37	0.56
1:F:825:MET:HG2	1:F:961:PHE:CZ	2.40	0.56
1:C:726:VAL:HG22	1:C:745:LYS:HG3	1.86	0.56
1:A:946:ILE:HD12	1:A:971:MET:HE3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:HIS:CB	1:B:990:PRO:N	2.67	0.56
1:D:732:ILE:O	1:D:732:ILE:HG13	2.03	0.56
1:D:991:SER:OG	1:D:992:PRO:CD	2.54	0.56
1:E:803:ARG:O	1:E:806:LYS:HD2	2.06	0.56
1:F:835:HIS:CE1	1:F:837:ASP:O	2.58	0.56
1:F:995:SER:O	1:F:999:ARG:HG3	2.05	0.56
1:G:769:VAL:O	1:G:769:VAL:HG22	2.04	0.56
1:G:881:MET:CE	1:G:885:SER:HB3	2.25	0.56
1:H:715:ILE:HG12	1:H:728:LYS:O	2.06	0.56
1:C:940:THR:CG2	1:C:943:VAL:HG23	2.30	0.56
1:A:775:CYS:HB2	1:A:853:ILE:O	2.06	0.56
1:D:845:VAL:HG12	1:D:845:VAL:O	2.05	0.56
1:F:835:HIS:HE1	1:F:837:ASP:O	1.87	0.56
1:F:889:ARG:HD2	4:F:1209:HOH:O	2.04	0.56
1:G:700:ASN:OD1	1:G:700:ASN:C	2.42	0.56
1:D:961:PHE:HA	1:D:964:LEU:HB2	1.88	0.56
1:E:876:VAL:HG11	1:E:889:ARG:HH12	1.70	0.56
1:E:879:LYS:HD3	1:E:915:TYR:HB2	1.87	0.56
1:E:913:LYS:CD	1:E:913:LYS:N	2.68	0.56
1:H:835:HIS:CD2	1:H:856:PHE:CB	2.89	0.56
1:C:723:PHE:O	1:C:748:ARG:HG3	2.06	0.56
1:C:878:ILE:HG22	1:C:923:ILE:HG21	1.87	0.56
1:B:905:TRP:CE2	1:B:909:THR:HG21	2.41	0.56
1:E:806:LYS:HB2	1:E:910:PHE:HB3	1.86	0.56
1:F:700:ASN:HB2	1:F:703:LEU:HD12	1.86	0.56
1:H:766:MET:HE3	1:H:777:LEU:HD22	1.87	0.56
1:H:777:LEU:C	1:H:778:LEU:HD23	2.24	0.56
1:A:931:GLU:O	1:A:932:ARG:HD3	2.06	0.56
1:B:708:LYS:HB2	1:B:711:GLU:CG	2.35	0.56
1:B:716:LYS:HB3	1:B:728:LYS:HB3	1.86	0.56
1:D:821:ILE:HG23	1:D:853:ILE:HD11	1.87	0.56
1:B:780:ILE:HD13	1:B:782:LEU:CD2	2.34	0.56
1:D:815:LEU:HD21	1:D:979:LEU:HD12	1.81	0.56
1:D:938:ILE:HD11	1:D:979:LEU:CD2	2.35	0.56
1:F:790:MET:HG2	2:F:1101:816:CLA	2.42	0.56
1:A:841:ARG:NH2	1:A:841:ARG:CG	2.62	0.56
1:H:925:SER:O	1:H:929:LYS:HG3	2.06	0.56
1:H:935:GLN:CB	1:H:944:TYR:CG	2.88	0.56
1:H:946:ILE:HG22	1:H:947:MET:N	2.21	0.56
1:H:946:ILE:CG2	1:H:947:MET:N	2.69	0.56
1:C:795:PHE:HE2	1:C:1002:MET:HE1	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:879:LYS:HG2	1:E:923:ILE:CD1	2.36	0.55
1:G:705:ARG:HG3	1:G:706:ILE:N	2.21	0.55
1:C:1007:MET:SD	1:C:1008:ASP:O	2.64	0.55
1:A:846:LYS:HE3	1:A:1005:GLU:OE1	2.07	0.55
1:A:945:MET:HE2	1:E:909:THR:HG22	1.87	0.55
1:E:941:ILE:CG1	1:E:945:MET:HE2	2.36	0.55
1:F:850:HIS:O	1:F:850:HIS:CD2	2.60	0.55
1:C:926:ILE:HA	1:C:929:LYS:HB2	1.87	0.55
1:A:815[A]:LEU:HG	1:A:979:LEU:CD1	2.36	0.55
1:A:878:ILE:CD1	4:A:1214:HOH:O	2.41	0.55
1:B:878:ILE:HG23	1:B:886:ILE:HD13	1.87	0.55
1:B:947:MET:O	1:B:950:CYS:HB2	2.07	0.55
1:D:773:HIS:CE1	1:D:850:HIS:CE1	2.94	0.55
1:E:765:VAL:O	1:E:768:SER:CB	2.54	0.55
1:G:949:LYS:O	1:G:952:MET:CG	2.53	0.55
1:C:941:ILE:C	1:C:941:ILE:CD1	2.69	0.55
1:A:999:ARG:O	1:A:1003:ASP:C	2.44	0.55
1:B:831:ARG:HB3	1:B:833:LEU:CD1	2.36	0.55
1:D:805:HIS:HD2	4:D:1202:HOH:O	1.83	0.55
1:H:817:TRP:O	1:H:821:ILE:CG1	2.49	0.55
2:H:1101:816:N3	2:H:1101:816:CAR	2.70	0.55
1:A:705:ARG:HD3	1:A:707:LEU:CD2	2.36	0.55
1:A:811:SER:HB3	1:A:984:ASP:OD1	2.06	0.55
1:B:997:PHE:CD1	1:B:997:PHE:C	2.78	0.55
1:D:803:ARG:HG2	1:D:911:GLY:HA3	1.88	0.55
1:H:729:GLY:HA3	1:H:744:ILE:HD11	1.89	0.55
1:B:717:VAL:CG2	1:B:727:TYR:HE2	2.18	0.55
1:D:765:VAL:CG1	1:D:766:MET:N	2.66	0.55
1:E:803:ARG:CG	1:E:911:GLY:HA3	2.33	0.55
1:E:1003:ASP:OD1	1:E:1005:GLU:HG2	2.06	0.55
1:A:830:ASP:CB	1:C:717:VAL:HG11	2.32	0.55
1:E:783:THR:O	1:E:784:SER:C	2.44	0.55
1:E:816:ASN:O	1:E:820:GLN:HG3	2.06	0.55
1:F:770:ASP:C	1:F:770:ASP:OD1	2.44	0.55
1:F:923:ILE:HA	1:F:926:ILE:HD11	1.88	0.55
1:F:977:ARG:NH2	1:G:926:ILE:HD12	2.22	0.55
1:G:971:MET:HA	1:G:978:TYR:CE2	2.42	0.55
1:H:974:ASP:O	1:H:978:TYR:HD2	1.89	0.55
1:C:825:MET:CG	1:C:838:LEU:HD21	2.36	0.55
1:A:813:TYR:OH	1:A:990:PRO:HG3	2.07	0.55
1:A:974:ASP:OD2	1:E:929:LYS:HE3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:845:VAL:CG1	1:F:847:THR:O	2.55	0.55
1:F:999:ARG:O	1:F:1003:ASP:N	2.39	0.55
1:C:765:VAL:HG12	1:C:766:MET:N	2.22	0.55
1:B:943:VAL:HG21	1:B:979:LEU:CD2	2.37	0.55
1:D:772:PRO:O	1:D:852:LYS:HG2	2.07	0.55
1:E:799:LEU:O	1:E:803:ARG:HG3	2.07	0.55
1:E:809:ILE:CG2	1:E:810:GLY:N	2.70	0.55
1:F:803:ARG:HG2	1:F:911:GLY:HA3	1.89	0.55
1:F:811:SER:HA	1:F:981:ILE:CD1	2.37	0.55
1:G:890:ILE:HG22	1:G:890:ILE:O	2.06	0.55
1:G:940:THR:CG2	1:G:978:TYR:O	2.54	0.55
1:A:974:ASP:OD2	1:E:929:LYS:CE	2.55	0.55
1:D:974:ASP:HB3	1:D:977:ARG:HB3	1.89	0.55
1:E:793:MET:HG3	1:E:844:LEU:HD13	1.88	0.55
1:G:774:VAL:CG1	1:G:856:PHE:CE2	2.90	0.55
1:C:839:ALA:CB	1:C:841:ARG:CG	2.85	0.55
1:A:797:CYS:HB2	1:A:800:ASP:OD2	2.07	0.54
1:D:938:ILE:CG1	1:D:979:LEU:HD23	2.37	0.54
1:E:854:THR:O	1:E:855:ASP:HB2	2.07	0.54
1:F:811:SER:HB2	1:F:981:ILE:HD12	1.87	0.54
1:F:977:ARG:HG2	1:F:977:ARG:HH21	1.73	0.54
1:G:822:ALA:CB	1:G:965:ILE:HG12	2.37	0.54
1:H:986:ARG:CB	1:H:986:ARG:CZ	2.84	0.54
1:B:809:ILE:HG21	1:B:814:LEU:HD11	1.89	0.54
1:D:846:LYS:C	1:D:847:THR:CG2	2.75	0.54
1:F:966:ILE:CG2	1:F:970:LYS:HE3	2.37	0.54
1:G:847:THR:OG1	1:G:848:PRO:CD	2.55	0.54
1:H:879:LYS:HD3	1:H:923:ILE:CD1	2.35	0.54
1:C:839:ALA:HB1	1:C:841:ARG:HG3	1.85	0.54
1:B:898:TRP:CH2	1:B:927:LEU:HD13	2.43	0.54
1:D:817:TRP:HA	1:D:820:GLN:HB2	1.90	0.54
1:E:847:THR:CG2	1:E:850:HIS:HB3	2.29	0.54
1:E:941:ILE:HG23	1:E:945:MET:HE3	1.89	0.54
1:C:842:ASN:O	1:C:854:THR:CG2	2.54	0.54
1:D:811:SER:HB2	1:D:981:ILE:CG1	2.37	0.54
1:E:817:TRP:O	1:E:821:ILE:HD12	2.08	0.54
1:G:806:LYS:CD	1:G:806:LYS:O	2.53	0.54
1:H:778:LEU:HG	1:H:790:MET:HA	1.88	0.54
1:B:813:TYR:OH	1:B:990:PRO:HG3	2.08	0.54
1:B:972:ALA:CB	1:B:1011:VAL:CG1	2.78	0.54
1:E:814:LEU:HD23	1:E:817:TRP:CZ3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:778:LEU:HD23	1:F:790:MET:CA	2.33	0.54
1:H:987:MET:HE1	4:H:1214:HOH:O	2.05	0.54
1:E:790:MET:CE	1:E:791:GLN:O	2.56	0.54
1:E:898:TRP:CD1	1:E:898:TRP:C	2.81	0.54
1:F:707:LEU:C	1:F:711:GLU:HG3	2.27	0.54
1:H:743:ALA:CB	2:H:1101:816:C6	2.86	0.54
1:H:897:VAL:HA	1:H:900:TYR:HB3	1.90	0.54
1:C:897:VAL:HG12	1:C:950:CYS:SG	2.47	0.54
1:A:717:VAL:CG2	1:A:727:TYR:CE2	2.89	0.54
1:B:941:ILE:HG23	1:B:942:ASP:OD1	2.08	0.54
1:D:703:LEU:O	1:D:776:ARG:NH1	2.37	0.54
1:D:892:THR:H	1:D:895:SER:HG	1.55	0.54
1:E:783:THR:CG2	1:E:784:SER:H	2.21	0.54
1:F:825:MET:HE1	1:F:835:HIS:HB3	1.90	0.54
1:C:714:LYS:HD3	1:C:727:TYR:CD1	2.43	0.54
1:B:783:THR:CG2	1:B:784:SER:H	2.20	0.54
1:G:932:ARG:HH11	1:G:932:ARG:CB	2.19	0.54
1:H:726:VAL:HG22	1:H:745:LYS:HB2	1.88	0.54
1:C:825:MET:SD	1:C:838:LEU:HD23	2.40	0.54
1:E:790:MET:HE2	2:E:1101:816:NAB	2.21	0.54
1:E:883:LEU:HD22	1:E:953:ILE:CD1	2.38	0.54
1:G:823:LYS:CE	1:G:1008:ASP:OD2	2.53	0.54
1:C:962:ARG:NH1	4:C:1205:HOH:O	2.41	0.54
1:E:836:ARG:HD2	1:E:860:LYS:HA	1.90	0.53
1:F:832:ARG:O	1:F:832:ARG:CG	2.56	0.53
1:H:805:HIS:HB3	1:H:809:ILE:HG13	1.90	0.53
1:C:955:ALA:O	1:C:958:ARG:HG2	2.07	0.53
1:C:977:ARG:CD	1:C:977:ARG:C	2.76	0.53
1:C:981:ILE:HG21	1:C:987:MET:CE	2.37	0.53
1:A:700:ASN:CB	1:A:703:LEU:CD1	2.86	0.53
1:A:738:VAL:CG2	4:A:1232:HOH:O	2.54	0.53
1:B:811:SER:HB3	1:B:984:ASP:OD2	2.07	0.53
1:E:717:VAL:HG13	1:E:727:TYR:HE2	1.73	0.53
1:G:766:MET:HE2	1:G:777:LEU:HD22	1.91	0.53
1:H:707:LEU:CD1	1:H:789:ILE:CD1	2.38	0.53
1:H:925:SER:O	1:H:929:LYS:CG	2.56	0.53
1:C:790:MET:HG2	2:C:1101:816:CLA	2.45	0.53
1:A:705:ARG:CD	1:A:707:LEU:CD2	2.85	0.53
1:B:718:LEU:HD11	1:B:728:LYS:HB2	1.90	0.53
1:D:830:ASP:HA	1:G:720:SER:HB2	1.89	0.53
1:D:999:ARG:HA	1:D:1003:ASP:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:799:LEU:O	1:G:802:VAL:HG23	2.07	0.53
1:D:790:MET:HG2	1:D:791:GLN:N	2.24	0.53
1:E:913:LYS:N	1:E:913:LYS:HD2	2.22	0.53
1:F:708:LYS:N	1:F:711:GLU:OE2	2.30	0.53
1:A:938:ILE:HG13	1:A:938:ILE:O	2.08	0.53
1:B:894:GLN:CB	1:B:955:ALA:HB1	2.39	0.53
1:G:847:THR:OG1	1:G:848:PRO:HD2	2.08	0.53
1:H:831:ARG:HB3	1:H:833:LEU:CD1	2.38	0.53
1:A:813:TYR:CZ	1:A:990:PRO:HD3	2.44	0.53
1:F:704:LEU:HD23	1:F:764:TYR:CE1	2.43	0.53
1:F:909:THR:O	1:F:910:PHE:HB2	2.07	0.53
1:C:922:GLU:O	1:C:926:ILE:HG23	2.09	0.53
1:A:762:GLU:OE1	1:A:861:LEU:HD23	2.09	0.53
1:H:803:ARG:HG2	1:H:911:GLY:HA3	1.90	0.53
1:C:765:VAL:O	1:C:768:SER:HB2	2.08	0.53
1:A:767:ALA:O	1:A:776:ARG:NH1	2.37	0.53
1:A:777:LEU:CD1	1:A:789:ILE:O	2.57	0.53
1:A:798:LEU:C	1:A:798:LEU:CD1	2.65	0.53
1:A:815[B]:LEU:CD2	1:A:979:LEU:HD12	2.38	0.53
1:D:1006:ASP:OD1	1:D:1006:ASP:N	2.37	0.53
2:E:1101:816:NAB	2:E:1101:816:CAN	2.72	0.53
1:F:701:GLN:OE1	1:F:701:GLN:HA	2.08	0.53
1:G:757:LYS:HD2	1:G:758:GLU:N	2.23	0.53
1:C:971:MET:HA	1:C:978:TYR:CE2	2.44	0.53
1:A:923:ILE:CA	1:A:926:ILE:HG12	2.34	0.53
1:A:940:THR:HG23	1:A:941:ILE:N	2.24	0.53
1:B:705:ARG:HG2	1:B:707:LEU:HD23	1.89	0.53
1:E:743:ALA:O	1:E:744:ILE:CD1	2.57	0.53
1:G:821:ILE:HG22	1:G:900:TYR:CE1	2.43	0.53
1:G:851:VAL:C	1:G:852:LYS:HG2	2.27	0.53
1:H:776:ARG:O	1:H:778:LEU:HD21	2.08	0.53
1:H:962:ARG:C	1:H:965:ILE:HG13	2.28	0.53
1:A:880:TRP:CZ2	1:A:906:GLU:OE2	2.62	0.53
1:F:781:CYS:SG	1:F:783:THR:HG23	2.49	0.53
1:F:879:LYS:NZ	1:F:918:ILE:O	2.36	0.53
1:G:773:HIS:CE1	1:G:820:GLN:HG2	2.43	0.53
1:G:998:TYR:HE2	4:G:1227:HOH:O	1.92	0.53
1:C:714:LYS:HA	1:C:729:GLY:HA2	1.90	0.53
1:C:782:LEU:C	1:C:783:THR:HG23	2.29	0.52
1:C:898:TRP:CD1	1:C:898:TRP:C	2.81	0.52
1:D:842:ASN:O	1:D:854:THR:CG2	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:726:VAL:HG23	1:E:745:LYS:HD2	1.92	0.52
1:B:894:GLN:HB3	1:B:955:ALA:HB1	1.91	0.52
1:E:821:ILE:HA	1:E:853:ILE:HD11	1.92	0.52
1:F:747:LEU:HG	1:F:788:LEU:CD1	2.37	0.52
1:F:778:LEU:HD22	1:F:778:LEU:N	2.24	0.52
1:H:971:MET:O	1:H:974:ASP:C	2.48	0.52
1:D:846:LYS:HD2	1:D:850:HIS:HD2	1.74	0.52
1:D:876:VAL:HG12	1:D:877:PRO:HD2	1.91	0.52
1:D:894:GLN:C	1:D:897:VAL:HG23	2.30	0.52
1:H:858:LEU:O	1:H:861:LEU:HB2	2.08	0.52
1:A:707:LEU:HD22	1:A:711:GLU:CD	2.30	0.52
1:D:981:ILE:HB	1:D:984:ASP:CB	2.24	0.52
1:E:745:LYS:O	1:E:787:GLN:HA	2.10	0.52
1:G:766:MET:CE	1:G:777:LEU:HD22	2.39	0.52
1:H:954:ASP:HB3	1:H:957:SER:OG	2.10	0.52
1:C:825:MET:CG	1:C:838:LEU:CD2	2.88	0.52
1:E:771:ASN:OD1	1:E:772:PRO:N	2.42	0.52
1:C:714:LYS:CE	1:C:787:GLN:NE2	2.67	0.52
1:C:817:TRP:CD1	1:C:851:VAL:HG11	2.45	0.52
1:B:798:LEU:HB2	1:B:843:VAL:CG1	2.36	0.52
1:D:942:ASP:O	1:D:946:ILE:HG13	2.09	0.52
1:G:728:LYS:HG3	1:G:792:LEU:HD13	1.90	0.52
1:H:769:VAL:HG11	1:H:856:PHE:CZ	2.45	0.52
1:A:799:LEU:HB2	1:A:840:ALA:HB3	1.91	0.52
1:E:773:HIS:O	1:E:853:ILE:HG13	2.09	0.52
1:H:945:MET:HE1	3:H:1103:EDO:H22	1.91	0.52
1:E:835:HIS:CE1	1:E:837:ASP:O	2.63	0.52
1:F:800:ASP:O	1:F:804:GLU:HG3	2.09	0.52
1:G:1007:MET:HG2	1:G:1008:ASP:O	2.09	0.52
1:H:718:LEU:HD21	1:H:728:LYS:HB2	1.92	0.52
1:A:705:ARG:HG2	1:A:706:ILE:O	2.10	0.52
1:A:757:LYS:N	1:A:757:LYS:CD	2.73	0.52
1:D:878:ILE:HG13	1:D:881:MET:HE2	1.92	0.52
1:G:819:VAL:HG22	1:G:968:PHE:HB3	1.92	0.52
1:H:1007:MET:SD	1:H:1008:ASP:O	2.68	0.52
1:C:712:PHE:CZ	1:C:787:GLN:OE1	2.63	0.52
1:C:780:ILE:HD12	1:C:787:GLN:O	2.07	0.52
1:C:929:LYS:HD2	1:C:931:GLU:OE2	2.10	0.52
1:B:762:GLU:O	1:B:766:MET:HG3	2.10	0.51
1:F:945:MET:CA	1:F:948:VAL:HG23	2.40	0.51
1:G:790:MET:HG2	2:G:1101:816:CBF	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:849:GLN:HB3	1:C:1010:VAL:CG1	2.41	0.51
1:C:894:GLN:NE2	1:C:958:ARG:O	2.42	0.51
1:E:780:ILE:O	1:E:780:ILE:HG22	2.10	0.51
1:E:950:CYS:O	1:E:958:ARG:CG	2.58	0.51
1:G:771:ASN:HB3	1:G:774:VAL:HG23	1.92	0.51
1:H:708:LYS:CG	1:H:711:GLU:OE2	2.58	0.51
1:H:716:LYS:CG	1:H:717:VAL:N	2.73	0.51
1:C:808:ASN:HB3	4:C:1222:HOH:O	2.10	0.51
1:C:827:TYR:CZ	1:C:831:ARG:HD2	2.44	0.51
1:B:915:TYR:OH	1:B:927:LEU:HD21	2.10	0.51
1:E:759:ILE:CD1	1:E:780:ILE:HD12	2.28	0.51
1:E:799:LEU:HD22	1:E:841:ARG:HB3	1.93	0.51
1:F:790:MET:CE	2:F:1101:816:NAB	2.72	0.51
1:F:900:TYR:HH	1:F:968:PHE:HE2	1.58	0.51
1:F:945:MET:HA	1:F:948:VAL:CG2	2.40	0.51
2:F:1101:816:CAR	4:F:1231:HOH:O	2.57	0.51
1:H:708:LYS:HG3	1:H:711:GLU:HB2	1.93	0.51
1:F:726:VAL:CG2	1:F:745:LYS:HE2	2.41	0.51
1:A:888:HIS:HA	1:D:888:HIS:O	2.11	0.51
1:B:900:TYR:HH	1:B:968:PHE:HE2	1.56	0.51
1:G:924:SER:O	1:G:928:GLU:CG	2.56	0.51
1:B:898:TRP:CZ2	1:B:927:LEU:CD1	2.92	0.51
1:D:806:LYS:HB2	1:D:910:PHE:HB3	1.92	0.51
1:F:991:SER:CB	1:F:992:PRO:CD	2.83	0.51
1:C:713:LYS:HG3	1:C:713:LYS:O	2.11	0.51
1:A:932:ARG:HB3	1:A:951:TRP:CE3	2.45	0.51
1:D:825:MET:HG3	1:D:838:LEU:HD22	1.92	0.51
1:E:922:GLU:O	1:E:926:ILE:HG23	2.10	0.51
1:F:949:LYS:O	1:F:952:MET:HB2	2.10	0.51
1:G:806:LYS:O	1:G:806:LYS:HE2	2.09	0.51
1:A:721:GLY:HA3	4:A:1207:HOH:O	2.10	0.51
1:C:795:PHE:HE2	1:C:1002:MET:CE	2.23	0.51
1:C:846:LYS:O	1:C:847:THR:HG22	2.10	0.51
1:A:806:LYS:O	1:A:806:LYS:HD3	2.09	0.51
1:B:851:VAL:O	1:B:851:VAL:CG2	2.59	0.51
1:E:806:LYS:HG2	1:E:807:ASP:N	2.25	0.51
2:G:1101:816:N3	2:G:1101:816:CAR	2.74	0.51
1:A:700:ASN:N	1:A:703:LEU:CD1	2.73	0.51
1:B:788:LEU:O	2:B:1101:816:CLA	2.66	0.51
1:B:977:ARG:HE	1:D:931:GLU:HB2	1.75	0.51
1:E:992:PRO:HD2	1:E:993:THR:H	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:955:ALA:O	1:F:958:ARG:CG	2.53	0.51
1:G:925:SER:O	1:G:929:LYS:HG2	2.11	0.51
1:G:940:THR:HG23	1:G:943:VAL:H	1.75	0.51
1:H:707:LEU:HD13	1:H:789:ILE:CG1	2.35	0.51
1:C:899:SER:O	1:C:902:VAL:HG23	2.11	0.51
1:A:783:THR:CG2	1:A:784:SER:H	2.21	0.50
1:D:940:THR:HG22	1:D:943:VAL:CG2	2.34	0.50
1:E:707:LEU:HD11	1:E:789:ILE:CG1	2.31	0.50
1:F:1008:ASP:O	1:F:1008:ASP:OD2	2.30	0.50
1:G:743:ALA:HB2	2:G:1101:816:N1	2.27	0.50
1:G:745:LYS:NZ	1:G:855:ASP:OD1	2.40	0.50
1:A:949:LYS:O	1:A:958:ARG:HG3	2.11	0.50
1:B:1003:ASP:C	1:B:1003:ASP:OD1	2.48	0.50
1:D:932:ARG:HH11	1:D:932:ARG:CG	2.14	0.50
1:E:950:CYS:HA	1:E:958:ARG:HG2	1.93	0.50
1:G:774:VAL:HG12	1:G:856:PHE:HE2	1.76	0.50
1:H:767:ALA:O	1:H:776:ARG:NH1	2.44	0.50
1:B:809:ILE:O	1:B:809:ILE:HG22	2.10	0.50
1:D:939:CYS:SG	1:D:943:VAL:CG1	2.99	0.50
1:D:940:THR:CB	1:D:978:TYR:O	2.58	0.50
1:F:932:ARG:HH22	1:F:953:ILE:HD13	1.76	0.50
1:E:819:VAL:HG23	1:E:968:PHE:HB3	1.91	0.50
1:F:850:HIS:CD2	1:F:850:HIS:C	2.84	0.50
1:F:894:GLN:O	1:F:897:VAL:HB	2.11	0.50
1:F:945:MET:HA	1:F:948:VAL:HG23	1.94	0.50
1:A:850:HIS:ND1	1:A:1003:ASP:OD2	2.45	0.50
1:B:1003:ASP:OD1	1:B:1003:ASP:O	2.30	0.50
1:E:919:PRO:HB2	1:E:922:GLU:HG3	1.93	0.50
1:F:776:ARG:NH1	4:F:1203:HOH:O	2.38	0.50
1:F:902:VAL:O	1:F:905:TRP:HB3	2.11	0.50
1:F:999:ARG:O	1:F:1003:ASP:O	2.30	0.50
1:G:943:VAL:HG21	1:G:979:LEU:HD23	1.92	0.50
1:G:1012:ASP:O	1:G:1014:ASP:OD1	2.30	0.50
1:C:817:TRP:CD1	1:C:851:VAL:HG13	2.46	0.50
1:C:881:MET:CE	1:C:886:ILE:HG13	2.38	0.50
1:D:837:ASP:O	1:D:837:ASP:OD1	2.30	0.50
1:E:999:ARG:O	1:E:1003:ASP:O	2.30	0.50
1:C:770:ASP:OD1	1:C:770:ASP:O	2.30	0.50
1:C:947:MET:HB3	1:C:951:TRP:CH2	2.47	0.50
1:A:945:MET:O	1:A:949:LYS:HG3	2.10	0.50
1:A:1013:ALA:O	1:A:1014:ASP:O	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:985:GLU:HG2	1:F:986:ARG:N	2.27	0.50
1:G:719:GLY:HA3	2:G:1101:816:CAS	2.42	0.50
1:A:932:ARG:HH22	1:A:953:ILE:HD11	1.76	0.50
1:B:846:LYS:O	1:B:847:THR:HG22	2.11	0.50
1:D:707:LEU:HD23	1:D:711:GLU:CG	2.41	0.50
1:E:848:PRO:HD2	1:E:998:TYR:CE1	2.47	0.50
1:G:773:HIS:ND1	1:G:820:GLN:CB	2.71	0.50
1:A:743:ALA:O	2:A:1101:816:CLA	2.67	0.50
1:A:846:LYS:HD3	1:A:852:LYS:HD2	1.94	0.50
1:B:737:LYS:HD2	1:B:737:LYS:N	2.26	0.50
1:B:821:ILE:CG2	1:B:853:ILE:HD11	2.42	0.50
1:F:731:TRP:CE3	1:F:740:ILE:HG13	2.47	0.50
1:F:898:TRP:CD1	1:F:898:TRP:C	2.85	0.50
1:G:718:LEU:HD21	1:G:728:LYS:HB2	1.93	0.50
1:G:975:PRO:HG3	1:G:1013:ALA:HB2	1.94	0.50
1:C:935:GLN:HB2	1:C:944:TYR:CD1	2.47	0.50
1:A:985:GLU:HG2	1:A:986:ARG:N	2.27	0.49
1:D:818:CYS:SG	1:D:904:VAL:HG13	2.51	0.49
1:F:717:VAL:HG22	1:F:727:TYR:HE2	1.71	0.49
1:C:756:ASN:ND2	1:C:782:LEU:HD22	2.27	0.49
1:C:860:LYS:O	1:C:861:LEU:O	2.30	0.49
1:C:940:THR:CG2	1:C:943:VAL:H	2.25	0.49
1:A:888:HIS:O	1:D:888:HIS:HB3	2.11	0.49
1:B:932:ARG:HG3	1:B:951:TRP:CE3	2.48	0.49
1:D:814:LEU:HD23	1:D:817:TRP:CZ3	2.47	0.49
1:D:856:PHE:O	1:D:856:PHE:CG	2.63	0.49
1:E:726:VAL:HG22	1:E:745:LYS:HD2	1.93	0.49
1:F:849:GLN:N	1:F:849:GLN:CD	2.65	0.49
1:G:912:SER:HA	1:G:913:LYS:HE3	1.94	0.49
1:C:781:CYS:HB3	1:C:787:GLN:HB2	1.94	0.49
1:C:999:ARG:HG2	1:C:1003:ASP:HB3	1.94	0.49
1:A:780:ILE:HG12	1:A:781:CYS:N	2.27	0.49
1:B:704:LEU:HD23	1:B:764:TYR:CE1	2.47	0.49
1:B:999:ARG:CG	1:B:999:ARG:NH1	2.73	0.49
1:D:839:ALA:HB3	1:D:842:ASN:HD22	1.77	0.49
1:E:803:ARG:NE	1:E:911:GLY:O	2.45	0.49
1:F:811:SER:CB	1:F:984:ASP:OD2	2.55	0.49
1:G:967:GLU:O	1:G:971:MET:HG3	2.12	0.49
1:H:879:LYS:HB3	1:H:915:TYR:HD2	1.77	0.49
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.46	0.49
1:E:821:ILE:HG21	1:E:900:TYR:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:892:THR:H	1:G:895:SER:HB3	1.77	0.49
1:H:758:GLU:O	1:H:758:GLU:OE2	2.30	0.49
1:C:977:ARG:HG3	1:C:978:TYR:N	2.27	0.49
1:A:732:ILE:HG23	1:A:732:ILE:O	2.12	0.49
1:B:831:ARG:NH2	4:B:1204:HOH:O	2.45	0.49
1:D:771:ASN:ND2	1:D:772:PRO:HD2	2.27	0.49
1:F:917:GLY:C	1:F:918:ILE:HD13	2.33	0.49
1:F:949:LYS:HB3	1:F:959:PRO:HD3	1.94	0.49
1:G:881:MET:CE	1:G:885:SER:CB	2.89	0.49
1:H:806:LYS:HG3	1:H:807:ASP:N	2.27	0.49
1:H:902:VAL:O	1:H:906:GLU:HG3	2.13	0.49
1:C:938:ILE:HG13	1:C:939:CYS:N	2.27	0.49
1:B:898:TRP:HZ2	1:B:927:LEU:CD1	2.26	0.49
1:E:941:ILE:HG23	1:C:934:PRO:HG3	1.93	0.49
1:F:770:ASP:OD1	1:F:770:ASP:O	2.30	0.49
1:G:802:VAL:HG12	1:G:809:ILE:CD1	2.42	0.49
1:H:708:LYS:HG3	1:H:711:GLU:OE2	2.12	0.49
1:H:758:GLU:OE1	1:H:762:GLU:OE1	2.30	0.49
1:C:884:GLU:HG2	1:C:885:SER:H	1.77	0.49
1:B:981:ILE:O	1:B:984:ASP:HB2	2.13	0.49
1:F:820:GLN:NE2	1:F:1010:VAL:HG12	2.28	0.49
1:G:774:VAL:HG12	1:G:856:PHE:CE2	2.48	0.49
1:H:802:VAL:HG12	1:H:809:ILE:HD12	1.94	0.49
1:H:847:THR:O	1:H:850:HIS:O	2.30	0.49
1:C:898:TRP:CH2	1:C:927:LEU:HD13	2.47	0.49
1:C:908:MET:CE	1:C:979:LEU:CD2	2.79	0.49
2:C:1101:816:NAB	2:C:1101:816:CAN	2.76	0.49
1:B:995:SER:O	1:B:999:ARG:HG2	2.12	0.49
1:E:718:LEU:HG	1:E:728:LYS:N	2.28	0.49
1:G:1007:MET:HE1	1:G:1008:ASP:O	2.13	0.49
1:H:809:ILE:CG2	1:H:810:GLY:N	2.75	0.49
1:C:707:LEU:CD1	1:C:789:ILE:CD1	2.89	0.49
1:C:782:LEU:C	1:C:783:THR:CG2	2.81	0.49
1:A:726:VAL:HG23	1:A:745:LYS:HG3	1.92	0.49
1:B:949:LYS:O	1:B:952:MET:CG	2.61	0.49
1:D:769:VAL:O	1:D:769:VAL:CG2	2.61	0.49
1:E:992:PRO:CD	1:E:993:THR:H	2.26	0.49
1:G:822:ALA:HB1	1:G:965:ILE:HG12	1.93	0.49
1:H:903:THR:HA	1:H:906:GLU:HG3	1.93	0.49
1:C:905:TRP:O	1:C:909:THR:CG2	2.56	0.49
1:A:774:VAL:CG2	1:A:824:GLY:O	2.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:TRP:NE1	1:A:906:GLU:OE2	2.44	0.49
1:D:965:ILE:O	1:D:969:SER:OG	2.31	0.49
1:E:876:VAL:HG11	1:E:889:ARG:NH1	2.28	0.49
1:C:745:LYS:O	1:C:787:GLN:HA	2.13	0.49
1:A:745:LYS:NZ	4:A:1207:HOH:O	2.46	0.48
1:A:999:ARG:NH2	1:A:1006:ASP:HA	2.28	0.48
1:D:767:ALA:O	1:D:776:ARG:CG	2.60	0.48
1:F:845:VAL:HG12	1:F:847:THR:C	2.34	0.48
1:C:759:ILE:HA	1:C:762:GLU:HG3	1.94	0.48
1:C:783:THR:OG1	1:C:785:THR:O	2.30	0.48
1:C:898:TRP:CE3	1:C:958:ARG:NH1	2.80	0.48
1:C:961:PHE:O	1:C:965:ILE:CD1	2.30	0.48
1:A:793:MET:CE	1:A:844:LEU:HB2	2.43	0.48
1:A:898:TRP:CZ2	1:A:927:LEU:CD1	2.96	0.48
1:D:848:PRO:HD2	1:D:998:TYR:CE1	2.48	0.48
1:F:909:THR:HB	1:F:912:SER:HB2	1.94	0.48
1:G:717:VAL:HG22	1:G:727:TYR:CD2	2.48	0.48
1:G:940:THR:HG22	1:G:978:TYR:O	2.14	0.48
1:C:756:ASN:CG	1:C:782:LEU:HD22	2.33	0.48
1:C:823:LYS:HG2	1:C:965:ILE:HG12	1.94	0.48
1:C:846:LYS:C	1:C:847:THR:CG2	2.81	0.48
1:A:708:LYS:N	1:A:711:GLU:OE2	2.42	0.48
1:A:819:VAL:CG1	1:A:823:LYS:HE3	2.42	0.48
1:B:729:GLY:HA3	1:B:744:ILE:HD11	1.95	0.48
1:D:783:THR:CG2	1:D:784:SER:H	2.08	0.48
1:D:803:ARG:NH2	1:D:911:GLY:O	2.40	0.48
1:E:723:PHE:CE2	1:E:859:ALA:CA	2.78	0.48
1:E:768:SER:OG	1:E:831:ARG:NH1	2.45	0.48
1:F:713:LYS:HA	4:F:1223:HOH:O	2.13	0.48
1:H:825:MET:HE3	1:H:961:PHE:CE2	2.49	0.48
1:H:884:GLU:HG2	1:H:885:SER:N	2.28	0.48
1:B:949:LYS:O	1:B:952:MET:HG2	2.13	0.48
1:D:795:PHE:CZ	1:D:848:PRO:HD3	2.48	0.48
1:E:771:ASN:OD1	1:E:773:HIS:N	2.30	0.48
1:E:783:THR:O	1:E:785:THR:N	2.46	0.48
1:F:736:GLU:N	4:F:1206:HOH:O	2.46	0.48
1:C:713:LYS:HD2	4:C:1206:HOH:O	2.14	0.48
1:A:811:SER:OG	1:A:975:PRO:HB2	2.13	0.48
1:A:837:ASP:O	1:A:842:ASN:ND2	2.43	0.48
1:B:816:ASN:O	1:B:820:GLN:HG3	2.14	0.48
1:D:723:PHE:O	1:D:747:LEU:HD23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:808:ASN:OD1	1:D:808:ASN:O	2.30	0.48
1:F:989:LEU:HD23	1:F:990:PRO:CA	2.42	0.48
1:G:821:ILE:HG22	1:G:900:TYR:HE1	1.79	0.48
1:C:908:MET:HB3	1:C:936:PRO:HG2	1.95	0.48
1:A:758:GLU:OE2	1:A:758:GLU:O	2.30	0.48
1:A:815[A]:LEU:O	1:A:818:CYS:HB2	2.14	0.48
1:B:809:ILE:N	1:B:987:MET:CE	2.77	0.48
1:B:932:ARG:HG3	1:B:951:TRP:HE3	1.79	0.48
1:D:815:LEU:HG	1:D:979:LEU:HD13	1.94	0.48
1:F:799:LEU:O	1:F:802:VAL:CG2	2.61	0.48
1:G:884:GLU:HG2	1:G:885:SER:N	2.29	0.48
1:G:944:TYR:O	1:G:947:MET:CB	2.61	0.48
1:H:969:SER:O	1:H:972:ALA:HB3	2.13	0.48
1:C:726:VAL:CG2	1:C:745:LYS:HE2	2.42	0.48
1:C:955:ALA:HA	1:C:958:ARG:NE	2.29	0.48
1:A:831:ARG:O	1:A:832:ARG:HB2	2.13	0.48
1:B:737:LYS:CD	1:B:737:LYS:C	2.81	0.48
1:D:941:ILE:O	1:D:941:ILE:HG13	2.14	0.48
1:D:941:ILE:HG12	1:D:945:MET:HE3	1.95	0.48
1:G:793:MET:H	2:G:1101:816:C2	2.26	0.48
1:H:835:HIS:NE2	1:H:854:THR:O	2.40	0.48
1:H:991:SER:OG	1:H:994:ASP:OD2	2.30	0.48
1:A:815[B]:LEU:O	1:A:818:CYS:HB2	2.14	0.48
1:A:904:VAL:O	1:A:908:MET:HG2	2.13	0.48
1:E:806:LYS:CE	4:E:1207:HOH:O	2.56	0.48
1:G:825:MET:HE3	1:G:825:MET:HB2	1.59	0.48
1:H:714:LYS:NZ	1:H:787:GLN:HE22	2.12	0.48
1:A:765:VAL:CG1	1:A:766:MET:N	2.76	0.48
1:B:846:LYS:HD3	1:B:852:LYS:HD2	1.96	0.48
1:E:706:ILE:HG13	1:E:780:ILE:HG22	1.96	0.48
1:E:708:LYS:O	1:E:711:GLU:N	2.43	0.48
1:E:898:TRP:CZ2	1:E:927:LEU:HD22	2.49	0.48
1:F:707:LEU:CB	1:F:711:GLU:CD	2.82	0.48
1:C:803:ARG:O	1:C:806:LYS:HG2	2.14	0.48
1:A:894:GLN:HB3	1:A:955:ALA:HB1	1.96	0.48
1:B:726:VAL:CG2	1:B:745:LYS:CE	2.91	0.48
1:B:815:LEU:O	1:B:818:CYS:HB2	2.14	0.48
1:F:881:MET:HE3	1:F:886:ILE:CG1	2.42	0.48
1:F:960:LYS:HA	4:F:1228:HOH:O	2.13	0.48
1:H:762:GLU:CB	1:H:861:LEU:CD2	2.90	0.48
1:A:938:ILE:HB	1:A:980:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:ARG:HD3	1:B:833:LEU:HD11	1.95	0.47
1:B:834:VAL:CG2	1:B:893:HIS:CD2	2.91	0.47
1:B:940:THR:HG23	1:B:942:ASP:N	2.29	0.47
1:E:855:ASP:OD2	1:E:858:LEU:HD23	2.13	0.47
1:F:717:VAL:HG22	1:F:727:TYR:CD2	2.49	0.47
1:A:881:MET:CE	1:A:885:SER:HB3	2.40	0.47
1:B:809:ILE:CG2	1:B:814:LEU:HD11	2.44	0.47
1:B:831:ARG:O	1:B:832:ARG:CB	2.61	0.47
1:E:759:ILE:O	1:E:763:ALA:N	2.35	0.47
1:F:879:LYS:HD3	1:F:915:TYR:HB2	1.96	0.47
1:F:898:TRP:CZ2	1:F:927:LEU:HD13	2.49	0.47
1:G:703:LEU:HD23	1:G:703:LEU:H	1.76	0.47
1:H:878:ILE:CG2	1:H:923:ILE:HG13	2.44	0.47
1:H:970:LYS:HA	1:H:973:ARG:HD2	1.96	0.47
1:A:793:MET:HE2	1:A:844:LEU:CD1	2.40	0.47
1:B:835:HIS:CG	1:B:856:PHE:CB	2.95	0.47
1:B:931:GLU:O	1:B:932:ARG:CD	2.58	0.47
1:F:731:TRP:CZ3	1:F:740:ILE:HG13	2.49	0.47
1:G:798:LEU:HG	1:G:907:LEU:HD21	1.95	0.47
1:G:940:THR:CB	1:G:978:TYR:O	2.62	0.47
1:H:708:LYS:HG3	1:H:711:GLU:CG	2.43	0.47
1:H:717:VAL:HG22	1:H:727:TYR:CE2	2.49	0.47
1:C:704:LEU:HB2	1:C:767:ALA:HB2	1.94	0.47
1:C:765:VAL:CG1	1:C:766:MET:N	2.76	0.47
1:C:846:LYS:HG3	1:C:847:THR:CG2	2.44	0.47
1:C:975:PRO:HD2	1:C:1013:ALA:CB	2.43	0.47
1:C:975:PRO:CD	1:C:1013:ALA:HB2	2.42	0.47
1:B:843:VAL:HG22	1:B:853:ILE:HG12	1.97	0.47
1:D:796:GLY:O	1:D:845:VAL:N	2.34	0.47
1:E:805:HIS:O	1:E:808:ASN:O	2.33	0.47
1:F:878:ILE:HD13	1:F:881:MET:HE1	1.96	0.47
1:C:714:LYS:HA	1:C:729:GLY:CA	2.45	0.47
1:C:811:SER:CB	1:C:984:ASP:OD1	2.58	0.47
1:A:762:GLU:CD	1:A:861:LEU:HD21	2.34	0.47
1:B:966:ILE:HG22	1:B:970:LYS:HE3	1.96	0.47
1:D:767:ALA:O	1:D:776:ARG:HD2	2.13	0.47
1:G:855:ASP:OD1	1:G:858:LEU:CD2	2.62	0.47
1:H:776:ARG:O	1:H:778:LEU:HD23	2.14	0.47
1:C:771:ASN:ND2	1:C:772:PRO:HD2	2.29	0.47
1:C:856:PHE:HD1	1:C:857:GLY:H	1.51	0.47
1:A:793:MET:HE3	1:A:844:LEU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:HB2	1:A:840:ALA:CB	2.44	0.47
1:A:900:TYR:O	1:A:904:VAL:CG2	2.59	0.47
1:A:927:LEU:HD11	4:A:1213:HOH:O	2.14	0.47
1:B:835:HIS:ND1	1:B:856:PHE:HA	2.30	0.47
1:A:856:PHE:O	1:A:856:PHE:CG	2.68	0.47
1:B:882:ALA:HA	1:B:898:TRP:CE2	2.50	0.47
1:B:935:GLN:CG	1:B:944:TYR:CG	2.93	0.47
1:D:894:GLN:HA	1:D:897:VAL:CG2	2.45	0.47
1:E:765:VAL:O	1:E:768:SER:OG	2.30	0.47
1:E:905:TRP:O	1:E:909:THR:OG1	2.30	0.47
1:E:973:ARG:HG2	1:E:973:ARG:HH11	1.80	0.47
1:F:795:PHE:HB2	1:F:845:VAL:O	2.15	0.47
1:F:817:TRP:CD1	1:F:851:VAL:CG2	2.97	0.47
1:F:935:GLN:HB3	1:F:944:TYR:CD2	2.50	0.47
1:G:758:GLU:O	1:G:761:ASP:HB2	2.15	0.47
1:H:962:ARG:HA	1:H:965:ILE:CG1	2.40	0.47
1:C:855:ASP:HA	2:C:1101:816:CAK	2.44	0.47
1:C:999:ARG:O	1:C:1003:ASP:C	2.52	0.47
1:B:729:GLY:HA3	1:B:744:ILE:CD1	2.44	0.47
1:D:846:LYS:C	1:D:847:THR:HG22	2.35	0.47
1:F:926:ILE:O	1:F:930:GLY:N	2.46	0.47
1:F:999:ARG:HA	1:F:1003:ASP:HB2	1.95	0.47
1:A:771:ASN:OD1	1:A:772:PRO:HD2	2.15	0.47
1:A:898:TRP:CD1	1:A:898:TRP:C	2.88	0.47
1:A:938:ILE:O	1:A:938:ILE:CG1	2.63	0.47
1:B:717:VAL:HG23	1:B:727:TYR:CE2	2.49	0.47
1:B:880:TRP:NE1	1:B:906:GLU:OE2	2.36	0.47
1:E:943:VAL:HG21	1:E:979:LEU:CD2	2.45	0.47
1:F:729:GLY:HA3	1:F:744:ILE:CD1	2.37	0.47
1:H:729:GLY:HA3	1:H:744:ILE:CD1	2.45	0.47
1:H:831:ARG:CB	1:H:833:LEU:HD12	2.45	0.47
1:C:816:ASN:O	1:C:820:GLN:CG	2.59	0.47
1:A:992:PRO:O	1:A:996:ASN:HB2	2.14	0.47
1:B:813:TYR:OH	1:B:990:PRO:HB3	2.15	0.47
1:B:835:HIS:HE2	1:B:838:LEU:HB2	1.80	0.47
1:E:707:LEU:HD13	1:E:789:ILE:HG12	1.92	0.47
1:D:748:ARG:O	1:D:749:GLU:C	2.53	0.46
1:D:812:GLN:NE2	1:D:1011:VAL:O	2.43	0.46
1:E:795:PHE:HB2	1:E:845:VAL:HB	1.96	0.46
1:E:795:PHE:N	1:E:795:PHE:CD2	2.84	0.46
1:F:844:LEU:O	1:F:851:VAL:HG12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:974:ASP:O	1:H:978:TYR:CD2	2.67	0.46
1:A:999:ARG:O	1:A:1003:ASP:O	2.34	0.46
1:B:771:ASN:HD21	1:B:772:PRO:HD2	1.70	0.46
1:B:778:LEU:HD11	1:B:791:GLN:CG	2.38	0.46
1:B:783:THR:HG22	1:B:784:SER:H	1.75	0.46
1:F:926:ILE:HB	1:F:931:GLU:HG3	1.97	0.46
1:G:707:LEU:HD13	1:G:789:ILE:HD13	1.97	0.46
1:A:940:THR:CG2	1:A:942:ASP:H	2.28	0.46
1:B:712:PHE:CE2	1:B:789:ILE:HD11	2.50	0.46
1:B:988:HIS:CA	1:B:989:LEU:C	2.84	0.46
1:D:706:ILE:N	1:D:706:ILE:CD1	2.78	0.46
1:D:795:PHE:CB	1:D:845:VAL:CG1	2.93	0.46
1:F:772:PRO:HB3	1:F:1007:MET:HA	1.97	0.46
1:F:839:ALA:O	1:F:843:VAL:HG23	2.15	0.46
1:F:995:SER:O	1:F:999:ARG:CG	2.62	0.46
1:C:777:LEU:HB2	2:C:1101:816:CAA	2.45	0.46
1:C:780:ILE:O	1:C:780:ILE:CG2	2.62	0.46
1:C:942:ASP:OD2	1:C:942:ASP:N	2.43	0.46
1:A:966:ILE:HG22	1:A:970:LYS:HE3	1.96	0.46
1:B:905:TRP:CD2	1:B:933:LEU:HD13	2.50	0.46
1:E:892:THR:O	1:E:895:SER:HB2	2.15	0.46
1:F:855:ASP:HA	1:F:858:LEU:HD13	1.97	0.46
1:F:888:HIS:HB2	1:F:890:ILE:HG13	1.97	0.46
1:G:943:VAL:O	1:G:946:ILE:HB	2.15	0.46
1:H:825:MET:HG2	1:H:853:ILE:HD12	1.97	0.46
1:A:769:VAL:HG21	1:A:856:PHE:CZ	2.51	0.46
1:A:774:VAL:HG21	1:A:824:GLY:O	2.16	0.46
1:A:894:GLN:CB	1:A:955:ALA:HB1	2.46	0.46
1:E:829:GLU:HA	1:E:893:HIS:CE1	2.50	0.46
1:H:707:LEU:HD13	1:H:789:ILE:HD13	0.57	0.46
1:C:714:LYS:NZ	4:C:1204:HOH:O	2.41	0.46
1:A:812:GLN:HE21	1:A:812:GLN:HB2	1.49	0.46
1:B:704:LEU:HD23	1:B:764:TYR:CD1	2.50	0.46
1:B:793:MET:HE2	1:B:844:LEU:HD12	1.98	0.46
1:D:826:ASN:HB2	1:D:961:PHE:HB3	1.97	0.46
1:D:844:LEU:HG	1:D:854:THR:HG21	1.98	0.46
1:D:970:LYS:HA	1:D:973:ARG:HG3	1.97	0.46
1:C:905:TRP:CE3	1:C:909:THR:HG21	2.50	0.46
1:A:716:LYS:HB3	1:A:728:LYS:HB3	1.97	0.46
1:A:834:VAL:CB	4:A:1209:HOH:O	2.49	0.46
1:D:926:ILE:HB	1:D:931:GLU:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:846:LYS:CE	1:E:1003:ASP:OD2	2.64	0.46
1:G:900:TYR:O	1:G:904:VAL:HG23	2.16	0.46
1:H:715:ILE:HD11	1:H:728:LYS:CD	2.45	0.46
1:D:717:VAL:CG1	1:D:727:TYR:HE2	2.15	0.46
1:E:881:MET:HE2	1:E:886:ILE:HG12	1.94	0.46
1:E:945:MET:HE3	1:C:934:PRO:CG	2.42	0.46
1:D:897:VAL:HG11	1:D:959:PRO:O	2.15	0.46
1:E:892:THR:H	1:E:895:SER:HB2	1.81	0.46
1:F:835:HIS:O	1:F:896:ASP:CG	2.54	0.46
1:C:777:LEU:HD12	1:C:789:ILE:O	2.15	0.46
1:C:836:ARG:HG2	1:C:891:TYR:CG	2.51	0.46
1:A:811:SER:CB	1:A:984:ASP:OD2	2.64	0.46
1:B:939:CYS:SG	1:B:943:VAL:HG11	2.56	0.46
1:E:950:CYS:HA	1:E:958:ARG:CG	2.46	0.46
1:E:977:ARG:CG	1:C:918:ILE:HD11	2.42	0.46
1:G:946:ILE:HD12	1:G:971:MET:CE	2.46	0.46
1:C:968:PHE:O	1:C:971:MET:HB2	2.16	0.46
1:A:811:SER:HB3	1:A:984:ASP:OD2	2.16	0.45
1:B:821:ILE:HG23	1:B:853:ILE:HD11	1.97	0.45
1:B:961:PHE:HA	1:B:964:LEU:HB2	1.98	0.45
1:E:793:MET:O	2:E:1101:816:C2	2.64	0.45
1:E:798:LEU:CD2	1:E:907:LEU:HD21	2.45	0.45
1:G:940:THR:HG23	1:G:942:ASP:N	2.31	0.45
1:C:769:VAL:O	1:C:769:VAL:HG22	2.17	0.45
1:C:825:MET:HB3	1:C:961:PHE:CE1	2.52	0.45
1:C:856:PHE:CD1	1:C:857:GLY:CA	2.98	0.45
1:C:908:MET:HE3	1:C:979:LEU:CD2	2.37	0.45
1:A:880:TRP:HA	1:A:902:VAL:HG21	1.98	0.45
1:B:780:ILE:CD1	1:B:782:LEU:HD22	2.42	0.45
1:B:910:PHE:CE2	1:B:938:ILE:CD1	2.99	0.45
1:B:977:ARG:O	1:D:918:ILE:HD11	2.16	0.45
1:D:833:LEU:HD13	1:D:856:PHE:CE1	2.52	0.45
1:D:961:PHE:O	1:D:965:ILE:HG13	2.15	0.45
1:E:708:LYS:O	1:E:711:GLU:HB2	2.16	0.45
1:E:759:ILE:CG2	1:E:760:LEU:N	2.79	0.45
1:E:836:ARG:CD	1:E:860:LYS:HA	2.45	0.45
1:F:707:LEU:HB2	1:F:711:GLU:CD	2.36	0.45
1:F:929:LYS:HA	1:F:929:LYS:HD2	1.71	0.45
1:H:708:LYS:O	1:H:712:PHE:CE1	2.69	0.45
1:H:743:ALA:CB	2:H:1101:816:NAB	2.78	0.45
1:H:762:GLU:HG2	1:H:861:LEU:HD23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ASN:CB	1:A:703:LEU:HD11	2.46	0.45
1:A:767:ALA:CB	1:A:777:LEU:O	2.64	0.45
1:B:798:LEU:HD12	1:B:801:TYR:HB3	1.97	0.45
1:B:881:MET:CE	1:B:891:TYR:CE1	2.99	0.45
1:E:904:VAL:CG1	1:E:947:MET:HE2	2.46	0.45
1:G:718:LEU:HD11	1:G:792:LEU:HD12	1.97	0.45
1:G:790:MET:HE3	1:G:791:GLN:O	2.17	0.45
1:C:908:MET:HE1	1:C:979:LEU:CD2	2.37	0.45
1:B:895:SER:O	1:B:898:TRP:HB3	2.16	0.45
1:F:999:ARG:HA	1:F:1003:ASP:HB3	1.96	0.45
1:G:861:LEU:HD23	1:G:861:LEU:N	2.31	0.45
1:G:897:VAL:HA	1:G:900:TYR:HB3	1.98	0.45
1:H:778:LEU:CD2	1:H:778:LEU:H	2.06	0.45
1:H:952:MET:HE2	1:H:952:MET:HB3	1.70	0.45
1:B:783:THR:O	1:B:784:SER:C	2.54	0.45
1:D:950:CYS:HA	1:D:958:ARG:HG2	1.98	0.45
1:E:818:CYS:O	1:E:900:TYR:OH	2.31	0.45
1:F:813:TYR:CE1	1:F:989:LEU:HB2	2.52	0.45
1:F:923:ILE:O	1:F:927:LEU:HG	2.17	0.45
1:G:915:TYR:CE1	1:G:926:ILE:CD1	2.93	0.45
1:A:708:LYS:O	1:A:711:GLU:CG	2.64	0.45
1:A:900:TYR:HH	1:A:968:PHE:HE2	1.63	0.45
1:A:972:ALA:O	1:A:975:PRO:HG3	2.17	0.45
1:E:991:SER:OG	1:E:992:PRO:CD	2.64	0.45
1:G:777:LEU:HD11	1:G:788:LEU:HB3	1.97	0.45
1:G:944:TYR:O	1:G:948:VAL:N	2.45	0.45
1:C:780:ILE:O	1:C:780:ILE:HG22	2.15	0.45
1:D:719:GLY:HA3	2:D:1101:816:CAO	2.46	0.45
1:E:783:THR:C	1:E:785:THR:N	2.69	0.45
1:E:961:PHE:HA	1:E:964:LEU:HB2	1.98	0.45
1:G:990:PRO:HB2	1:G:994:ASP:HB2	1.99	0.45
1:C:720:SER:OG	1:C:725:THR:HG22	2.17	0.45
1:C:940:THR:HG23	1:C:942:ASP:N	2.31	0.45
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.50	0.45
1:A:915:TYR:OH	1:A:927:LEU:HD21	2.17	0.45
1:B:835:HIS:O	1:B:835:HIS:CD2	2.70	0.45
1:D:886:ILE:HG21	1:D:924:SER:HB2	1.99	0.45
1:D:938:ILE:HG12	1:D:939:CYS:N	2.32	0.45
1:E:850:HIS:ND1	1:E:1003:ASP:OD2	2.32	0.45
1:E:914:PRO:O	1:E:915:TYR:C	2.55	0.45
1:E:973:ARG:HH11	1:E:973:ARG:CG	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:733:PRO:HB2	1:F:736:GLU:CB	2.44	0.45
1:G:855:ASP:OD1	1:G:858:LEU:HD22	2.17	0.45
1:G:858:LEU:HD12	1:G:861:LEU:HG	1.99	0.45
1:H:739:LYS:HB3	1:H:739:LYS:HE3	1.57	0.45
1:C:932:ARG:HH22	1:C:953:ILE:HD11	1.81	0.45
1:B:717:VAL:HG23	1:B:727:TYR:CD2	2.52	0.45
1:D:729:GLY:HA3	1:D:744:ILE:CD1	2.47	0.45
1:E:826:ASN:O	1:E:829:GLU:HB3	2.17	0.45
1:C:825:MET:CB	1:C:961:PHE:CE1	2.99	0.45
1:C:878:ILE:CG2	1:C:886:ILE:HD11	2.28	0.45
1:C:906:GLU:HA	1:C:909:THR:HG1	1.82	0.45
1:A:831:ARG:O	1:A:832:ARG:CB	2.63	0.45
1:A:966:ILE:O	1:A:970:LYS:HG3	2.16	0.45
1:B:999:ARG:HB3	1:B:999:ARG:CZ	2.47	0.45
1:D:939:CYS:SG	1:D:943:VAL:HG11	2.57	0.45
1:D:977:ARG:HG2	1:D:978:TYR:CE2	2.52	0.45
1:E:837:ASP:OD1	1:E:838:LEU:N	2.50	0.45
1:E:971:MET:HA	1:E:978:TYR:CE2	2.51	0.45
1:G:943:VAL:HG21	1:G:979:LEU:CD2	2.46	0.45
1:H:816:ASN:O	1:H:820:GLN:HG3	2.17	0.45
1:H:913:LYS:NZ	4:H:1204:HOH:O	2.49	0.45
1:C:715:ILE:HD11	1:C:728:LYS:HD3	1.99	0.45
1:C:780:ILE:HD13	1:C:780:ILE:HA	1.62	0.45
1:A:885:SER:HB3	1:A:891:TYR:CE1	2.52	0.44
1:B:723:PHE:HB3	1:B:858:LEU:HD23	1.99	0.44
1:B:898:TRP:CE3	1:B:951:TRP:HA	2.52	0.44
1:G:938:ILE:HG13	1:G:939:CYS:N	2.31	0.44
1:H:971:MET:HA	1:H:978:TYR:CE2	2.52	0.44
1:A:793:MET:CE	1:A:844:LEU:CB	2.96	0.44
1:B:777:LEU:HD12	1:B:789:ILE:O	2.17	0.44
1:B:835:HIS:CE1	1:B:837:ASP:O	2.70	0.44
1:D:757:LYS:HD2	1:D:761:ASP:CG	2.37	0.44
1:E:879:LYS:HG2	1:E:923:ILE:HD13	1.99	0.44
1:F:836:ARG:CB	1:F:859:ALA:HB3	2.38	0.44
1:G:765:VAL:O	1:G:768:SER:HB3	2.16	0.44
1:H:764:TYR:HD1	1:H:764:TYR:HA	1.71	0.44
1:H:935:GLN:HB2	1:H:944:TYR:CD1	2.52	0.44
1:A:719:GLY:HA3	2:A:1101:816:CAS	2.48	0.44
1:B:961:PHE:O	1:B:965:ILE:HG13	2.17	0.44
1:F:944:TYR:O	1:F:948:VAL:HG23	2.16	0.44
1:F:977:ARG:O	1:G:918:ILE:HD11	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:825:MET:CE	1:G:838:LEU:HD22	2.47	0.44
1:H:881:MET:HE1	1:H:891:TYR:OH	2.17	0.44
1:H:965:ILE:O	1:H:969:SER:OG	2.30	0.44
1:C:835:HIS:NE2	1:C:856:PHE:N	2.65	0.44
1:A:762:GLU:OE1	1:A:861:LEU:HD21	2.17	0.44
1:B:999:ARG:O	1:B:1003:ASP:C	2.55	0.44
1:E:941:ILE:HG13	1:E:945:MET:CE	2.48	0.44
1:G:821:ILE:CG2	1:G:900:TYR:HE1	2.30	0.44
1:G:850:HIS:HD2	1:G:851:VAL:N	2.14	0.44
1:G:879:LYS:CG	1:G:915:TYR:HB2	2.47	0.44
1:G:925:SER:O	1:G:929:LYS:CG	2.65	0.44
1:C:889:ARG:HD3	1:C:889:ARG:HA	1.36	0.44
1:B:923:ILE:HA	1:B:926:ILE:HG12	1.98	0.44
1:D:831:ARG:HE	1:D:831:ARG:HB3	1.74	0.44
1:D:949:LYS:HB2	1:D:949:LYS:HE3	1.60	0.44
1:E:745:LYS:HZ1	1:E:858:LEU:CD2	2.31	0.44
1:E:949:LYS:HB2	1:E:949:LYS:HE3	1.48	0.44
1:E:961:PHE:O	1:E:964:LEU:N	2.50	0.44
1:G:855:ASP:HA	2:G:1101:816:CAK	2.47	0.44
1:H:936:PRO:HA	1:H:937:PRO:HD3	1.90	0.44
1:H:952:MET:HB2	1:H:958:ARG:HG2	1.99	0.44
1:C:717:VAL:HG22	1:C:727:TYR:CD2	2.52	0.44
1:C:890:ILE:O	1:C:890:ILE:HG22	2.18	0.44
1:A:849:GLN:OE1	1:A:995:SER:CB	2.61	0.44
1:A:849:GLN:HE21	1:A:849:GLN:H	1.64	0.44
1:B:793:MET:HE2	1:B:844:LEU:CD1	2.48	0.44
1:E:861:LEU:HD22	1:E:861:LEU:HA	1.76	0.44
1:F:708:LYS:CA	1:F:711:GLU:CG	2.96	0.44
1:G:883:LEU:HD22	1:G:953:ILE:HD12	1.99	0.44
1:G:902:VAL:O	1:G:906:GLU:HG3	2.18	0.44
1:C:730:LEU:HD12	1:C:739:LYS:HB3	2.00	0.44
1:C:747:LEU:HD21	1:C:788:LEU:HD11	1.99	0.44
1:A:715:ILE:HG12	1:A:728:LYS:O	2.17	0.44
1:A:736:GLU:OE2	1:A:736:GLU:HA	2.18	0.44
1:E:743:ALA:O	1:E:744:ILE:HD12	2.18	0.44
1:F:714:LYS:HE2	1:F:787:GLN:OE1	2.18	0.44
1:F:954:ASP:O	1:F:957:SER:OG	2.34	0.44
1:G:898:TRP:HZ3	1:G:952:MET:O	2.01	0.44
1:H:913:LYS:HA	1:H:914:PRO:HD3	1.84	0.44
1:C:769:VAL:HG11	1:C:856:PHE:CE2	2.44	0.44
1:C:772:PRO:O	1:C:852:LYS:HG2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:935:GLN:HA	1:C:936:PRO:HD3	1.76	0.44
1:B:777:LEU:CD2	1:B:788:LEU:HD22	2.38	0.44
1:D:707:LEU:CD2	1:D:711:GLU:CG	2.96	0.44
1:D:933:LEU:HB3	1:D:934:PRO:HD2	2.00	0.44
1:E:703:LEU:N	1:E:703:LEU:HD23	2.33	0.44
1:F:747:LEU:CG	1:F:788:LEU:HD11	2.43	0.44
1:A:835:HIS:CE1	1:A:837:ASP:O	2.70	0.44
1:D:782:LEU:O	1:D:783:THR:OG1	2.35	0.44
1:E:774:VAL:HG11	1:E:828:LEU:HD21	2.00	0.44
1:E:780:ILE:O	1:E:780:ILE:CG2	2.63	0.44
1:G:889:ARG:NH1	1:G:889:ARG:HG3	2.31	0.44
1:H:741:PRO:C	1:H:742:VAL:HG13	2.37	0.44
1:C:715:ILE:HD11	1:C:728:LYS:CD	2.48	0.44
1:C:799:LEU:O	1:C:802:VAL:CG2	2.66	0.44
1:C:806:LYS:HB2	1:C:806:LYS:HE2	1.38	0.44
1:B:967:GLU:O	1:B:971:MET:HG3	2.18	0.43
1:D:729:GLY:HA3	1:D:744:ILE:HD12	2.00	0.43
1:D:799:LEU:O	1:D:802:VAL:CG2	2.65	0.43
1:D:879:LYS:H	1:D:879:LYS:HG2	1.56	0.43
1:D:893:HIS:O	1:D:896:ASP:HB2	2.19	0.43
1:D:942:ASP:OD1	1:D:942:ASP:N	2.40	0.43
1:F:708:LYS:CA	1:F:711:GLU:HG3	2.47	0.43
1:F:908:MET:HE3	1:F:979:LEU:HD21	2.00	0.43
1:B:760:LEU:HD12	1:B:760:LEU:HA	1.84	0.43
1:B:802:VAL:HG11	1:B:907:LEU:CD2	2.46	0.43
1:B:813:TYR:HE1	1:B:988:HIS:O	2.01	0.43
1:B:982:GLN:H	1:B:982:GLN:CD	2.13	0.43
1:E:908:MET:O	1:E:938:ILE:CG2	2.66	0.43
1:G:798:LEU:HD12	1:G:798:LEU:C	2.39	0.43
1:G:944:TYR:O	1:G:947:MET:N	2.51	0.43
1:H:938:ILE:HA	1:H:980:VAL:O	2.18	0.43
1:H:945:MET:HE1	3:H:1103:EDO:O2	2.18	0.43
1:H:945:MET:HE3	3:H:1104:EDO:H22	1.99	0.43
1:A:735:GLY:N	4:A:1203:HOH:O	2.52	0.43
1:A:783:THR:CG2	1:A:784:SER:N	2.73	0.43
1:A:811:SER:HB3	1:A:984:ASP:CG	2.38	0.43
1:A:843:VAL:C	1:A:844:LEU:HD23	2.38	0.43
1:B:904:VAL:O	1:B:908:MET:HG2	2.18	0.43
1:B:926:ILE:O	1:B:929:LYS:HB2	2.18	0.43
1:D:830:ASP:O	1:G:725:THR:HG23	2.18	0.43
1:D:966:ILE:O	1:D:970:LYS:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:707:LEU:HD22	1:F:712:PHE:HD1	1.83	0.43
1:F:878:ILE:CG2	1:F:923:ILE:HG21	2.48	0.43
1:A:958:ARG:HA	1:A:959:PRO:HD3	1.86	0.43
1:B:708:LYS:HB2	1:B:711:GLU:HG2	1.99	0.43
1:B:977:ARG:NE	1:D:931:GLU:HB2	2.33	0.43
1:D:774:VAL:HG11	1:D:828:LEU:HD21	1.99	0.43
1:D:898:TRP:CZ2	1:D:927:LEU:HD13	2.54	0.43
1:E:844:LEU:HD23	1:E:854:THR:CG2	2.47	0.43
1:E:893:HIS:O	1:E:896:ASP:HB2	2.19	0.43
1:F:799:LEU:O	1:F:802:VAL:HG22	2.17	0.43
1:F:813:TYR:OH	1:F:849:GLN:NE2	2.51	0.43
1:G:790:MET:CE	1:G:791:GLN:O	2.67	0.43
1:G:823:LYS:CA	1:G:965:ILE:HD11	2.45	0.43
1:B:705:ARG:HG2	1:B:707:LEU:CD2	2.48	0.43
1:B:940:THR:CG2	1:B:978:TYR:O	2.66	0.43
1:D:992:PRO:HD2	1:D:993:THR:H	1.84	0.43
1:D:999:ARG:O	1:D:1003:ASP:C	2.57	0.43
1:F:897:VAL:CG2	4:F:1228:HOH:O	2.62	0.43
1:G:985:GLU:CG	1:G:986:ARG:N	2.81	0.43
1:H:976:GLN:HG2	1:H:984:ASP:OD2	2.19	0.43
1:C:925:SER:O	1:C:929:LYS:N	2.46	0.43
1:A:731:TRP:CE3	1:A:740:ILE:HD13	2.54	0.43
1:B:730:LEU:HB3	1:B:739:LYS:HB3	2.00	0.43
1:E:913:LYS:NZ	4:E:1203:HOH:O	2.52	0.43
1:F:898:TRP:HZ2	1:F:927:LEU:HD13	1.83	0.43
1:F:973:ARG:O	1:F:1013:ALA:HA	2.19	0.43
1:H:766:MET:CE	1:H:777:LEU:HD22	2.47	0.43
1:C:745:LYS:O	1:C:788:LEU:HD12	2.17	0.43
1:C:897:VAL:HG21	1:C:959:PRO:O	2.18	0.43
1:A:893:HIS:HA	1:A:896:ASP:HB2	2.01	0.43
1:A:1013:ALA:O	1:A:1014:ASP:C	2.56	0.43
1:B:760:LEU:HD13	1:B:782:LEU:CD2	2.48	0.43
1:B:790:MET:HE1	1:B:844:LEU:CD1	2.49	0.43
1:B:941:ILE:HG23	1:B:942:ASP:N	2.33	0.43
1:D:703:LEU:C	1:D:776:ARG:HH12	2.18	0.43
1:E:950:CYS:O	1:E:958:ARG:HG2	2.18	0.43
1:F:926:ILE:HA	1:F:929:LYS:HB2	2.01	0.43
1:F:977:ARG:HH21	1:F:977:ARG:CG	2.31	0.43
1:G:952:MET:HE2	1:G:957:SER:CB	2.49	0.43
1:C:881:MET:CE	1:C:886:ILE:CG1	2.91	0.43
1:A:805:HIS:HB3	1:A:809:ILE:CG1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:TYR:CE1	1:B:988:HIS:O	2.72	0.43
1:B:846:LYS:C	1:B:847:THR:CG2	2.87	0.43
1:B:939:CYS:SG	1:B:943:VAL:CG1	3.07	0.43
1:E:771:ASN:OD1	1:E:772:PRO:HD2	2.19	0.43
1:G:977:ARG:NH2	1:G:978:TYR:CE1	2.86	0.43
1:G:991:SER:HB2	1:G:994:ASP:OD2	2.18	0.43
1:H:745:LYS:HB2	1:H:745:LYS:HE3	1.49	0.43
1:B:831:ARG:HB3	1:B:833:LEU:HD12	1.99	0.43
1:F:972:ALA:CB	1:F:1011:VAL:HG11	2.43	0.43
1:F:1007:MET:CG	1:F:1008:ASP:O	2.64	0.43
1:G:952:MET:HE2	1:G:957:SER:HB3	2.01	0.43
1:H:782:LEU:C	1:H:783:THR:HG23	2.39	0.43
1:H:943:VAL:HG12	1:H:947:MET:HE3	2.01	0.43
1:A:885:SER:HA	1:A:890:ILE:H	1.84	0.43
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.54	0.43
1:F:884:GLU:O	1:F:888:HIS:N	2.32	0.43
1:G:821:ILE:CG2	1:G:900:TYR:CE1	3.02	0.43
1:H:714:LYS:HZ1	1:H:787:GLN:HE22	1.65	0.43
1:H:768:SER:OG	1:H:831:ARG:NH2	2.52	0.43
1:C:790:MET:HE2	1:C:791:GLN:O	2.18	0.43
1:C:846:LYS:HG3	1:C:847:THR:HG23	2.01	0.43
1:C:940:THR:HG22	1:C:943:VAL:CG2	2.38	0.43
1:A:846:LYS:HD3	1:A:852:LYS:CD	2.49	0.42
1:D:885:SER:O	1:D:889:ARG:HA	2.18	0.42
1:D:902:VAL:O	1:D:905:TRP:HB3	2.19	0.42
1:F:771:ASN:HD21	1:F:772:PRO:HD2	1.73	0.42
1:G:776:ARG:NH1	1:G:776:ARG:HG2	2.35	0.42
1:G:971:MET:O	1:G:974:ASP:N	2.51	0.42
1:H:729:GLY:C	1:H:730:LEU:HD23	2.40	0.42
1:H:935:GLN:HA	1:H:936:PRO:HD3	1.74	0.42
1:B:856:PHE:O	1:B:856:PHE:CG	2.72	0.42
1:B:945:MET:CE	1:D:909:THR:CG2	2.91	0.42
1:D:777:LEU:HD11	1:D:788:LEU:CB	2.50	0.42
1:E:772:PRO:O	1:E:852:LYS:HG2	2.18	0.42
1:E:884:GLU:OE2	1:E:895:SER:OG	2.33	0.42
1:E:913:LYS:O	1:E:916:ASP:HB2	2.18	0.42
1:E:941:ILE:HG23	1:E:945:MET:CE	2.49	0.42
1:F:1006:ASP:OD2	1:F:1006:ASP:N	2.52	0.42
1:H:743:ALA:CB	2:H:1101:816:N1	2.83	0.42
1:H:878:ILE:HG22	1:H:923:ILE:HG13	2.01	0.42
1:C:795:PHE:CE2	1:C:1002:MET:CE	3.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:984:ASP:OD2	1:C:984:ASP:O	2.37	0.42
1:C:991:SER:HB2	1:C:992:PRO:CD	2.50	0.42
1:A:974:ASP:OD2	1:E:929:LYS:HE2	2.19	0.42
1:B:889:ARG:HD2	1:B:889:ARG:HA	1.83	0.42
1:D:821:ILE:HG22	1:D:900:TYR:HE1	1.84	0.42
1:D:950:CYS:O	1:D:958:ARG:CG	2.67	0.42
1:D:1008:ASP:OD1	1:D:1009:ASP:N	2.51	0.42
1:E:793:MET:CE	1:E:844:LEU:HD12	2.49	0.42
1:E:814:LEU:HD11	1:E:910:PHE:HE1	1.84	0.42
1:E:818:CYS:SG	1:E:904:VAL:CG2	3.05	0.42
1:F:1008:ASP:OD2	1:F:1008:ASP:C	2.58	0.42
1:G:772:PRO:HB2	1:G:773:HIS:CD2	2.54	0.42
1:H:757:LYS:O	1:H:757:LYS:HD3	2.20	0.42
1:H:903:THR:O	1:H:906:GLU:HB2	2.19	0.42
1:C:1007:MET:CG	1:C:1008:ASP:N	2.68	0.42
1:A:707:LEU:HB3	1:A:712:PHE:HE1	1.85	0.42
1:A:878:ILE:CD1	1:A:920:ALA:HB1	2.49	0.42
1:D:732:ILE:HA	1:D:733:PRO:HD2	1.92	0.42
1:D:845:VAL:HG13	1:D:847:THR:O	2.19	0.42
1:E:712:PHE:CE2	1:E:744:ILE:HG13	2.54	0.42
1:F:813:TYR:HE1	1:F:989:LEU:HA	1.83	0.42
1:G:726:VAL:HG22	1:G:745:LYS:HG3	2.01	0.42
1:G:889:ARG:HA	1:G:889:ARG:HD2	1.53	0.42
1:C:855:ASP:H	2:C:1101:816:CAH	2.33	0.42
1:D:714:LYS:HB3	1:D:744:ILE:HD13	2.00	0.42
1:D:901:GLY:O	1:D:905:TRP:N	2.47	0.42
1:D:941:ILE:HG13	1:D:945:MET:HG3	2.01	0.42
1:E:730:LEU:HD23	1:E:730:LEU:HA	1.61	0.42
1:E:795:PHE:H	1:E:795:PHE:HD2	1.66	0.42
1:F:805:HIS:O	1:F:809:ILE:CG1	2.67	0.42
1:F:977:ARG:HH21	1:G:926:ILE:HD12	1.85	0.42
1:F:999:ARG:HB3	1:F:1003:ASP:HB3	2.01	0.42
1:G:938:ILE:HB	1:G:980:VAL:O	2.20	0.42
1:H:704:LEU:HB3	1:H:764:TYR:CE1	2.54	0.42
1:A:738:VAL:HG22	1:A:739:LYS:N	2.35	0.42
1:A:922:GLU:OE2	1:A:926:ILE:HG22	2.18	0.42
1:A:933:LEU:HA	1:A:934:PRO:HD3	1.79	0.42
1:B:884:GLU:OE1	1:B:958:ARG:NH1	2.41	0.42
1:B:890:ILE:O	1:B:890:ILE:HG22	2.19	0.42
1:D:757:LYS:HD3	1:D:761:ASP:OD1	2.18	0.42
1:D:877:PRO:HB2	1:D:880:TRP:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:941:ILE:CG1	1:D:945:MET:HE3	2.49	0.42
1:E:806:LYS:O	1:E:910:PHE:CE2	2.73	0.42
1:H:716:LYS:HG2	1:H:717:VAL:N	2.34	0.42
1:H:845:VAL:HG12	1:H:847:THR:C	2.36	0.42
1:C:707:LEU:HD11	1:C:789:ILE:CD1	2.35	0.42
1:A:946:ILE:CD1	1:A:971:MET:HE3	2.39	0.42
1:B:733:PRO:HB2	1:B:736:GLU:CB	2.46	0.42
1:E:819:VAL:CG2	1:E:968:PHE:HB3	2.50	0.42
1:F:778:LEU:HD22	1:F:778:LEU:H	1.84	0.42
1:G:773:HIS:CE1	1:G:820:GLN:CG	3.03	0.42
1:H:935:GLN:CD	1:H:944:TYR:CD2	2.91	0.42
1:C:758:GLU:OE2	1:C:759:ILE:HA	2.19	0.42
1:C:884:GLU:HG2	1:C:885:SER:N	2.34	0.42
1:A:821:ILE:O	1:A:825:MET:HG2	2.19	0.42
1:B:898:TRP:CZ3	1:B:951:TRP:O	2.73	0.42
1:B:966:ILE:CG2	1:B:970:LYS:HE3	2.49	0.42
1:D:894:GLN:HA	1:D:897:VAL:HG23	2.02	0.42
1:D:950:CYS:O	1:D:958:ARG:HG2	2.20	0.42
1:E:806:LYS:CG	1:E:807:ASP:N	2.83	0.42
1:E:835:HIS:NE2	1:E:856:PHE:HA	2.35	0.42
1:G:712:PHE:CZ	1:G:781:CYS:SG	3.13	0.42
1:H:729:GLY:O	1:H:730:LEU:HD23	2.18	0.42
1:H:741:PRO:C	1:H:742:VAL:CG1	2.88	0.42
1:C:849:GLN:N	1:C:849:GLN:CD	2.72	0.42
1:C:973:ARG:O	1:C:1013:ALA:CA	2.66	0.42
1:A:782:LEU:O	1:A:783:THR:OG1	2.35	0.42
1:B:829:GLU:HG3	1:B:893:HIS:CG	2.55	0.42
1:F:769:VAL:HB	1:F:827:TYR:HE2	1.85	0.42
1:F:776:ARG:O	2:F:1101:816:CAA	2.68	0.42
1:G:831:ARG:NH2	4:G:1206:HOH:O	2.52	0.42
1:G:876:VAL:HG11	1:G:889:ARG:HH21	1.85	0.42
1:H:732:ILE:HA	1:H:733:PRO:HD3	1.84	0.42
1:A:900:TYR:CD2	1:A:900:TYR:C	2.93	0.42
1:B:813:TYR:CE1	1:B:990:PRO:HD3	2.55	0.42
1:D:942:ASP:CG	1:F:934:PRO:HG3	2.40	0.42
1:D:989:LEU:CB	1:D:990:PRO:HD2	2.50	0.42
1:F:811:SER:HB3	1:F:984:ASP:CG	2.39	0.42
1:H:798:LEU:HD12	1:H:798:LEU:HA	1.75	0.42
1:H:856:PHE:O	1:H:856:PHE:CD1	2.73	0.42
1:C:733:PRO:HB2	1:C:736:GLU:HB2	2.01	0.42
2:C:1101:816:CAP	2:C:1101:816:CAV	2.98	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:GLU:OE2	1:A:926:ILE:HG21	2.20	0.41
1:B:790:MET:HG2	2:B:1101:816:CLA	2.57	0.41
1:B:923:ILE:O	1:B:926:ILE:HG12	2.19	0.41
1:E:904:VAL:HG12	1:E:905:TRP:N	2.33	0.41
1:E:913:LYS:HZ2	1:E:913:LYS:HG2	1.66	0.41
1:F:748:ARG:HG2	1:F:748:ARG:H	1.44	0.41
1:F:989:LEU:HD23	1:F:990:PRO:C	2.40	0.41
1:G:760:LEU:HD12	1:G:760:LEU:HA	1.73	0.41
1:G:1012:ASP:OD1	1:G:1013:ALA:N	2.53	0.41
1:H:793:MET:HA	1:H:794:PRO:HD3	1.89	0.41
1:H:918:ILE:HA	1:H:919:PRO:HD3	1.94	0.41
1:C:740:ILE:HA	1:C:741:PRO:HD3	1.86	0.41
1:A:769:VAL:HG21	1:A:856:PHE:HZ	1.85	0.41
1:A:858:LEU:HD13	1:A:858:LEU:HA	1.85	0.41
1:B:759:ILE:HD12	1:B:759:ILE:N	2.29	0.41
1:B:811:SER:OG	1:B:975:PRO:CB	2.66	0.41
1:D:812:GLN:HG2	1:D:975:PRO:HG3	2.00	0.41
1:D:923:ILE:O	1:D:926:ILE:CG1	2.63	0.41
1:E:723:PHE:CE2	1:E:859:ALA:CB	3.03	0.41
1:E:723:PHE:O	1:E:747:LEU:HD23	2.20	0.41
1:F:806:LYS:HB3	1:F:910:PHE:HB3	2.00	0.41
1:F:841:ARG:HH12	1:F:877:PRO:HB3	1.84	0.41
1:H:708:LYS:HG2	1:H:711:GLU:OE2	2.19	0.41
1:C:793:MET:HE2	1:C:844:LEU:HB2	2.01	0.41
1:C:838:LEU:HD12	1:C:839:ALA:N	2.34	0.41
1:A:815[B]:LEU:CD2	1:A:979:LEU:CD1	2.97	0.41
1:E:731:TRP:HB3	1:E:740:ILE:HB	2.01	0.41
1:G:822:ALA:HB3	1:G:965:ILE:HG12	2.02	0.41
1:H:841:ARG:CG	1:H:842:ASN:N	2.83	0.41
1:A:878:ILE:HD13	1:A:920:ALA:HB1	2.01	0.41
1:D:771:ASN:CB	1:D:774:VAL:HG23	2.16	0.41
1:D:931:GLU:H	1:D:931:GLU:HG2	1.45	0.41
1:D:944:TYR:O	1:D:948:VAL:HG23	2.20	0.41
1:G:1007:MET:CE	1:G:1010:VAL:CG1	2.96	0.41
1:H:809:ILE:O	1:H:987:MET:SD	2.79	0.41
1:H:831:ARG:HB3	1:H:833:LEU:HD12	2.00	0.41
1:C:850:HIS:HD2	1:C:851:VAL:N	2.18	0.41
1:A:898:TRP:HZ2	1:A:927:LEU:HD13	1.79	0.41
1:B:815:LEU:O	1:B:819:VAL:CG2	2.66	0.41
1:F:839:ALA:HB3	1:F:841:ARG:HG2	2.02	0.41
1:F:923:ILE:O	1:F:926:ILE:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:PHE:HD1	1:C:857:GLY:CA	2.27	0.41
1:A:818:CYS:SG	1:A:904:VAL:HG13	2.61	0.41
1:B:955:ALA:HA	1:B:958:ARG:NH1	2.36	0.41
1:G:852:LYS:HE3	1:G:852:LYS:HB3	1.84	0.41
1:G:883:LEU:CD2	1:G:953:ILE:HD12	2.50	0.41
1:H:900:TYR:O	1:H:904:VAL:HG23	2.20	0.41
1:C:775:CYS:N	1:C:853:ILE:O	2.51	0.41
1:C:997:PHE:O	1:C:1001:LEU:HD12	2.20	0.41
1:A:700:ASN:CA	1:A:703:LEU:HD12	2.48	0.41
1:A:888:HIS:O	1:D:888:HIS:CB	2.68	0.41
1:B:705:ARG:HD3	1:B:707:LEU:CD2	2.44	0.41
1:E:712:PHE:HE2	1:E:744:ILE:HG13	1.85	0.41
1:E:718:LEU:HB2	1:E:727:TYR:HA	2.02	0.41
1:F:835:HIS:CD2	1:F:856:PHE:CB	3.02	0.41
1:C:892:THR:H	1:C:895:SER:HB3	1.85	0.41
1:C:966:ILE:HG22	1:C:967:GLU:N	2.34	0.41
1:A:835:HIS:ND1	1:A:835:HIS:C	2.74	0.41
1:A:982:GLN:OE1	1:A:982:GLN:CA	2.69	0.41
1:B:767:ALA:O	1:B:776:ARG:CG	2.69	0.41
1:B:775:CYS:HB2	1:B:853:ILE:O	2.21	0.41
1:B:777:LEU:HD21	1:B:788:LEU:CD2	2.41	0.41
1:E:705:ARG:O	1:E:779:GLY:HA2	2.20	0.41
1:E:723:PHE:HE2	1:E:859:ALA:CB	2.33	0.41
1:H:771:ASN:HA	1:H:772:PRO:HD3	1.95	0.41
1:C:880:TRP:CZ2	1:C:906:GLU:OE2	2.74	0.41
1:B:801:TYR:CE1	1:B:805:HIS:CE1	3.09	0.41
1:B:835:HIS:CB	1:B:856:PHE:HA	2.42	0.41
1:B:961:PHE:O	1:B:965:ILE:N	2.45	0.41
1:D:793:MET:HA	1:D:794:PRO:HD2	1.97	0.41
1:D:827:TYR:O	1:D:830:ASP:HB2	2.21	0.41
1:E:723:PHE:N	1:E:723:PHE:CD1	2.89	0.41
1:F:762:GLU:H	1:F:762:GLU:HG2	1.59	0.41
1:G:802:VAL:HG12	1:G:809:ILE:HD12	2.03	0.41
1:G:908:MET:HG3	1:G:939:CYS:SG	2.61	0.41
1:H:762:GLU:HG2	1:H:861:LEU:CD2	2.51	0.41
1:C:716:LYS:HG3	1:C:717:VAL:H	1.80	0.41
1:C:835:HIS:HE2	1:C:856:PHE:N	2.18	0.41
1:C:972:ALA:C	1:C:975:PRO:HD3	2.37	0.41
1:A:778:LEU:HG	1:A:790:MET:HA	2.03	0.41
1:A:813:TYR:OH	1:A:990:PRO:CD	2.68	0.41
1:A:976:GLN:H	1:A:976:GLN:HG2	1.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:717:VAL:HG13	1:E:727:TYR:CE2	2.55	0.41
1:F:884:GLU:HG2	1:F:885:SER:H	1.82	0.41
1:F:935:GLN:HB3	1:F:944:TYR:CE2	2.56	0.41
1:G:960:LYS:HA	4:G:1203:HOH:O	2.19	0.41
1:H:905:TRP:CZ2	1:H:933:LEU:HD22	2.56	0.41
1:D:961:PHE:O	1:D:964:LEU:N	2.54	0.40
1:E:898:TRP:CH2	1:E:927:LEU:HD22	2.56	0.40
1:H:744:ILE:HA	1:H:788:LEU:O	2.20	0.40
1:C:736:GLU:OE2	1:C:736:GLU:CA	2.54	0.40
1:A:811:SER:OG	1:A:975:PRO:CB	2.68	0.40
1:B:782:LEU:HA	1:B:782:LEU:HD13	1.75	0.40
1:B:820:GLN:NE2	1:B:849:GLN:O	2.50	0.40
1:G:898:TRP:CZ3	1:G:952:MET:O	2.75	0.40
1:H:783:THR:OG1	1:H:785:THR:O	2.37	0.40
1:H:791:GLN:HG3	1:H:792:LEU:N	2.36	0.40
1:H:859:ALA:O	1:H:862:LEU:C	2.59	0.40
1:C:703:LEU:HD13	1:C:768:SER:HA	2.03	0.40
1:C:827:TYR:OH	1:C:831:ARG:HD2	2.22	0.40
1:C:879:LYS:NZ	1:C:918:ILE:O	2.43	0.40
1:A:898:TRP:HZ2	1:A:927:LEU:CD1	2.34	0.40
1:B:938:ILE:HG22	1:B:979:LEU:HB3	2.03	0.40
1:B:952:MET:O	1:B:958:ARG:CZ	2.70	0.40
1:D:707:LEU:HD23	1:D:711:GLU:CD	2.42	0.40
1:D:812:GLN:CG	1:D:975:PRO:HG2	2.51	0.40
1:D:814:LEU:HD11	1:D:910:PHE:HE1	1.87	0.40
1:D:836:ARG:HG2	1:D:891:TYR:CD1	2.56	0.40
1:E:729:GLY:N	1:E:742:VAL:O	2.52	0.40
1:F:744:ILE:HG23	1:F:789:ILE:HG13	2.04	0.40
1:H:811:SER:N	1:H:981:ILE:HD12	2.37	0.40
1:H:890:ILE:O	1:H:890:ILE:HG22	2.17	0.40
1:C:987:MET:HG3	1:C:987:MET:O	2.22	0.40
1:A:790:MET:HG3	1:A:791:GLN:O	2.21	0.40
1:A:815[B]:LEU:CD1	1:A:979:LEU:HD11	2.51	0.40
1:B:905:TRP:CZ3	1:B:914:PRO:HA	2.57	0.40
1:G:799:LEU:HD13	1:G:840:ALA:HB3	2.03	0.40
1:G:953:ILE:HB	4:G:1207:HOH:O	2.21	0.40
1:G:971:MET:O	1:G:974:ASP:C	2.59	0.40
1:H:758:GLU:O	1:H:758:GLU:OE1	2.38	0.40
1:C:758:GLU:OE2	1:C:759:ILE:CA	2.69	0.40
1:C:1007:MET:HG2	1:C:1008:ASP:C	2.40	0.40
1:A:709:GLU:H	1:A:709:GLU:HG2	1.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:MET:HE3	1:A:844:LEU:CB	2.52	0.40
1:A:841:ARG:HH21	1:A:841:ARG:CG	2.02	0.40
1:B:1002:MET:HE2	1:B:1002:MET:HB2	1.85	0.40
1:E:885:SER:O	1:E:889:ARG:CA	2.69	0.40
1:F:979:LEU:HD23	1:F:979:LEU:HA	1.89	0.40
1:G:730:LEU:HD13	1:G:739:LYS:CB	2.32	0.40
1:G:757:LYS:C	1:G:757:LYS:HD2	2.41	0.40
1:G:773:HIS:O	1:G:852:LYS:HA	2.22	0.40
1:G:792:LEU:HA	2:G:1101:816:N1	2.37	0.40
1:H:708:LYS:HG3	1:H:711:GLU:CD	2.42	0.40
1:H:777:LEU:N	2:H:1101:816:CAA	2.85	0.40
1:H:968:PHE:HA	1:H:971:MET:HG3	2.04	0.40
1:C:977:ARG:CD	1:C:977:ARG:O	2.70	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	296/331 (89%)	290 (98%)	6 (2%)	0	100	100
1	B	293/331 (88%)	286 (98%)	7 (2%)	0	100	100
1	C	289/331 (87%)	285 (99%)	4 (1%)	0	100	100
1	D	291/331 (88%)	282 (97%)	9 (3%)	0	100	100
1	E	291/331 (88%)	286 (98%)	5 (2%)	0	100	100
1	F	291/331 (88%)	287 (99%)	4 (1%)	0	100	100
1	G	294/331 (89%)	291 (99%)	3 (1%)	0	100	100
1	H	292/331 (88%)	286 (98%)	6 (2%)	0	100	100
All	All	2337/2648 (88%)	2293 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	254/288 (88%)	191 (75%)	63 (25%)	0	2
1	B	246/288 (85%)	184 (75%)	62 (25%)	0	2
1	C	248/288 (86%)	166 (67%)	82 (33%)	0	0
1	D	234/288 (81%)	170 (73%)	64 (27%)	0	1
1	E	236/288 (82%)	175 (74%)	61 (26%)	0	1
1	F	245/288 (85%)	171 (70%)	74 (30%)	0	1
1	G	256/288 (89%)	196 (77%)	60 (23%)	1	3
1	H	252/288 (88%)	184 (73%)	68 (27%)	0	1
All	All	1971/2304 (86%)	1437 (73%)	534 (27%)	0	1

All (534) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	709	GLU
1	A	711	GLU
1	A	714	LYS
1	A	725	THR
1	A	732	ILE
1	A	739	LYS
1	A	745	LYS
1	A	746	GLU
1	A	757	LYS
1	A	758	GLU
1	A	762	GLU
1	A	765	VAL
1	A	769	VAL
1	A	780	ILE
1	A	788	LEU
1	A	789	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	790	MET
1	A	792	LEU
1	A	793	MET
1	A	797	CYS
1	A	798	LEU
1	A	802	VAL
1	A	806	LYS
1	A	807	ASP
1	A	808	ASN
1	A	809	ILE
1	A	811	SER
1	A	812	GLN
1	A	832	ARG
1	A	841	ARG
1	A	846	LYS
1	A	849	GLN
1	A	854	THR
1	A	855	ASP
1	A	858	LEU
1	A	889	ARG
1	A	896	ASP
1	A	913	LYS
1	A	921	SER
1	A	922	GLU
1	A	925	SER
1	A	928	GLU
1	A	935	GLN
1	A	938	ILE
1	A	939	CYS
1	A	940	THR
1	A	957	SER
1	A	967[A]	GLU
1	A	967[B]	GLU
1	A	973	ARG
1	A	976	GLN
1	A	980	VAL
1	A	982	GLN
1	A	987	MET
1	A	991	SER
1	A	994	ASP
1	A	1001	LEU
1	A	1002	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1006	ASP
1	A	1009	ASP
1	A	1010	VAL
1	A	1011	VAL
1	A	1012	ASP
1	B	701	GLN
1	B	709	GLU
1	B	711	GLU
1	B	713	LYS
1	B	734	GLU
1	B	737	LYS
1	B	758	GLU
1	B	760	LEU
1	B	762	GLU
1	B	768	SER
1	B	769	VAL
1	B	780	ILE
1	B	782	LEU
1	B	790	MET
1	B	792	LEU
1	B	793	MET
1	B	797	CYS
1	B	807	ASP
1	B	808	ASN
1	B	809	ILE
1	B	811	SER
1	B	831	ARG
1	B	832	ARG
1	B	833	LEU
1	B	835	HIS
1	B	836	ARG
1	B	841	ARG
1	B	843	VAL
1	B	846	LYS
1	B	847	THR
1	B	849	GLN
1	B	858	LEU
1	B	861	LEU
1	B	878	ILE
1	B	884	GLU
1	B	889	ARG
1	B	890	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	896	ASP
1	B	904	VAL
1	B	921	SER
1	B	923	ILE
1	B	925	SER
1	B	935	GLN
1	B	939	CYS
1	B	941	ILE
1	B	948	VAL
1	B	950	CYS
1	B	957	SER
1	B	971	MET
1	B	977	ARG
1	B	980	VAL
1	B	982	GLN
1	B	985	GLU
1	B	987	MET
1	B	991	SER
1	B	993	THR
1	B	997	PHE
1	B	1001	LEU
1	B	1002	MET
1	B	1004	GLU
1	B	1006	ASP
1	B	1012	ASP
1	D	703	LEU
1	D	705	ARG
1	D	706	ILE
1	D	708	LYS
1	D	713	LYS
1	D	714	LYS
1	D	715	ILE
1	D	728	LYS
1	D	732	ILE
1	D	738	VAL
1	D	742	VAL
1	D	757	LYS
1	D	765	VAL
1	D	774	VAL
1	D	780	ILE
1	D	785	THR
1	D	787	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	788	LEU
1	D	793	MET
1	D	797	CYS
1	D	802	VAL
1	D	803	ARG
1	D	804	GLU
1	D	806	LYS
1	D	811	SER
1	D	812	GLN
1	D	829	GLU
1	D	836	ARG
1	D	841	ARG
1	D	847	THR
1	D	858	LEU
1	D	876	VAL
1	D	879	LYS
1	D	885	SER
1	D	890	ILE
1	D	892	THR
1	D	895	SER
1	D	897	VAL
1	D	909	THR
1	D	913	LYS
1	D	921	SER
1	D	924	SER
1	D	925	SER
1	D	931	GLU
1	D	932	ARG
1	D	935	GLN
1	D	938	ILE
1	D	939	CYS
1	D	941	ILE
1	D	942	ASP
1	D	949	LYS
1	D	951	TRP
1	D	952	MET
1	D	957	SER
1	D	969	SER
1	D	973	ARG
1	D	974	ASP
1	D	979	LEU
1	D	986	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	987	MET
1	D	993	THR
1	D	994	ASP
1	D	995	SER
1	D	1002	MET
1	E	703	LEU
1	E	706	ILE
1	E	710	THR
1	E	711	GLU
1	E	714	LYS
1	E	717	VAL
1	E	718	LEU
1	E	725	THR
1	E	730	LEU
1	E	732	ILE
1	E	738	VAL
1	E	739	LYS
1	E	742	VAL
1	E	744	ILE
1	E	745	LYS
1	E	746	GLU
1	E	759	ILE
1	E	761	ASP
1	E	765	VAL
1	E	768	SER
1	E	769	VAL
1	E	774	VAL
1	E	780	ILE
1	E	782	LEU
1	E	789	ILE
1	E	797	CYS
1	E	804	GLU
1	E	806	LYS
1	E	808	ASN
1	E	809	ILE
1	E	811	SER
1	E	812	GLN
1	E	821	ILE
1	E	844	LEU
1	E	847	THR
1	E	851	VAL
1	E	853	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	856	PHE
1	E	861	LEU
1	E	876	VAL
1	E	884	GLU
1	E	892	THR
1	E	898	TRP
1	E	909	THR
1	E	913	LYS
1	E	921	SER
1	E	924	SER
1	E	925	SER
1	E	929	LYS
1	E	935	GLN
1	E	938	ILE
1	E	949	LYS
1	E	952	MET
1	E	956	ASP
1	E	957	SER
1	E	977	ARG
1	E	981	ILE
1	E	986	ARG
1	E	993	THR
1	E	998	TYR
1	E	1001	LEU
1	F	700	ASN
1	F	701	GLN
1	F	705	ARG
1	F	707	LEU
1	F	710	THR
1	F	714	LYS
1	F	716	LYS
1	F	725	THR
1	F	730	LEU
1	F	736	GLU
1	F	740	ILE
1	F	744	ILE
1	F	748	ARG
1	F	758	GLU
1	F	759	ILE
1	F	765	VAL
1	F	766	MET
1	F	770	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	777	LEU
1	F	780	ILE
1	F	781	CYS
1	F	782	LEU
1	F	786	VAL
1	F	791	GLN
1	F	792	LEU
1	F	797	CYS
1	F	807	ASP
1	F	808	ASN
1	F	811	SER
1	F	812	GLN
1	F	829	GLU
1	F	847	THR
1	F	849	GLN
1	F	851	VAL
1	F	853	ILE
1	F	856	PHE
1	F	858	LEU
1	F	861	LEU
1	F	876	VAL
1	F	879	LYS
1	F	889	ARG
1	F	890	ILE
1	F	892	THR
1	F	912	SER
1	F	913	LYS
1	F	918	ILE
1	F	923	ILE
1	F	924	SER
1	F	925	SER
1	F	926	ILE
1	F	929	LYS
1	F	931	GLU
1	F	938	ILE
1	F	943	VAL
1	F	945	MET
1	F	948	VAL
1	F	949	LYS
1	F	952	MET
1	F	953	ILE
1	F	958	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	963	GLU
1	F	967	GLU
1	F	970	LYS
1	F	977	ARG
1	F	987	MET
1	F	989	LEU
1	F	997	PHE
1	F	998	TYR
1	F	999	ARG
1	F	1002	MET
1	F	1003	ASP
1	F	1006	ASP
1	F	1007	MET
1	F	1010	VAL
1	G	703	LEU
1	G	705	ARG
1	G	706	ILE
1	G	707	LEU
1	G	710	THR
1	G	715	ILE
1	G	737	LYS
1	G	740	ILE
1	G	744	ILE
1	G	757	LYS
1	G	758	GLU
1	G	762	GLU
1	G	764	TYR
1	G	768	SER
1	G	769	VAL
1	G	792	LEU
1	G	793	MET
1	G	798	LEU
1	G	802	VAL
1	G	806	LYS
1	G	808	ASN
1	G	811	SER
1	G	825	MET
1	G	829	GLU
1	G	841	ARG
1	G	847	THR
1	G	851	VAL
1	G	852	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	855	ASP
1	G	876	VAL
1	G	879	LYS
1	G	889	ARG
1	G	890	ILE
1	G	895	SER
1	G	909	THR
1	G	913	LYS
1	G	918	ILE
1	G	921	SER
1	G	926	ILE
1	G	929	LYS
1	G	932	ARG
1	G	935	GLN
1	G	938	ILE
1	G	958	ARG
1	G	961	PHE
1	G	962	ARG
1	G	965	ILE
1	G	969	SER
1	G	973	ARG
1	G	977	ARG
1	G	989	LEU
1	G	995	SER
1	G	998	TYR
1	G	1002	MET
1	G	1004	GLU
1	G	1006	ASP
1	G	1007	MET
1	G	1008	ASP
1	G	1009	ASP
1	G	1014	ASP
1	H	701	GLN
1	H	705	ARG
1	H	707	LEU
1	H	710	THR
1	H	711	GLU
1	H	714	LYS
1	H	725	THR
1	H	737	LYS
1	H	738	VAL
1	H	739	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	740	ILE
1	H	745	LYS
1	H	757	LYS
1	H	758	GLU
1	H	760	LEU
1	H	762	GLU
1	H	764	TYR
1	H	765	VAL
1	H	766	MET
1	H	768	SER
1	H	776	ARG
1	H	778	LEU
1	H	780	ILE
1	H	782	LEU
1	H	784	SER
1	H	790	MET
1	H	797	CYS
1	H	802	VAL
1	H	803	ARG
1	H	806	LYS
1	H	808	ASN
1	H	821	ILE
1	H	832	ARG
1	H	851	VAL
1	H	861	LEU
1	H	862	LEU
1	H	876	VAL
1	H	879	LYS
1	H	899	SER
1	H	902	VAL
1	H	903	THR
1	H	912	SER
1	H	913	LYS
1	H	918	ILE
1	H	921	SER
1	H	924	SER
1	H	932	ARG
1	H	935	GLN
1	H	938	ILE
1	H	939	CYS
1	H	941	ILE
1	H	946	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	952	MET
1	H	953	ILE
1	H	961	PHE
1	H	965	ILE
1	H	971	MET
1	H	976	GLN
1	H	982	GLN
1	H	987	MET
1	H	995	SER
1	H	1002	MET
1	H	1005	GLU
1	H	1007	MET
1	H	1008	ASP
1	H	1009	ASP
1	H	1011	VAL
1	H	1015	GLU
1	C	700	ASN
1	C	701	GLN
1	C	704	LEU
1	C	706	ILE
1	C	707	LEU
1	C	713	LYS
1	C	714	LYS
1	C	717	VAL
1	C	718	LEU
1	C	720	SER
1	C	725	THR
1	C	730	LEU
1	C	744	ILE
1	C	746	GLU
1	C	748	ARG
1	C	758	GLU
1	C	759	ILE
1	C	762	GLU
1	C	765	VAL
1	C	769	VAL
1	C	770	ASP
1	C	778	LEU
1	C	780	ILE
1	C	784	SER
1	C	785	THR
1	C	788	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	790	MET
1	C	791	GLN
1	C	792	LEU
1	C	797	CYS
1	C	806	LYS
1	C	807	ASP
1	C	809	ILE
1	C	811	SER
1	C	812	GLN
1	C	828	LEU
1	C	829	GLU
1	C	831	ARG
1	C	832	ARG
1	C	833	LEU
1	C	838	LEU
1	C	841	ARG
1	C	846	LYS
1	C	847	THR
1	C	853	ILE
1	C	856	PHE
1	C	889	ARG
1	C	894	GLN
1	C	895	SER
1	C	902	VAL
1	C	908	MET
1	C	912	SER
1	C	913	LYS
1	C	918	ILE
1	C	921	SER
1	C	922	GLU
1	C	924	SER
1	C	925	SER
1	C	928	GLU
1	C	931	GLU
1	C	935	GLN
1	C	941	ILE
1	C	942	ASP
1	C	945	MET
1	C	949	LYS
1	C	950	CYS
1	C	953	ILE
1	C	958	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	962	ARG
1	C	963	GLU
1	C	966	ILE
1	C	970	LYS
1	C	973	ARG
1	C	977	ARG
1	C	982	GLN
1	C	986	ARG
1	C	998	TYR
1	C	1005	GLU
1	C	1006	ASP
1	C	1007	MET
1	C	1011	VAL
1	C	1012	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	771	ASN
1	B	849	GLN
1	B	893	HIS
1	B	894	GLN
1	B	982	GLN
1	D	773	HIS
1	D	805	HIS
1	D	808	ASN
1	D	850	HIS
1	E	935	GLN
1	F	771	ASN
1	F	835	HIS
1	G	849	GLN
1	H	701	GLN
1	H	787	GLN
1	H	976	GLN
1	C	787	GLN
1	C	808	ASN
1	C	835	HIS
1	C	888	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	H	1103	-	3,3,3	0.40	0	2,2,2	0.47	0
3	EDO	H	1102	-	3,3,3	0.33	0	2,2,2	0.50	0
2	816	B	1101	1	38,40,40	4.41	11 (28%)	46,57,57	2.32	10 (21%)
2	816	H	1101	1	38,40,40	4.37	11 (28%)	46,57,57	2.26	9 (19%)
2	816	D	1101	1	38,40,40	4.51	10 (26%)	46,57,57	2.18	7 (15%)
2	816	A	1101	1	38,40,40	4.29	11 (28%)	46,57,57	2.15	8 (17%)
3	EDO	G	1102	-	3,3,3	0.48	0	2,2,2	0.27	0
2	816	F	1101	1	38,40,40	3.63	10 (26%)	46,57,57	2.02	11 (23%)
2	816	G	1101	1	38,40,40	4.51	11 (28%)	46,57,57	2.30	10 (21%)
2	816	E	1101	1	38,40,40	4.03	11 (28%)	46,57,57	2.14	10 (21%)
2	816	C	1101	1	38,40,40	4.21	10 (26%)	46,57,57	2.19	10 (21%)
3	EDO	H	1104	-	3,3,3	0.55	0	2,2,2	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	H	1103	-	-	1/1/1/1	-
3	EDO	H	1102	-	-	1/1/1/1	-
2	816	B	1101	1	-	6/15/29/29	0/5/5/5
2	816	H	1101	1	-	5/15/29/29	0/5/5/5
2	816	D	1101	1	-	7/15/29/29	0/5/5/5
2	816	A	1101	1	-	6/15/29/29	0/5/5/5
3	EDO	G	1102	-	-	0/1/1/1	-
2	816	F	1101	1	-	7/15/29/29	0/5/5/5
2	816	G	1101	1	-	7/15/29/29	0/5/5/5
2	816	E	1101	1	-	5/15/29/29	0/5/5/5
2	816	C	1101	1	-	7/15/29/29	0/5/5/5
3	EDO	H	1104	-	-	1/1/1/1	-

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	816	NAZ-NBP	-21.51	1.11	1.37
2	D	1101	816	NAZ-NBP	-21.43	1.11	1.37
2	G	1101	816	NAZ-NBP	-20.65	1.12	1.37
2	H	1101	816	NAZ-NBP	-20.14	1.12	1.37
2	A	1101	816	NAZ-NBP	-19.87	1.13	1.37
2	C	1101	816	NAZ-NBP	-19.50	1.13	1.37
2	E	1101	816	NAZ-NBP	-18.53	1.14	1.37
2	F	1101	816	NAZ-NBP	-15.06	1.19	1.37
2	H	1101	816	CBH-CBJ	-12.30	1.32	1.49
2	D	1101	816	CBH-CBJ	-12.19	1.32	1.49
2	G	1101	816	CBH-CBJ	-11.93	1.32	1.49
2	C	1101	816	CBH-CBJ	-11.50	1.33	1.49
2	A	1101	816	CBH-CBJ	-11.36	1.33	1.49
2	B	1101	816	CBH-CBJ	-11.36	1.33	1.49
2	F	1101	816	CBH-CBJ	-11.04	1.33	1.49
2	E	1101	816	CBH-CBJ	-10.81	1.34	1.49
2	G	1101	816	CBF-CLA	-6.31	1.58	1.73
2	A	1101	816	CBF-CLA	-6.13	1.59	1.73
2	G	1101	816	CAA-CBD	-5.25	1.37	1.50
2	F	1101	816	CAA-CBD	-5.25	1.37	1.50
2	C	1101	816	CAA-CBD	-5.16	1.38	1.50
2	B	1101	816	CAA-CBD	-5.09	1.38	1.50
2	D	1101	816	CAA-CBD	-5.06	1.38	1.50
2	E	1101	816	CAA-CBD	-5.03	1.38	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	816	CAT-CBG	-5.01	1.38	1.50
2	G	1101	816	CAT-CBG	-5.00	1.38	1.50
2	A	1101	816	CAA-CBD	-4.98	1.38	1.50
2	H	1101	816	CAA-CBD	-4.97	1.38	1.50
2	E	1101	816	CAT-CBG	-4.93	1.38	1.50
2	C	1101	816	CBF-CLA	-4.91	1.62	1.73
2	D	1101	816	CAT-CBG	-4.84	1.38	1.50
2	F	1101	816	CAP-CAQ	4.66	1.53	1.30
2	H	1101	816	CAT-CBG	-4.61	1.39	1.50
2	F	1101	816	CAT-CBG	-4.61	1.39	1.50
2	H	1101	816	CBF-CLA	-4.58	1.62	1.73
2	C	1101	816	CAP-CAQ	4.55	1.52	1.30
2	D	1101	816	C2-N3	4.53	1.39	1.32
2	B	1101	816	CAP-CAQ	4.53	1.52	1.30
2	H	1101	816	CAP-CAQ	4.51	1.52	1.30
2	D	1101	816	CAP-CAQ	4.51	1.52	1.30
2	C	1101	816	CAT-CBG	-4.49	1.39	1.50
2	E	1101	816	CAP-CAQ	4.47	1.52	1.30
2	H	1101	816	C5-C4	-4.45	1.31	1.43
2	A	1101	816	CAP-CAQ	4.44	1.52	1.30
2	B	1101	816	CAT-CBG	-4.43	1.39	1.50
2	C	1101	816	C2-N3	4.40	1.39	1.32
2	G	1101	816	CAP-CAQ	4.36	1.51	1.30
2	G	1101	816	C2-N3	4.32	1.39	1.32
2	E	1101	816	C2-N3	4.31	1.39	1.32
2	D	1101	816	CBJ-NAZ	-4.28	1.31	1.35
2	G	1101	816	C5-C4	-4.24	1.31	1.43
2	A	1101	816	C5-C4	-4.22	1.31	1.43
2	H	1101	816	C2-N3	4.21	1.38	1.32
2	F	1101	816	C2-N3	4.20	1.38	1.32
2	B	1101	816	C2-N3	4.17	1.38	1.32
2	E	1101	816	CBF-CLA	-4.17	1.63	1.73
2	A	1101	816	C2-N3	4.16	1.38	1.32
2	B	1101	816	C5-C4	-4.14	1.32	1.43
2	F	1101	816	C5-C4	-4.14	1.32	1.43
2	C	1101	816	C5-C4	-4.07	1.32	1.43
2	F	1101	816	CBF-CLA	-4.06	1.64	1.73
2	D	1101	816	C5-C4	-4.05	1.32	1.43
2	G	1101	816	CBN-NBP	-3.98	1.43	1.49
2	D	1101	816	CBF-CLA	-3.97	1.64	1.73
2	E	1101	816	C5-C4	-3.87	1.32	1.43
2	G	1101	816	CBJ-NAZ	-3.45	1.32	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	816	CBJ-NAZ	-3.37	1.32	1.35
2	H	1101	816	CBJ-NAZ	-3.33	1.32	1.35
2	B	1101	816	CBJ-NAZ	-3.32	1.32	1.35
2	H	1101	816	CBN-NBP	-3.21	1.44	1.49
2	B	1101	816	CBF-CLA	-3.11	1.66	1.73
2	H	1101	816	C2-N1	3.07	1.39	1.33
2	G	1101	816	C2-N1	2.99	1.39	1.33
2	D	1101	816	C2-N1	2.95	1.39	1.33
2	A	1101	816	CBJ-NAZ	-2.91	1.32	1.35
2	E	1101	816	C2-N1	2.85	1.39	1.33
2	C	1101	816	C2-N1	2.78	1.39	1.33
2	F	1101	816	CBJ-NAZ	-2.65	1.33	1.35
2	A	1101	816	CBN-NBP	-2.60	1.45	1.49
2	F	1101	816	C2-N1	2.57	1.38	1.33
2	B	1101	816	C2-N1	2.54	1.38	1.33
2	E	1101	816	CBJ-NAZ	-2.47	1.33	1.35
2	E	1101	816	CBN-NBP	-2.47	1.45	1.49
2	B	1101	816	CBN-NBP	-2.43	1.45	1.49
2	A	1101	816	C2-N1	2.18	1.38	1.33

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1101	816	CAP-CAQ-CBC	-8.74	103.45	121.33
2	H	1101	816	CAP-CAQ-CBC	-7.97	105.02	121.33
2	B	1101	816	N3-C2-N1	-7.28	117.30	128.68
2	A	1101	816	N3-C2-N1	-7.21	117.41	128.68
2	F	1101	816	N3-C2-N1	-7.14	117.53	128.68
2	D	1101	816	CBJ-NAZ-NBP	7.05	110.80	105.17
2	G	1101	816	N3-C2-N1	-7.05	117.66	128.68
2	D	1101	816	N3-C2-N1	-6.95	117.81	128.68
2	C	1101	816	N3-C2-N1	-6.85	117.97	128.68
2	H	1101	816	N3-C2-N1	-6.80	118.06	128.68
2	B	1101	816	CBJ-NAZ-NBP	6.72	110.54	105.17
2	B	1101	816	CAP-CAQ-CBC	-6.65	107.73	121.33
2	D	1101	816	CAP-CAQ-CBC	-6.64	107.75	121.33
2	E	1101	816	N3-C2-N1	-6.59	118.38	128.68
2	C	1101	816	CAP-CAQ-CBC	-6.41	108.21	121.33
2	A	1101	816	CAP-CAQ-CBC	-6.41	108.21	121.33
2	E	1101	816	CAP-CAQ-CBC	-6.22	108.61	121.33
2	C	1101	816	CBJ-NAZ-NBP	6.08	110.03	105.17
2	E	1101	816	CBJ-NAZ-NBP	5.92	109.90	105.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	816	CBJ-NAZ-NBP	5.74	109.75	105.17
2	F	1101	816	CBJ-NAZ-NBP	5.38	109.47	105.17
2	H	1101	816	CAT-OBA-CBI	-5.32	107.30	117.76
2	G	1101	816	CBJ-NAZ-NBP	4.84	109.04	105.17
2	F	1101	816	CAP-CAQ-CBC	-4.75	111.61	121.33
2	H	1101	816	CBJ-NAZ-NBP	4.21	108.53	105.17
2	B	1101	816	CAT-OBA-CBI	-4.16	109.57	117.76
2	C	1101	816	CAT-OBA-CBI	-3.94	110.02	117.76
2	G	1101	816	CAT-OBA-CBI	-3.84	110.20	117.76
2	H	1101	816	CBN-CAV-NBO	-3.72	104.56	109.57
2	A	1101	816	CAT-OBA-CBI	-3.71	110.47	117.76
2	F	1101	816	CAT-OBA-CBI	-3.43	111.02	117.76
2	B	1101	816	CAO-CAS-NBO	-3.36	104.02	110.66
2	C	1101	816	CAS-NBO-CAV	3.36	119.78	113.06
2	F	1101	816	C5-C6-NAB	-3.30	116.71	122.67
2	D	1101	816	C5-C6-NAB	-3.30	116.71	122.67
2	D	1101	816	CBN-CAV-NBO	3.29	114.00	109.57
2	A	1101	816	C5-C6-NAB	-3.27	116.76	122.67
2	E	1101	816	C5-C6-NAB	-3.18	116.93	122.67
2	G	1101	816	C5-C6-NAB	-3.14	117.00	122.67
2	E	1101	816	CBI-CBF-CLA	-3.12	115.76	119.43
2	H	1101	816	C5-C6-NAB	-3.10	117.08	122.67
2	B	1101	816	C5-C6-NAB	-3.09	117.10	122.67
2	A	1101	816	CAQ-CBC-NBO	-2.99	114.20	117.66
2	G	1101	816	CAS-NBO-CAV	2.98	119.03	113.06
2	C	1101	816	C5-C6-NAB	-2.87	117.50	122.67
2	D	1101	816	CAS-NBO-CAV	2.77	118.61	113.06
2	A	1101	816	CAS-NBO-CAV	2.77	118.59	113.06
2	E	1101	816	CAN-CBF-CLA	2.75	122.94	118.49
2	D	1101	816	CAR-CAO-CAS	-2.73	107.03	110.85
2	H	1101	816	CAS-NBO-CAV	2.72	118.51	113.06
2	B	1101	816	CAK-CBG-NAY	-2.64	119.06	122.41
2	B	1101	816	CAT-CBG-NAY	2.57	120.93	115.71
2	F	1101	816	CAO-CAR-CBN	2.55	115.36	111.57
2	E	1101	816	CAO-CAS-NBO	-2.48	105.75	110.66
2	F	1101	816	CAN-CBF-CLA	2.44	122.43	118.49
2	A	1101	816	OAE-CBC-NBO	2.42	124.62	121.13
2	G	1101	816	CBI-CBF-CLA	-2.39	116.62	119.43
2	C	1101	816	CAQ-CBC-NBO	-2.37	114.92	117.66
2	F	1101	816	CAS-NBO-CAV	2.35	117.77	113.06
2	E	1101	816	CAS-NBO-CAV	2.35	117.76	113.06
2	G	1101	816	CAN-CBF-CLA	2.34	122.27	118.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	816	CAS-NBO-CAV	2.34	117.74	113.06
2	C	1101	816	CAT-CBG-NAY	2.30	120.37	115.71
2	E	1101	816	CAR-CAO-CAS	-2.29	107.65	110.85
2	H	1101	816	CAT-CBG-NAY	2.28	120.33	115.71
2	E	1101	816	CAT-OBA-CBI	-2.23	113.38	117.76
2	B	1101	816	CAO-CAR-CBN	2.21	114.85	111.57
2	F	1101	816	CBH-CBJ-NAZ	2.19	124.53	120.78
2	F	1101	816	CBI-CBF-CLA	-2.11	116.94	119.43
2	H	1101	816	CBH-CBJ-NAZ	2.11	124.39	120.78
2	G	1101	816	CBN-CAV-NBO	-2.08	106.76	109.57
2	C	1101	816	OAE-CBC-NBO	2.08	124.12	121.13
2	C	1101	816	CAN-CBF-CLA	2.07	121.83	118.49
2	F	1101	816	CAR-CBN-CAV	2.07	113.51	110.93
2	G	1101	816	CBJ-C5-C4	-2.00	102.79	106.55

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	816	CAL-CBH-CBJ-NAZ
2	B	1101	816	CAN-CBH-CBJ-NAZ
2	D	1101	816	CAL-CBH-CBJ-NAZ
2	D	1101	816	CAN-CBH-CBJ-NAZ
2	E	1101	816	CAP-CAQ-CBC-OAE
2	H	1101	816	CAL-CBH-CBJ-NAZ
2	H	1101	816	CAN-CBH-CBJ-NAZ
2	H	1101	816	CBG-CAT-OBA-CBI
2	F	1101	816	CBG-CAT-OBA-CBI
2	G	1101	816	CBG-CAT-OBA-CBI
2	E	1101	816	CAN-CBH-CBJ-NAZ
2	C	1101	816	CAN-CBH-CBJ-NAZ
2	A	1101	816	CAP-CAQ-CBC-OAE
2	C	1101	816	CAP-CAQ-CBC-OAE
2	E	1101	816	CAP-CAQ-CBC-NBO
2	C	1101	816	CAP-CAQ-CBC-NBO
2	B	1101	816	CBG-CAT-OBA-CBI
2	D	1101	816	CBG-CAT-OBA-CBI
2	C	1101	816	CBG-CAT-OBA-CBI
2	F	1101	816	CAN-CBH-CBJ-NAZ
2	C	1101	816	OBA-CAT-CBG-NAY
2	E	1101	816	CBG-CAT-OBA-CBI
2	E	1101	816	CAL-CBH-CBJ-NAZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	1101	816	CAL-CBH-CBJ-NAZ
2	C	1101	816	CAL-CBH-CBJ-NAZ
2	D	1101	816	CAP-CAQ-CBC-OAE
2	F	1101	816	CAP-CAQ-CBC-OAE
2	G	1101	816	CAP-CAQ-CBC-OAE
2	C	1101	816	OBA-CAT-CBG-CAK
2	G	1101	816	OBA-CAT-CBG-NAY
2	A	1101	816	CAP-CAQ-CBC-NBO
2	D	1101	816	CAP-CAQ-CBC-NBO
2	F	1101	816	CAP-CAQ-CBC-NBO
2	G	1101	816	CAP-CAQ-CBC-NBO
3	H	1103	EDO	O1-C1-C2-O2
2	A	1101	816	CAN-CBH-CBJ-NAZ
2	G	1101	816	OBA-CAT-CBG-CAK
2	B	1101	816	OBA-CAT-CBG-NAY
2	G	1101	816	CAN-CBH-CBJ-NAZ
2	A	1101	816	OBA-CAT-CBG-NAY
2	A	1101	816	OBA-CAT-CBG-CAK
2	F	1101	816	OBA-CAT-CBG-NAY
2	H	1101	816	OBA-CAT-CBG-NAY
2	B	1101	816	CAP-CAQ-CBC-OAE
3	H	1102	EDO	O1-C1-C2-O2
2	B	1101	816	OBA-CAT-CBG-CAK
2	H	1101	816	OBA-CAT-CBG-CAK
2	F	1101	816	OBA-CAT-CBG-CAK
2	A	1101	816	CAL-CBH-CBJ-NAZ
2	G	1101	816	CAL-CBH-CBJ-NAZ
3	H	1104	EDO	O1-C1-C2-O2
2	D	1101	816	OBA-CAT-CBG-NAY
2	D	1101	816	OBA-CAT-CBG-CAK

There are no ring outliers.

11 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1103	EDO	3	0
2	B	1101	816	6	0
2	H	1101	816	11	0
2	D	1101	816	11	0
2	A	1101	816	4	0
3	G	1102	EDO	2	0
2	F	1101	816	9	0

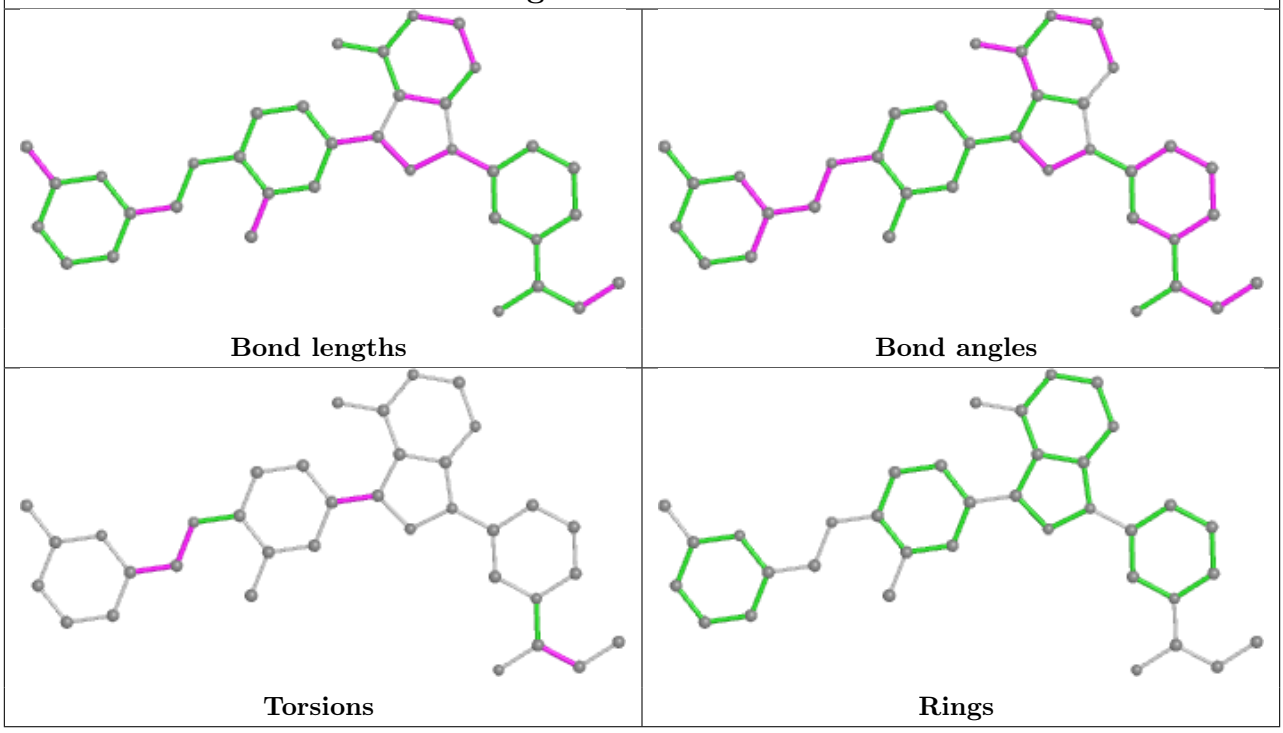
Continued on next page...

Continued from previous page...

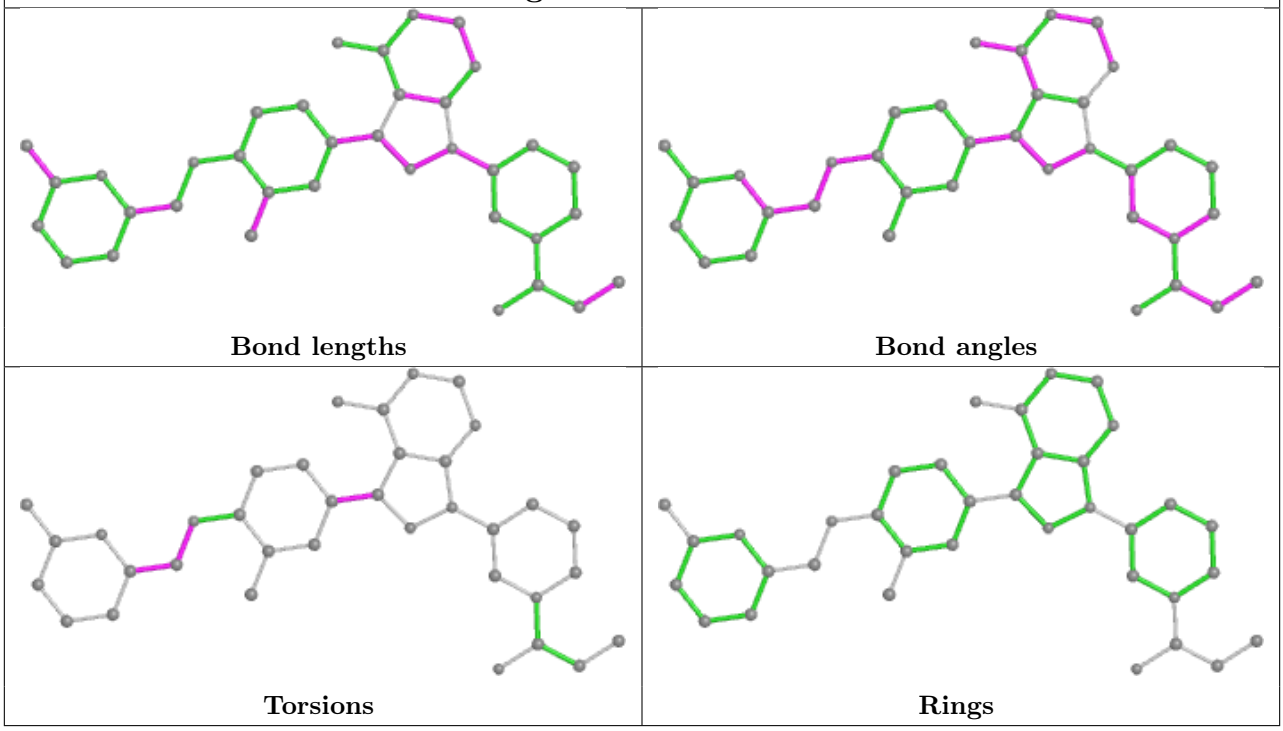
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1101	816	14	0
2	E	1101	816	8	0
2	C	1101	816	9	0
3	H	1104	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

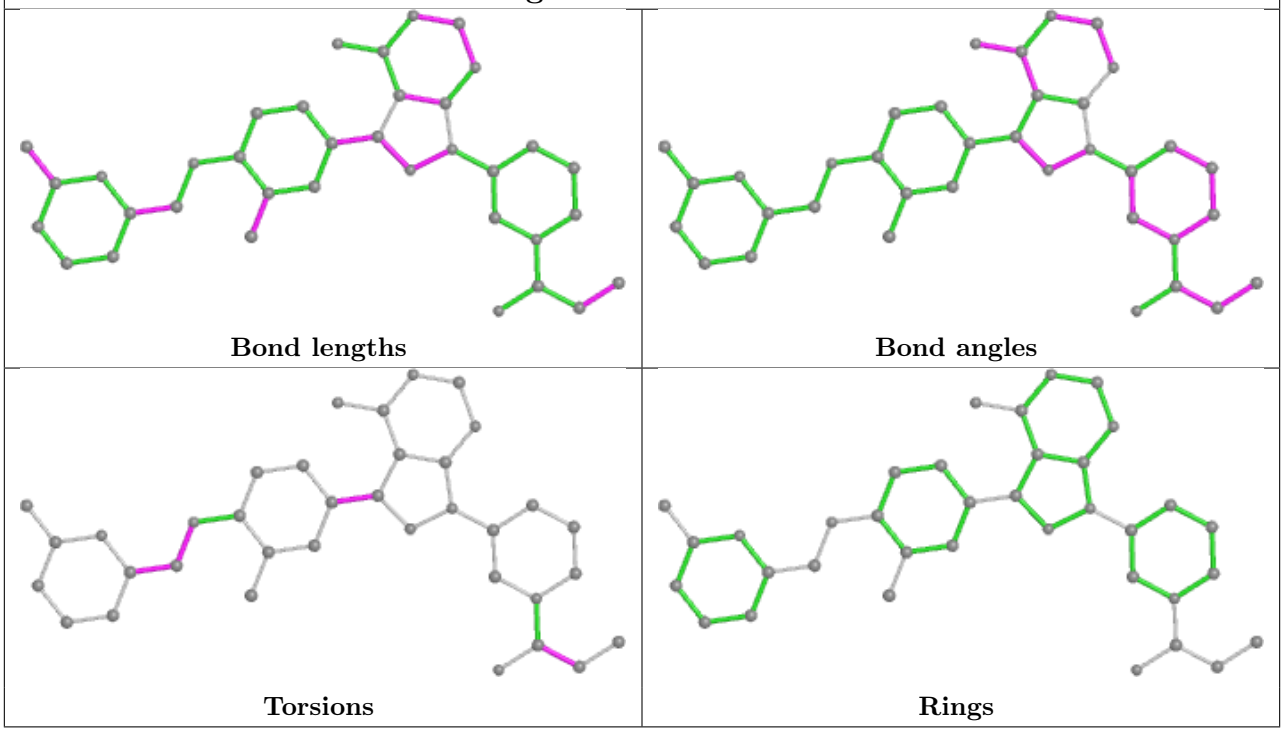
Ligand 816 B 1101



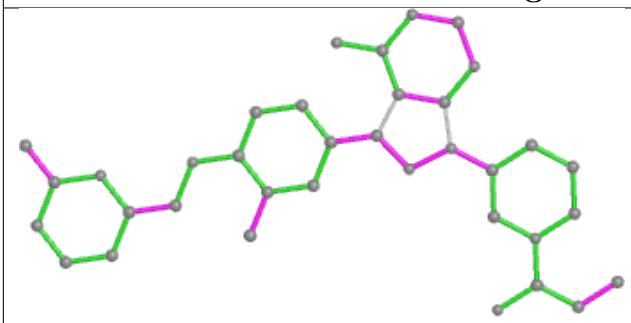
Ligand 816 H 1101



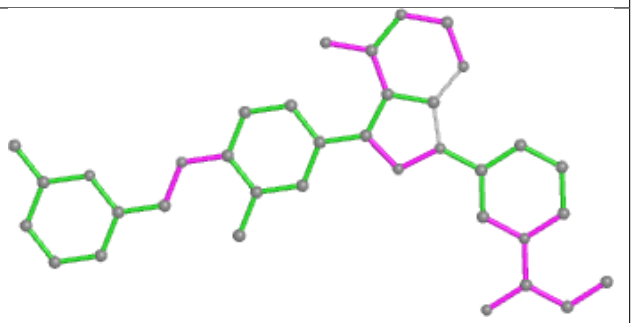
Ligand 816 D 1101



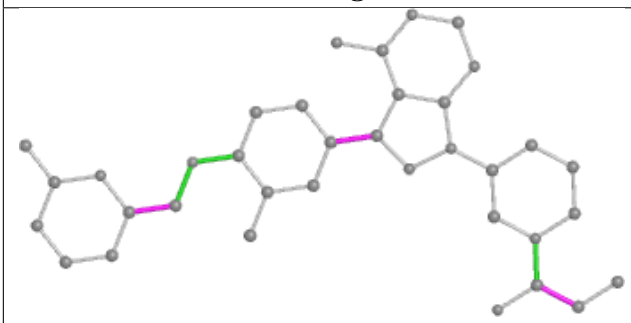
Ligand 816 A 1101



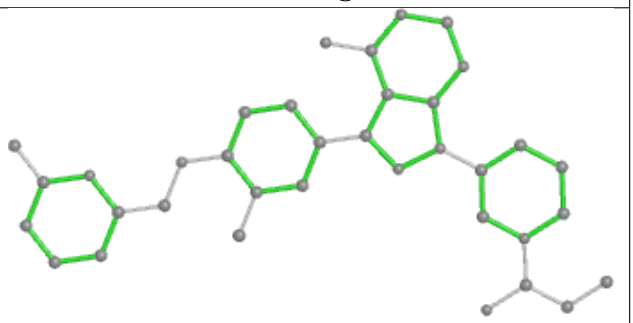
Bond lengths



Bond angles

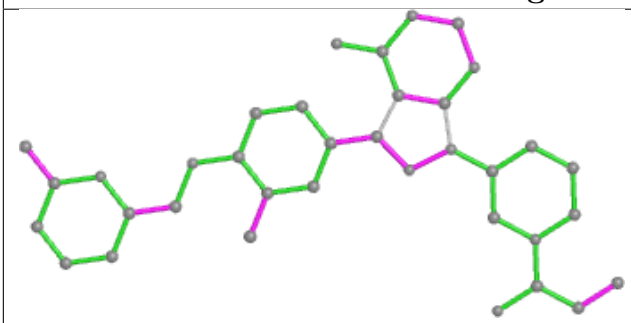


Torsions

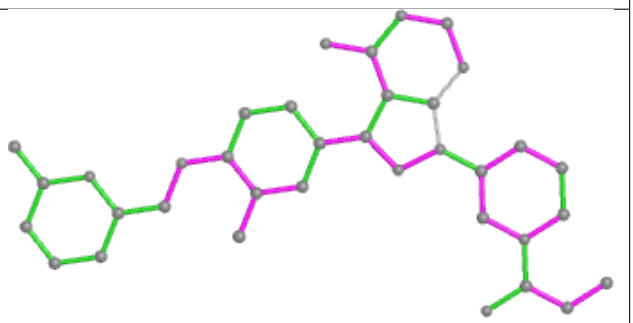


Rings

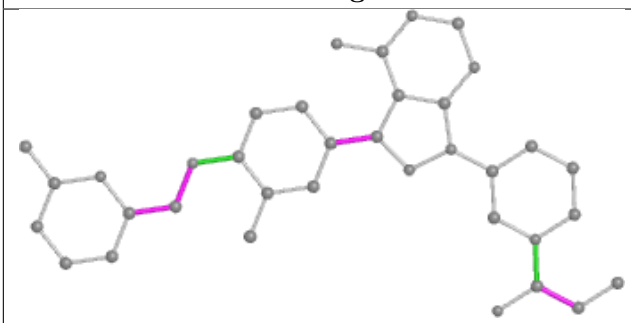
Ligand 816 F 1101



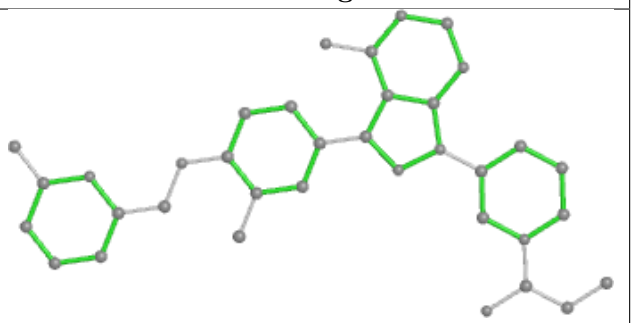
Bond lengths



Bond angles

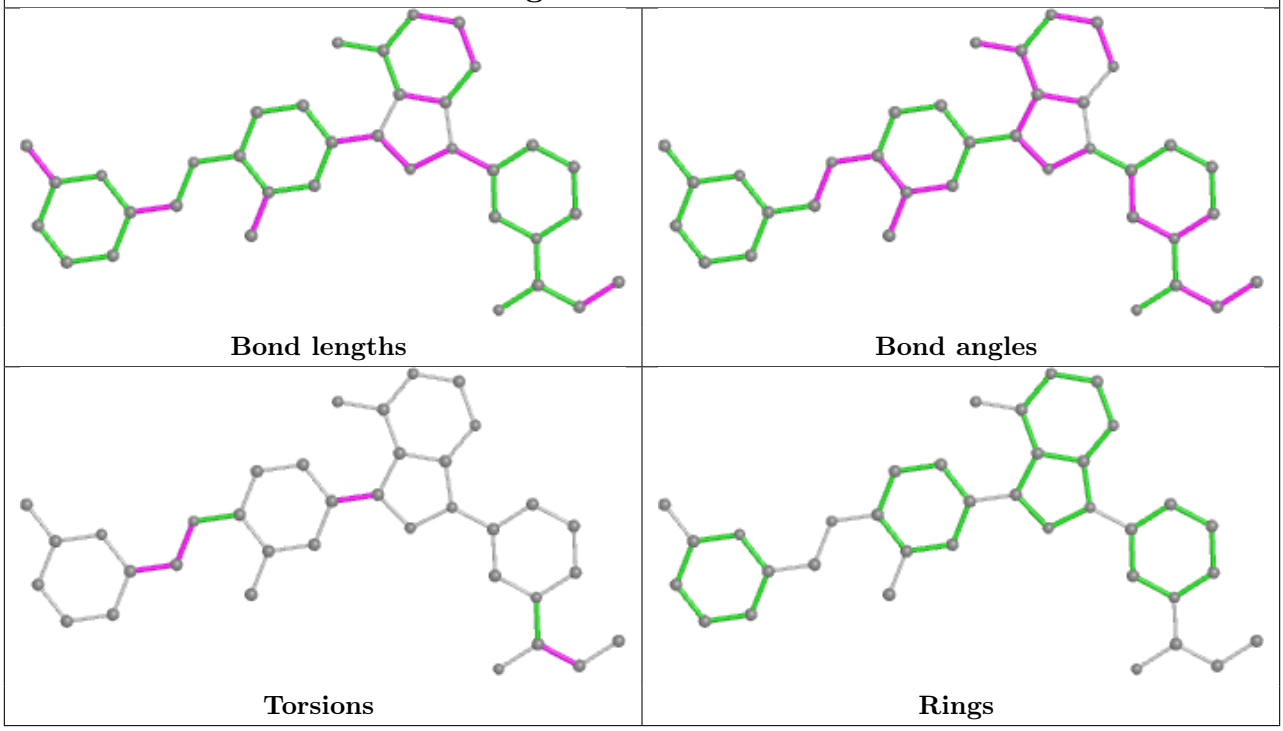


Torsions

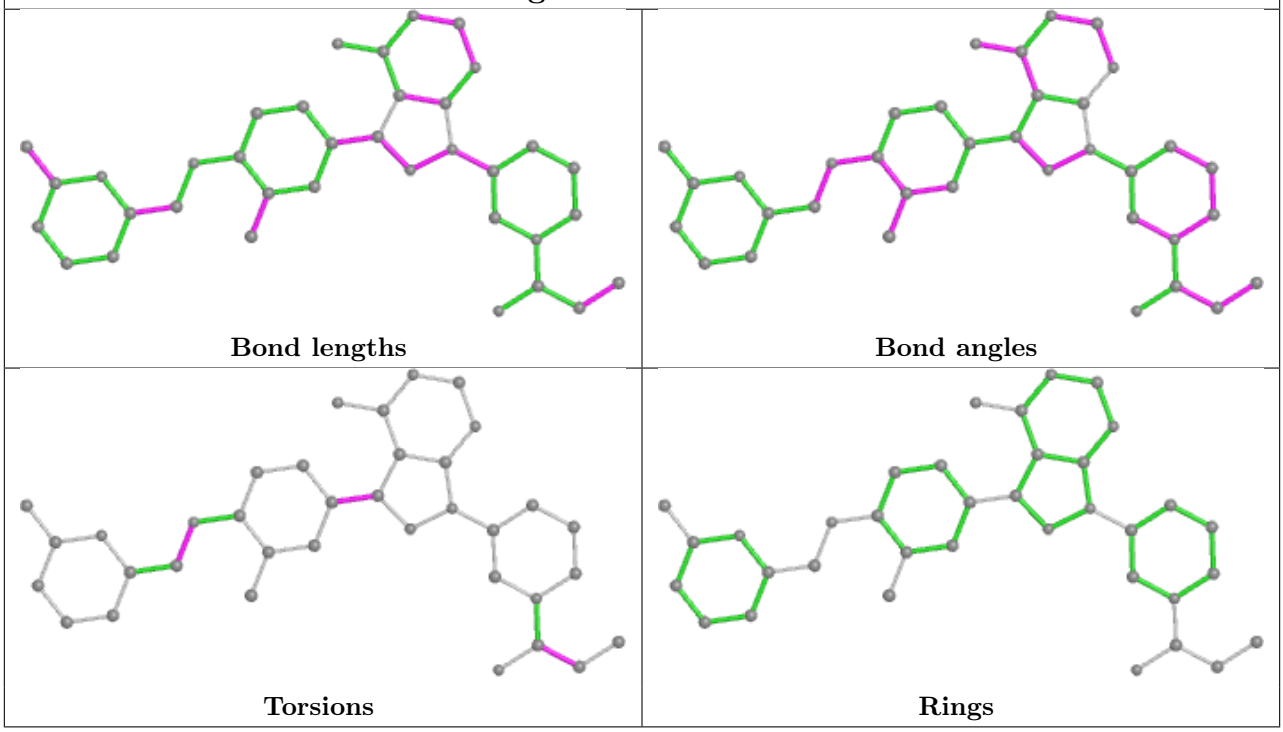


Rings

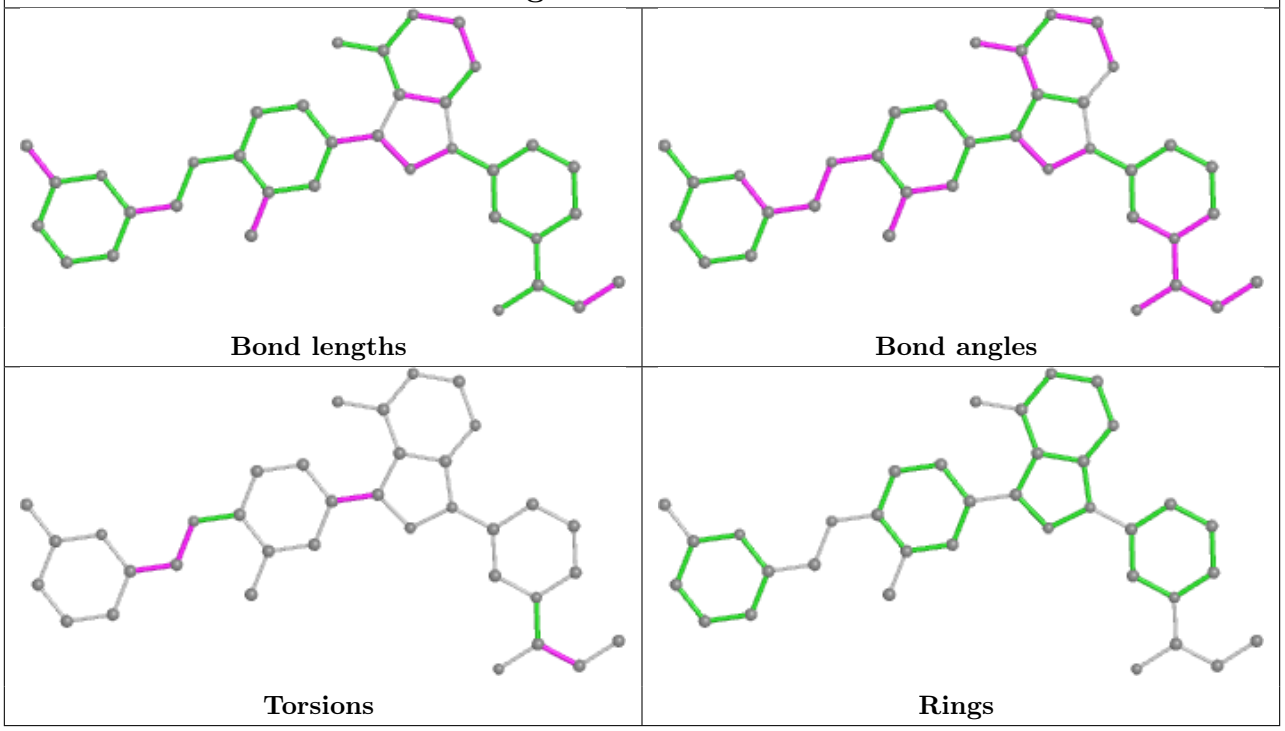
Ligand 816 G 1101



Ligand 816 E 1101



Ligand 816 C 1101



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	300/331 (90%)	-0.01	6 (2%) 65 46	29, 48, 89, 111	1 (0%)
1	B	299/331 (90%)	0.02	13 (4%) 35 17	29, 48, 85, 112	0
1	C	295/331 (89%)	0.13	17 (5%) 23 10	31, 52, 89, 125	2 (0%)
1	D	297/331 (89%)	0.00	14 (4%) 31 15	29, 48, 97, 121	1 (0%)
1	E	297/331 (89%)	0.03	22 (7%) 14 6	26, 49, 94, 112	0
1	F	297/331 (89%)	-0.02	5 (1%) 70 51	31, 48, 82, 93	0
1	G	299/331 (90%)	0.19	15 (5%) 28 13	31, 50, 88, 99	0
1	H	300/331 (90%)	0.03	5 (1%) 70 51	31, 48, 92, 107	0
All	All	2384/2648 (90%)	0.05	97 (4%) 37 19	26, 49, 89, 125	4 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	ASP	6.4
1	D	760	LEU	4.9
1	G	1013	ALA	4.7
1	D	763	ALA	4.6
1	E	1013	ALA	4.4
1	C	1009	ASP	4.3
1	E	860	LYS	4.3
1	B	762	GLU	4.2
1	F	859	ALA	4.1
1	D	1013	ALA	4.1
1	E	1014	ASP	4.0
1	G	699	PRO	4.0
1	G	1012	ASP	4.0
1	C	724	GLY	3.9
1	E	786	VAL	3.8
1	D	762	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	1016	TYR	3.6
1	E	763	ALA	3.5
1	B	1014	ASP	3.4
1	G	986	ARG	3.3
1	B	704	LEU	3.3
1	G	861	LEU	3.3
1	B	927	LEU	3.2
1	E	784	SER	3.2
1	G	760	LEU	3.1
1	B	764	TYR	3.1
1	B	1008	ASP	3.1
1	F	876	VAL	3.0
1	F	1009	ASP	3.0
1	C	1012	ASP	3.0
1	H	861	LEU	2.9
1	F	782	LEU	2.9
1	E	783	THR	2.9
1	C	745	LYS	2.9
1	E	859	ALA	2.8
1	A	915	TYR	2.8
1	G	764	TYR	2.8
1	A	1014	ASP	2.8
1	G	766	MET	2.8
1	C	788	LEU	2.7
1	D	859	ALA	2.7
1	B	807	ASP	2.7
1	E	761	ASP	2.6
1	E	785	THR	2.6
1	E	988	HIS	2.6
1	H	755	ALA	2.5
1	E	808	ASN	2.5
1	E	1008	ASP	2.5
1	C	725	THR	2.5
1	C	1013	ALA	2.5
1	D	764	TYR	2.5
1	A	877	PRO	2.5
1	G	1014	ASP	2.5
1	D	807	ASP	2.5
1	D	808	ASN	2.5
1	A	988	HIS	2.5
1	G	807	ASP	2.4
1	C	782	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	765	VAL	2.4
1	A	927	LEU	2.4
1	C	856	PHE	2.4
1	B	859	ALA	2.3
1	C	785	THR	2.3
1	C	746	GLU	2.3
1	E	991	SER	2.3
1	B	1012	ASP	2.3
1	C	781	CYS	2.3
1	B	782	LEU	2.3
1	E	782	LEU	2.3
1	C	754	LYS	2.3
1	E	707	LEU	2.3
1	D	759	ILE	2.3
1	D	1009	ASP	2.3
1	E	1012	ASP	2.2
1	G	701	GLN	2.2
1	E	766	MET	2.2
1	C	768	SER	2.2
1	D	1008	ASP	2.2
1	D	860	LYS	2.2
1	G	759	ILE	2.2
1	C	729	GLY	2.2
1	G	953	ILE	2.1
1	G	1011	VAL	2.1
1	E	807	ASP	2.1
1	D	991	SER	2.1
1	E	788	LEU	2.1
1	C	993	THR	2.1
1	D	707	LEU	2.1
1	G	993	THR	2.1
1	E	759	ILE	2.1
1	H	760	LEU	2.0
1	A	1009	ASP	2.0
1	B	1009	ASP	2.0
1	H	860	LYS	2.0
1	E	985	GLU	2.0
1	C	756	ASN	2.0
1	F	788	LEU	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 (i)

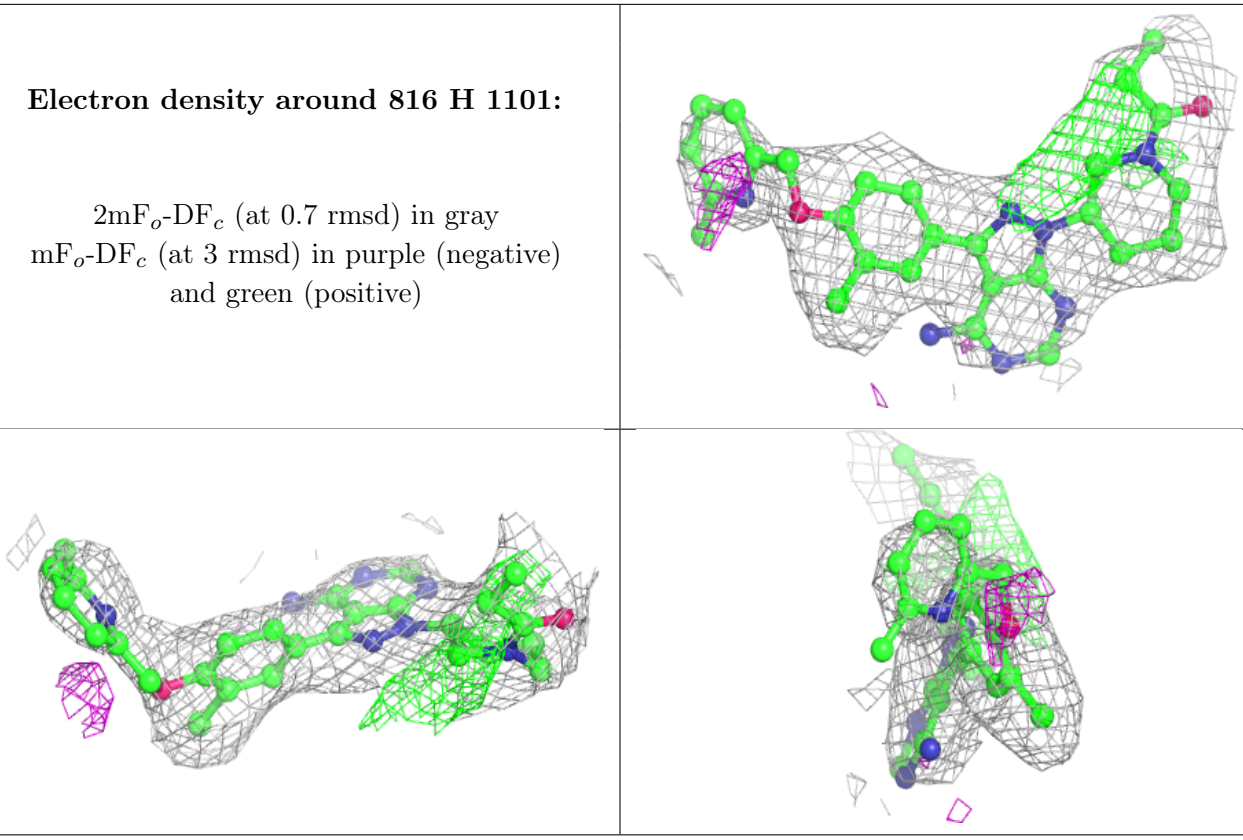
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	H	1104	4/4	0.56	0.47	71,71,71,71	0
3	EDO	H	1103	4/4	0.79	0.36	70,70,70,70	0
3	EDO	H	1102	4/4	0.80	0.22	65,65,65,65	0
2	816	H	1101	36/36	0.84	0.29	44,50,60,61	0
2	816	E	1101	36/36	0.85	0.26	42,56,66,70	0
2	816	C	1101	36/36	0.88	0.23	43,51,62,77	0
2	816	F	1101	36/36	0.88	0.25	33,45,50,62	0
3	EDO	G	1102	4/4	0.89	0.19	55,55,55,55	0
2	816	G	1101	36/36	0.89	0.26	40,51,62,67	0
2	816	D	1101	36/36	0.92	0.20	41,53,66,68	0
2	816	A	1101	36/36	0.92	0.20	31,39,51,61	0
2	816	B	1101	36/36	0.93	0.20	36,42,49,51	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

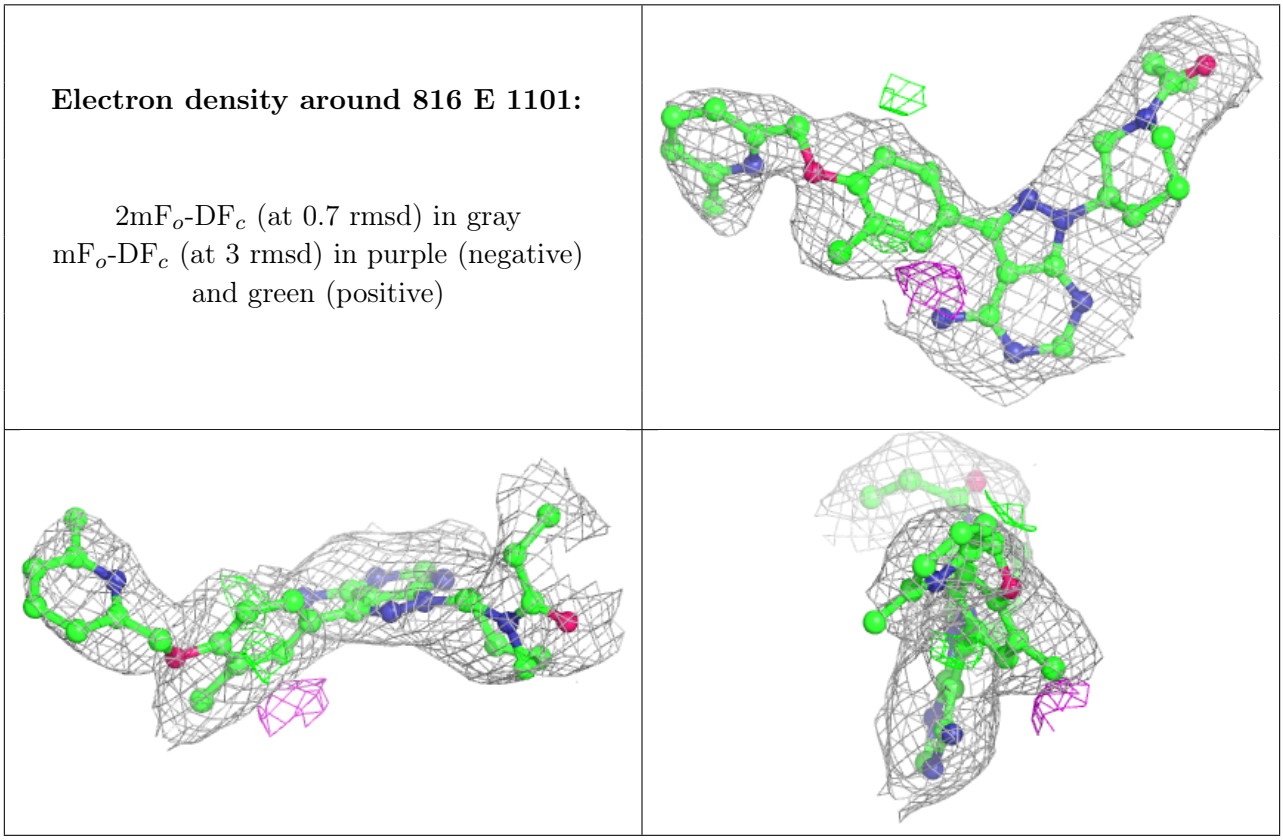
Electron density around 816 H 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



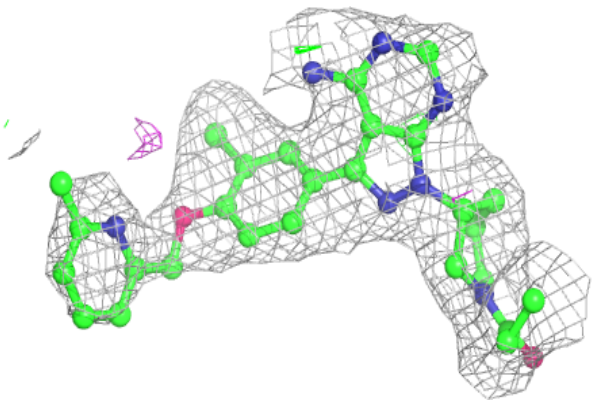
Electron density around 816 E 1101:

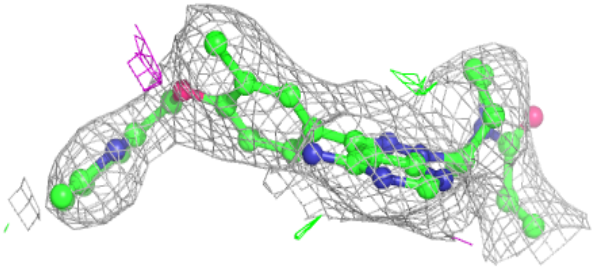
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

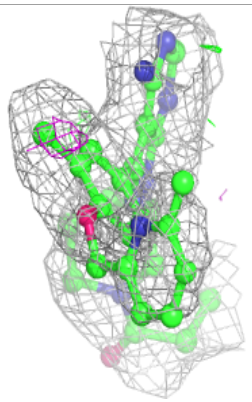


Electron density around 816 C 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

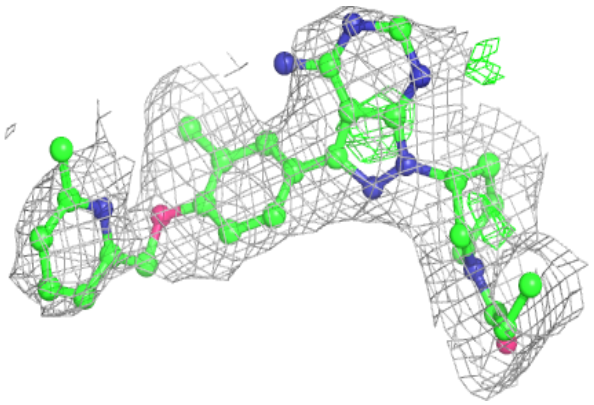


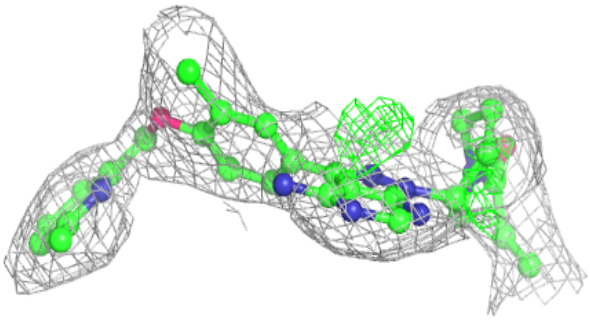


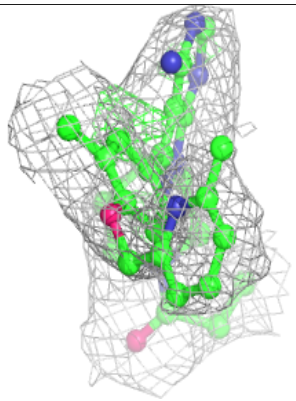


Electron density around 816 F 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

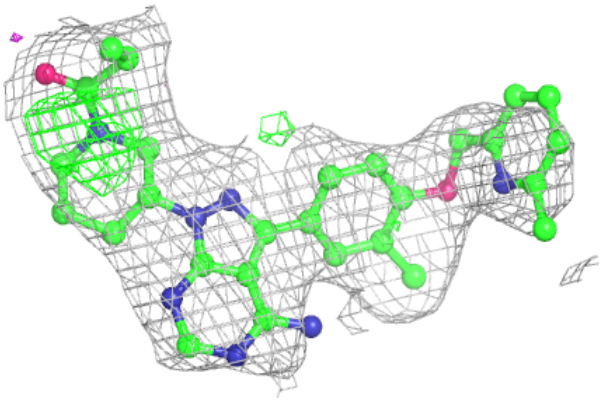


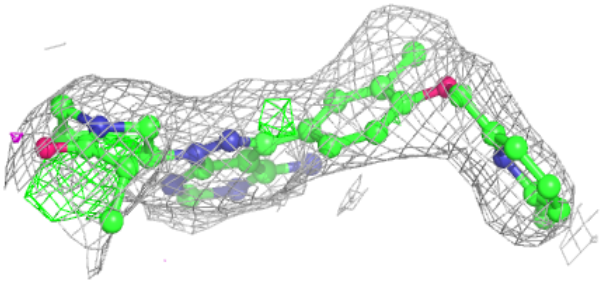


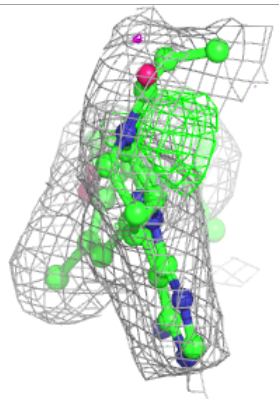


Electron density around 816 G 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

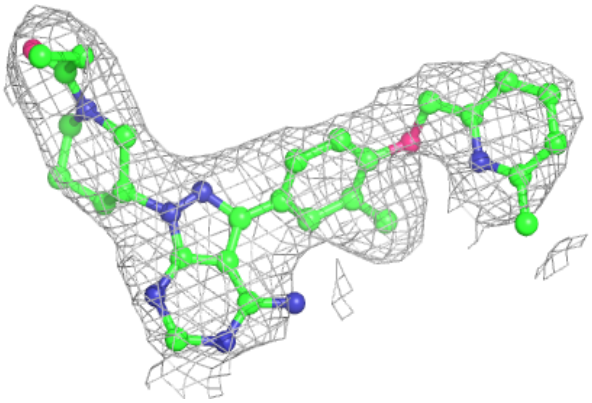


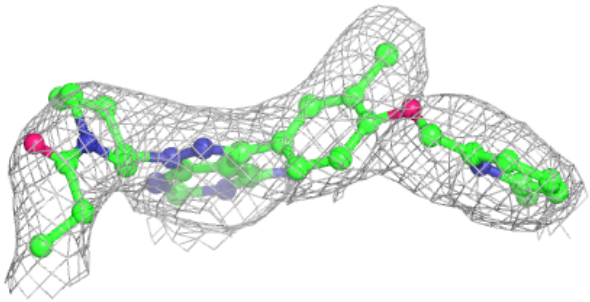


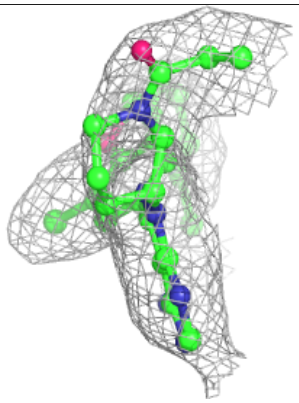


Electron density around 816 D 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

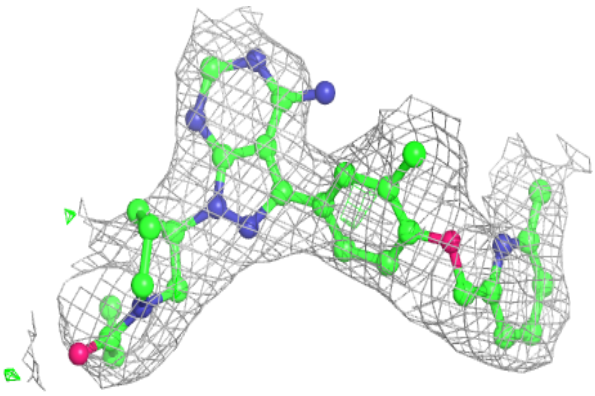


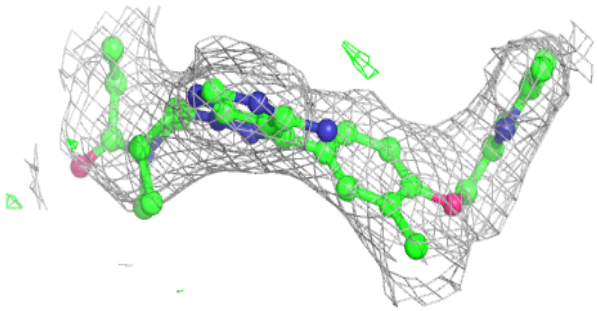


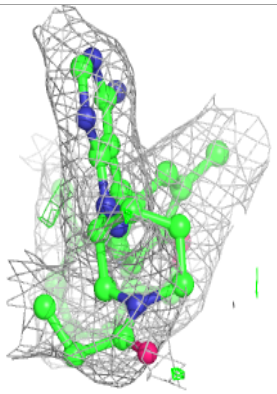


Electron density around 816 A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

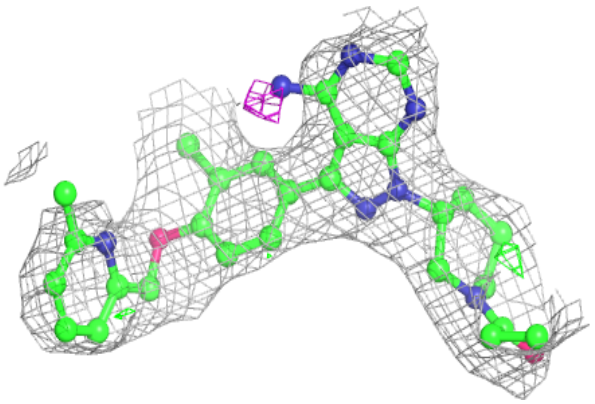


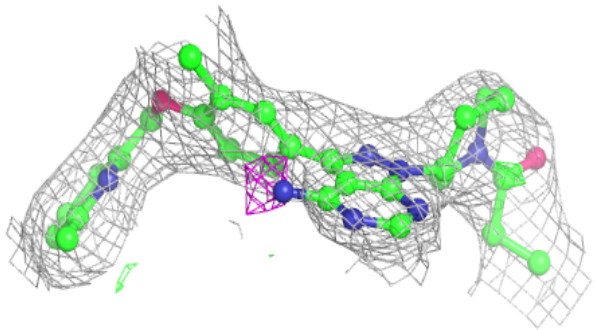


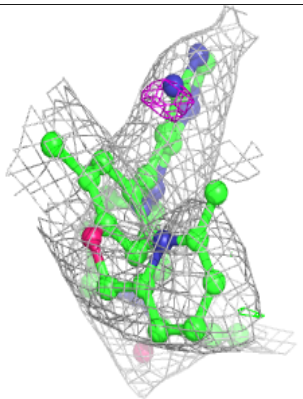


Electron density around 816 B 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.