



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:13 am BST

PDB ID : 1AM4
Title : COMPLEX BETWEEN CDC42HS.GMPPNP AND P50 RHOGAP (H. SAPI-
ENS)
Authors : Rittinger, K.; Walker, P.; Gamblin, S.J.; Smerdon, S.J.
Deposited on : 1997-06-22
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

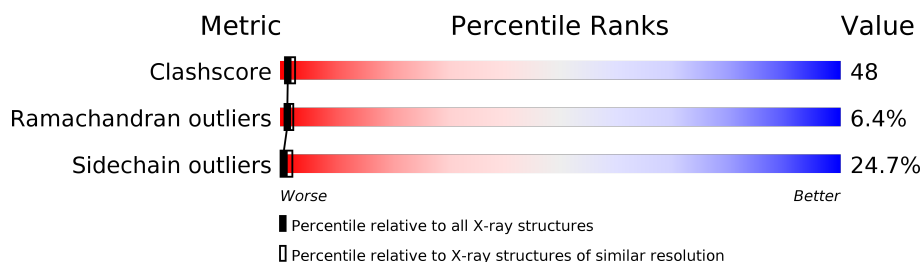
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	199	
1	B	199	
1	C	199	
2	D	177	
2	E	177	
2	F	177	

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
4	GNP	D	678	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9191 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 P50-RHOGAP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1593	1032	273	286	2			
1	B	199	Total	C	N	O	S	0	0	0
			1593	1032	273	286	2			
1	C	199	Total	C	N	O	S	0	0	0
			1593	1032	273	286	2			

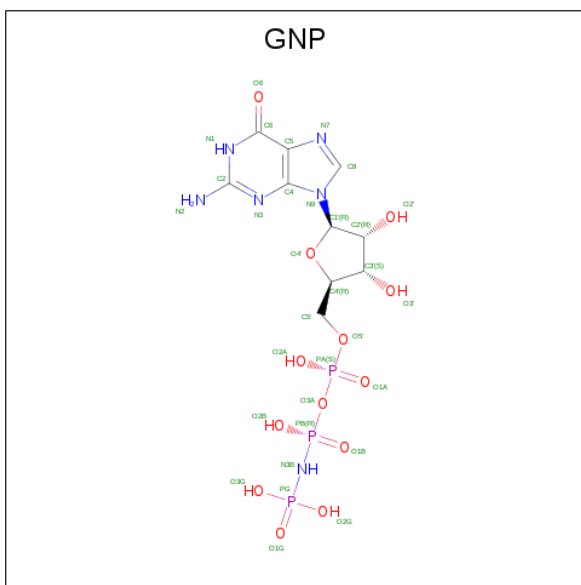
- Molecule 2 is a protein called CDC42HS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	174	Total	C	N	O	S	0	0	0
			1337	861	218	252	6			
2	E	174	Total	C	N	O	S	0	0	0
			1337	861	218	252	6			
2	F	174	Total	C	N	O	S	0	0	0
			1337	861	218	252	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	E	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	F	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 5 is water.

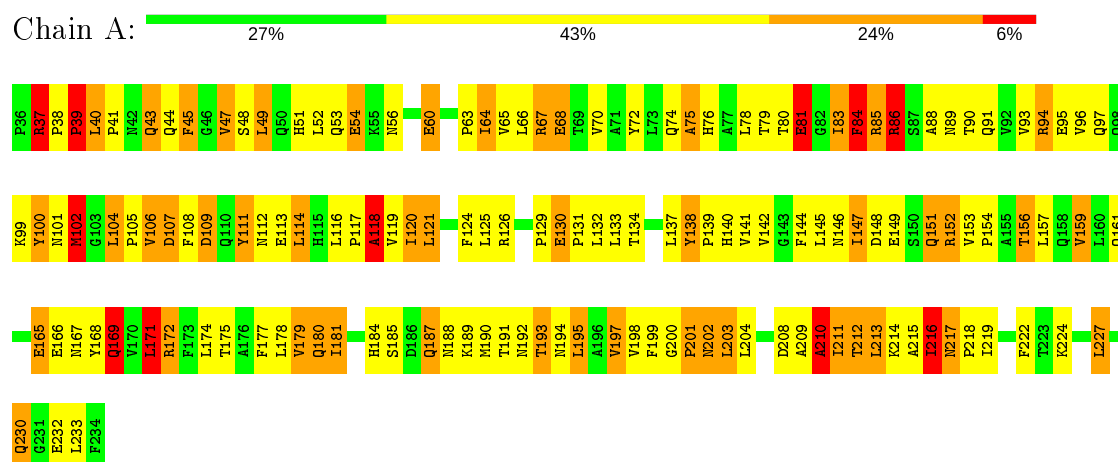
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	D	36	Total O 36 36	0	0
5	B	62	Total O 62 62	0	0
5	E	39	Total O 39 39	0	0
5	C	62	Total O 62 62	0	0
5	F	40	Total O 40 40	0	0

3 Residue-property plots

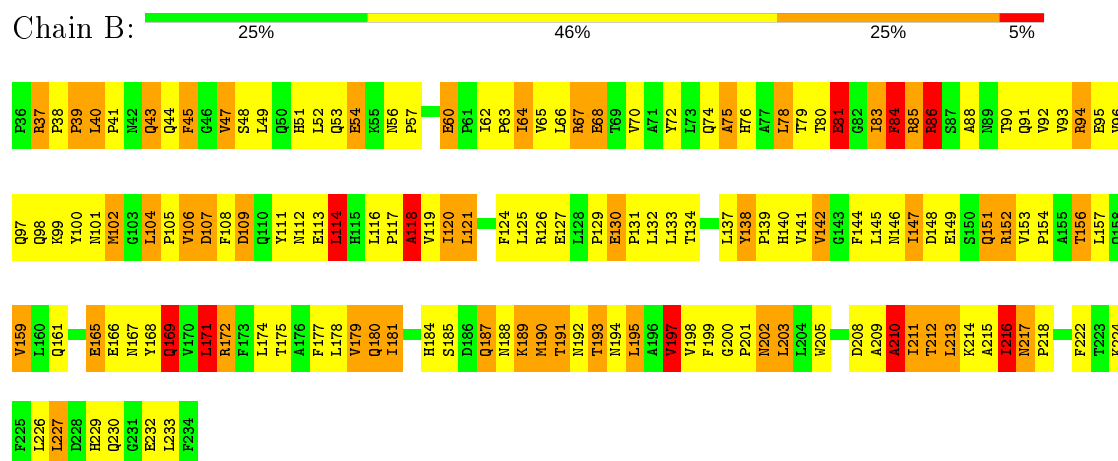
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

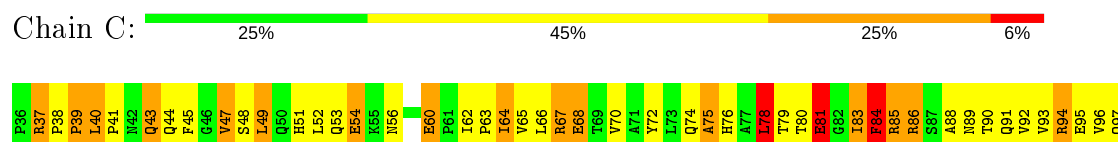
• Molecule 1: P50-RHOGAP

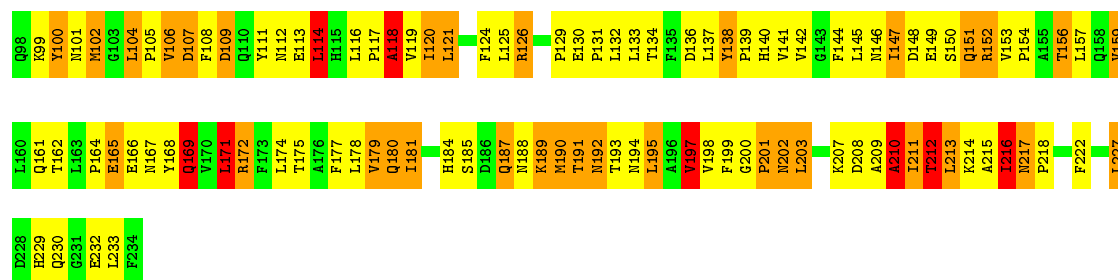


• Molecule 1: P50-RHOGAP

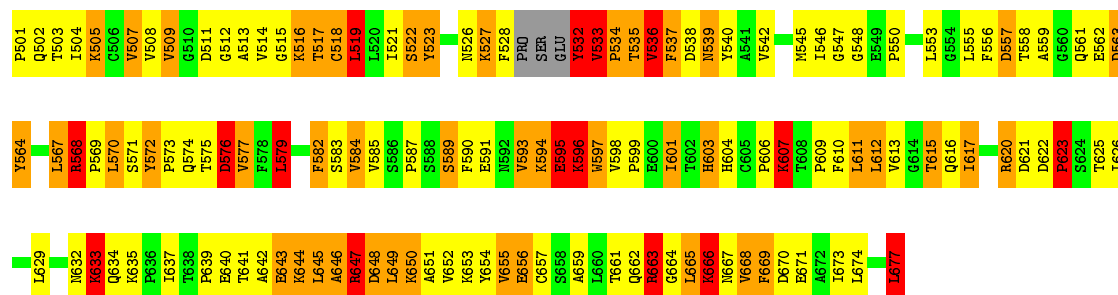
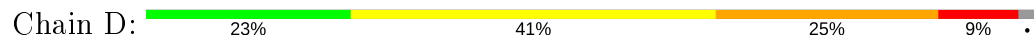


• Molecule 1: P50-RHOGAP

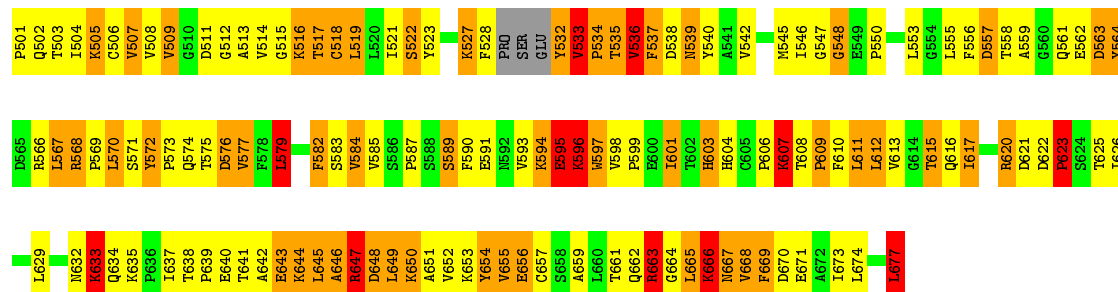
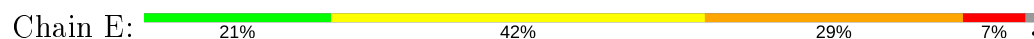




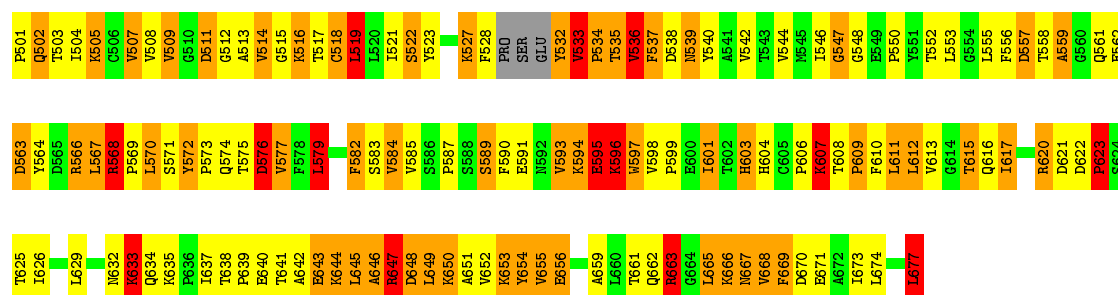
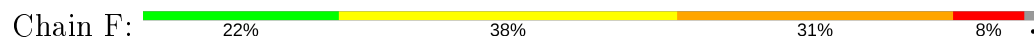
• Molecule 2: CDC42HS



• Molecule 2: CDC42HS



• Molecule 2: CDC42HS



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.11Å 78.12Å 78.10Å 90.01° 90.00° 90.05°	Depositor
Resolution (Å)	12.00 – 2.70	Depositor
% Data completeness (in resolution range)	96.0 (12.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.230 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9191	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	0/1633	2.14	68/2231 (3.0%)
1	B	0.92	0/1633	2.16	61/2231 (2.7%)
1	C	0.94	0/1633	2.16	65/2231 (2.9%)
2	D	0.97	0/1366	2.18	53/1860 (2.8%)
2	E	0.96	0/1366	2.18	52/1860 (2.8%)
2	F	0.95	0/1366	2.17	53/1860 (2.8%)
All	All	0.94	0/8997	2.16	352/12273 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
2	D	0	5
2	E	0	2
2	F	0	2
All	All	0	21

There are no bond length outliers.

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	647	ARG	CD-NE-CZ	19.40	150.76	123.60
2	E	647	ARG	CD-NE-CZ	19.30	150.61	123.60
2	D	647	ARG	CD-NE-CZ	19.27	150.58	123.60
1	C	85	ARG	NE-CZ-NH1	18.11	129.35	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ARG	NE-CZ-NH1	16.45	128.53	120.30
1	A	85	ARG	NE-CZ-NH1	15.60	128.10	120.30
1	C	67	ARG	NE-CZ-NH1	14.61	127.61	120.30
1	B	67	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	B	172	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	F	519	LEU	CA-CB-CG	11.96	142.81	115.30
2	E	519	LEU	CA-CB-CG	11.92	142.72	115.30
2	D	519	LEU	CA-CB-CG	11.40	141.53	115.30
1	C	172	ARG	CD-NE-CZ	10.96	138.95	123.60
2	D	557	ASP	CB-CG-OD2	10.91	128.12	118.30
2	E	557	ASP	CB-CG-OD2	10.71	127.94	118.30
1	C	172	ARG	NE-CZ-NH1	10.55	125.57	120.30
1	A	172	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	C	203	LEU	CA-CB-CG	10.36	139.12	115.30
1	B	203	LEU	CA-CB-CG	10.12	138.59	115.30
1	B	86	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	203	LEU	CA-CB-CG	10.08	138.49	115.30
1	A	86	ARG	NE-CZ-NH1	10.03	125.31	120.30
2	D	535	THR	CA-CB-OG1	-10.00	88.00	109.00
1	A	67	ARG	CD-NE-CZ	9.99	137.59	123.60
2	F	579	LEU	CA-CB-CG	9.95	138.18	115.30
2	E	647	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	B	138	TYR	CB-CG-CD2	-9.94	115.03	121.00
2	F	535	THR	CA-CB-OG1	-9.87	88.27	109.00
2	D	579	LEU	CA-CB-CG	9.84	137.94	115.30
1	B	81	GLU	CA-CB-CG	9.82	135.00	113.40
2	D	535	THR	CA-CB-CG2	9.78	126.10	112.40
1	A	138	TYR	CB-CG-CD2	-9.78	115.13	121.00
2	F	535	THR	CA-CB-CG2	9.74	126.04	112.40
2	E	535	THR	CA-CB-OG1	-9.66	88.71	109.00
1	C	148	ASP	CB-CG-OD2	-9.56	109.70	118.30
1	B	67	ARG	CD-NE-CZ	9.53	136.94	123.60
2	F	557	ASP	CB-CG-OD2	9.46	126.82	118.30
2	E	535	THR	CA-CB-CG2	9.45	125.63	112.40
2	E	579	LEU	CA-CB-CG	9.43	136.98	115.30
1	B	138	TYR	CB-CG-CD1	9.36	126.62	121.00
1	A	172	ARG	CD-NE-CZ	9.34	136.68	123.60
1	C	81	GLU	CA-CB-CG	9.27	133.79	113.40
2	E	532	TYR	CA-CB-CG	-9.26	95.80	113.40
1	A	138	TYR	CB-CG-CD1	9.23	126.54	121.00
1	A	81	GLU	CA-CB-CG	9.21	133.65	113.40
1	A	67	ARG	NE-CZ-NH1	9.12	124.86	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	532	TYR	CA-CB-CG	-9.05	96.20	113.40
2	D	532	TYR	CA-CB-CG	-9.05	96.21	113.40
1	B	60	GLU	CA-CB-CG	8.93	133.04	113.40
1	B	165	GLU	C-N-CA	8.91	143.99	121.70
2	E	532	TYR	CB-CG-CD1	-8.77	115.74	121.00
1	A	60	GLU	CA-CB-CG	8.69	132.51	113.40
1	C	67	ARG	CD-NE-CZ	8.37	135.32	123.60
1	C	60	GLU	CA-CB-CG	8.35	131.76	113.40
1	A	165	GLU	C-N-CA	8.35	142.57	121.70
2	D	647	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	148	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	C	165	GLU	C-N-CA	8.26	142.34	121.70
1	A	148	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	B	172	ARG	CD-NE-CZ	8.18	135.05	123.60
2	F	647	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	152	ARG	NE-CZ-NH2	8.11	124.35	120.30
1	C	152	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	C	166	GLU	CA-CB-CG	7.88	130.73	113.40
1	B	64	ILE	CB-CG1-CD1	7.87	135.92	113.90
1	A	64	ILE	CB-CG1-CD1	7.83	135.82	113.90
2	E	647	ARG	CG-CD-NE	7.57	127.70	111.80
2	F	647	ARG	CG-CD-NE	7.55	127.66	111.80
1	C	109	ASP	CB-CA-C	7.54	125.49	110.40
2	D	647	ARG	CG-CD-NE	7.53	127.61	111.80
1	A	168	TYR	CB-CG-CD2	7.49	125.49	121.00
2	D	615	THR	O-C-N	7.43	134.59	122.70
2	D	595	GLU	CG-CD-OE1	7.42	133.14	118.30
1	C	86	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	E	532	TYR	CB-CG-CD2	7.36	125.42	121.00
2	F	648	ASP	CB-CG-OD1	7.34	124.91	118.30
1	C	91	GLN	CB-CG-CD	7.33	130.65	111.60
1	B	166	GLU	CA-CB-CG	7.29	129.45	113.40
1	A	149	GLU	CG-CD-OE2	7.26	132.83	118.30
1	B	195	LEU	CA-CB-CG	7.23	131.94	115.30
1	B	91	GLN	CB-CG-CD	7.23	130.39	111.60
1	A	106	VAL	CA-CB-CG2	7.21	121.72	110.90
2	E	648	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	91	GLN	CB-CG-CD	7.21	130.34	111.60
2	F	669	PHE	CB-CA-C	7.19	124.77	110.40
2	D	648	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	109	ASP	CB-CA-C	7.18	124.76	110.40
1	B	149	GLU	CG-CD-OE2	7.14	132.58	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	595	GLU	CG-CD-OE1	7.10	132.50	118.30
1	A	195	LEU	CA-CB-CG	7.09	131.61	115.30
2	E	669	PHE	CB-CA-C	7.08	124.56	110.40
2	E	595	GLU	CG-CD-OE1	7.07	132.44	118.30
2	F	665	LEU	CA-CB-CG	7.05	131.52	115.30
1	B	106	VAL	CA-CB-CG2	7.05	121.47	110.90
1	A	166	GLU	CA-CB-CG	7.04	128.90	113.40
1	C	138	TYR	CB-CG-CD2	-7.04	116.78	121.00
2	D	656	GLU	OE1-CD-OE2	7.03	131.73	123.30
1	C	64	ILE	CB-CG1-CD1	7.00	133.51	113.90
1	C	121	LEU	CA-CB-CG	6.99	131.37	115.30
1	B	109	ASP	CB-CA-C	6.98	124.36	110.40
2	D	649	LEU	CB-CA-C	6.96	123.43	110.20
2	F	615	THR	O-C-N	6.94	133.80	122.70
1	C	195	LEU	CA-CB-CG	6.93	131.25	115.30
1	B	49	LEU	O-C-N	6.90	133.75	122.70
2	F	649	LEU	CB-CA-C	6.88	123.27	110.20
2	E	649	LEU	CB-CA-C	6.87	123.25	110.20
2	E	557	ASP	CB-CG-OD1	-6.85	112.14	118.30
2	E	615	THR	O-C-N	6.83	133.63	122.70
1	B	54	GLU	CA-CB-CG	6.82	128.41	113.40
2	D	665	LEU	CA-CB-CG	6.80	130.93	115.30
1	C	168	TYR	CB-CG-CD2	6.77	125.06	121.00
1	C	68	GLU	CA-C-O	-6.75	105.92	120.10
2	D	517	THR	CA-CB-OG1	-6.73	94.86	109.00
2	D	563	ASP	CB-CG-OD2	6.72	124.35	118.30
2	E	572	TYR	CB-CG-CD1	6.71	125.03	121.00
1	C	54	GLU	CA-CB-CG	6.71	128.16	113.40
2	D	562	GLU	CG-CD-OE1	6.67	131.64	118.30
2	D	570	LEU	C-N-CA	6.67	138.37	121.70
2	F	576	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	168	TYR	CB-CG-CD2	6.64	124.98	121.00
2	E	536	VAL	CA-CB-CG1	-6.63	100.95	110.90
2	F	517	THR	CA-CB-OG1	-6.63	95.07	109.00
1	C	191	THR	CA-CB-CG2	6.63	121.68	112.40
2	E	665	LEU	CA-CB-CG	6.63	130.54	115.30
1	C	85	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	D	669	PHE	CB-CA-C	6.62	123.64	110.40
1	A	54	GLU	CA-CB-CG	6.61	127.94	113.40
2	F	557	ASP	CB-CG-OD1	-6.60	112.36	118.30
2	D	536	VAL	CA-CB-CG1	-6.58	101.02	110.90
2	D	572	TYR	CB-CG-CD2	-6.54	117.08	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ARG	CG-CD-NE	6.52	125.50	111.80
1	B	121	LEU	CA-CB-CG	6.52	130.29	115.30
1	B	152	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	C	67	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	85	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	D	536	VAL	CB-CA-C	6.49	123.72	111.40
1	C	106	VAL	CA-CB-CG2	6.48	120.62	110.90
1	A	49	LEU	O-C-N	6.47	133.06	122.70
1	B	67	ARG	NE-CZ-NH2	-6.45	117.07	120.30
2	D	597	TRP	CA-CB-CG	-6.41	101.52	113.70
2	F	562	GLU	CG-CD-OE1	6.41	131.11	118.30
2	E	536	VAL	CB-CA-C	6.39	123.55	111.40
2	F	677	LEU	CB-CA-C	6.39	122.35	110.20
1	C	152	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	A	208	ASP	CB-CG-OD1	6.38	124.04	118.30
2	F	536	VAL	CB-CA-C	6.37	123.51	111.40
2	F	566	ARG	NE-CZ-NH2	-6.37	117.11	120.30
2	E	644	LYS	CA-C-O	6.36	133.46	120.10
1	B	227	LEU	CB-CA-C	6.32	122.21	110.20
2	F	568	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	169	GLN	CA-CB-CG	6.32	127.30	113.40
1	B	104	LEU	CB-CA-C	6.31	122.19	110.20
2	E	562	GLU	CG-CD-OE1	6.30	130.90	118.30
1	B	68	GLU	CA-C-O	-6.29	106.89	120.10
2	E	537	PHE	CA-CB-CG	6.29	129.00	113.90
2	F	537	PHE	CA-CB-CG	6.29	129.00	113.90
2	E	670	ASP	CB-CG-OD2	6.27	123.95	118.30
2	D	537	PHE	CA-CB-CG	6.25	128.90	113.90
1	A	68	GLU	CA-C-O	-6.25	106.98	120.10
1	C	49	LEU	O-C-N	6.25	132.69	122.70
2	D	532	TYR	CB-CG-CD1	-6.24	117.25	121.00
2	D	656	GLU	CG-CD-OE2	-6.24	105.83	118.30
2	D	518	CYS	CB-CA-C	6.23	122.87	110.40
1	B	127	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	C	149	GLU	CG-CD-OE2	6.20	130.70	118.30
1	B	86	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	F	518	CYS	CB-CA-C	6.18	122.75	110.40
1	C	227	LEU	CB-CA-C	6.17	121.93	110.20
2	F	536	VAL	CA-CB-CG1	-6.16	101.67	110.90
1	A	152	ARG	NE-CZ-NH1	-6.15	117.23	120.30
2	F	663	ARG	CD-NE-CZ	6.13	132.19	123.60
2	D	532	TYR	CB-CG-CD2	6.13	124.68	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	597	TRP	CA-CB-CG	-6.11	102.09	113.70
2	E	518	CYS	CB-CA-C	6.09	122.59	110.40
1	C	169	GLN	CB-CG-CD	6.09	127.43	111.60
2	E	677	LEU	CB-CA-C	6.08	121.76	110.20
2	D	557	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	C	104	LEU	CB-CA-C	6.08	121.75	110.20
2	E	656	GLU	OE1-CD-OE2	6.07	130.59	123.30
2	E	534	PRO	CA-C-O	6.06	134.73	120.20
1	A	37	ARG	NE-CZ-NH1	-6.05	117.27	120.30
2	E	671	GLU	CG-CD-OE1	6.05	130.39	118.30
1	B	88	ALA	C-N-CA	6.04	136.79	121.70
1	A	107	ASP	CB-CA-C	6.03	122.46	110.40
2	E	597	TRP	CA-CB-CG	-6.02	102.26	113.70
1	C	68	GLU	N-CA-CB	6.02	121.43	110.60
1	B	202	ASN	CB-CG-OD1	-6.02	109.57	121.60
1	B	152	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	169	GLN	CA-CB-CG	5.99	126.58	113.40
2	F	671	GLU	CG-CD-OE1	5.99	130.28	118.30
1	C	208	ASP	CB-CG-OD1	5.98	123.68	118.30
2	E	538	ASP	CB-CG-OD1	5.98	123.68	118.30
2	D	656	GLU	CA-CB-CG	5.97	126.53	113.40
1	A	171	LEU	CA-CB-CG	5.96	129.02	115.30
1	B	179	VAL	C-N-CA	5.96	136.61	121.70
1	B	169	GLN	CA-CB-CG	5.96	126.51	113.40
2	D	523	TYR	CB-CG-CD1	5.95	124.57	121.00
1	C	107	ASP	CB-CA-C	5.95	122.29	110.40
2	F	534	PRO	CA-C-O	5.94	134.46	120.20
2	E	644	LYS	C-N-CA	5.94	136.54	121.70
2	D	568	ARG	CD-NE-CZ	-5.93	115.29	123.60
2	F	568	ARG	CD-NE-CZ	-5.92	115.31	123.60
1	C	202	ASN	CB-CG-OD1	-5.92	109.77	121.60
2	F	656	GLU	CA-CB-CG	5.91	126.41	113.40
2	D	576	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	E	572	TYR	CB-CG-CD2	-5.90	117.46	121.00
2	E	656	GLU	CA-CB-CG	5.88	126.34	113.40
2	D	677	LEU	CB-CA-C	5.88	121.38	110.20
1	A	202	ASN	CB-CG-OD1	-5.88	109.84	121.60
1	A	68	GLU	N-CA-CB	5.88	121.18	110.60
1	C	88	ALA	C-N-CA	5.87	136.38	121.70
1	A	169	GLN	CB-CG-CD	5.85	126.81	111.60
1	B	171	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	88	ALA	C-N-CA	5.84	136.29	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LEU	CB-CA-C	5.83	121.28	110.20
1	B	169	GLN	CB-CG-CD	5.83	126.75	111.60
1	B	152	ARG	CG-CD-NE	5.82	124.02	111.80
1	C	76	HIS	CA-CB-CG	-5.81	103.72	113.60
1	A	227	LEU	CB-CA-C	5.81	121.24	110.20
1	B	68	GLU	N-CA-CB	5.81	121.06	110.60
1	B	130	GLU	CG-CD-OE2	-5.80	106.71	118.30
2	D	534	PRO	CA-C-O	5.79	134.09	120.20
1	A	159	VAL	O-C-N	5.78	131.95	122.70
1	A	145	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	120	ILE	CB-CA-C	5.76	123.11	111.60
1	C	190	MET	CA-CB-CG	5.75	123.07	113.30
1	C	100	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	C	201	PRO	C-N-CA	5.70	135.95	121.70
1	A	152	ARG	CG-CD-NE	5.69	123.76	111.80
2	D	671	GLU	CG-CD-OE1	5.69	129.67	118.30
1	B	107	ASP	CB-CA-C	5.68	121.77	110.40
2	E	570	LEU	C-N-CA	5.68	135.89	121.70
2	F	572	TYR	CB-CG-CD2	-5.68	117.59	121.00
2	D	568	ARG	NE-CZ-NH2	-5.67	117.46	120.30
2	D	644	LYS	C-N-CA	5.67	135.88	121.70
2	F	570	LEU	C-N-CA	5.67	135.88	121.70
2	D	564	TYR	CB-CG-CD2	5.67	124.40	121.00
1	B	145	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	102	MET	CA-CB-CG	5.64	122.90	113.30
1	A	121	LEU	CA-CB-CG	5.64	128.28	115.30
1	B	76	HIS	CA-CB-CG	-5.64	104.01	113.60
1	B	114	LEU	CA-CB-CG	5.64	128.27	115.30
1	C	89	ASN	CA-CB-CG	5.62	125.77	113.40
1	A	89	ASN	CA-CB-CG	5.62	125.77	113.40
2	E	562	GLU	CA-CB-CG	5.62	125.77	113.40
1	B	159	VAL	O-C-N	5.62	131.69	122.70
1	A	111	TYR	CB-CG-CD2	5.62	124.37	121.00
1	A	76	HIS	CA-CB-CG	-5.61	104.06	113.60
1	C	171	LEU	CA-CB-CG	5.60	128.17	115.30
1	C	159	VAL	O-C-N	5.58	131.63	122.70
1	A	49	LEU	CA-CB-CG	5.57	128.11	115.30
2	F	670	ASP	CB-CG-OD2	5.56	123.30	118.30
2	F	582	PHE	O-C-N	5.55	131.59	122.70
1	C	120	ILE	CB-CA-C	5.55	122.69	111.60
2	E	595	GLU	CG-CD-OE2	-5.54	107.22	118.30
2	F	644	LYS	CA-C-O	5.54	131.72	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	595	GLU	CG-CD-OE2	-5.53	107.24	118.30
2	D	538	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	84	PHE	N-CA-CB	-5.50	100.70	110.60
2	F	514	VAL	C-N-CA	5.49	133.84	122.30
1	B	118	ALA	CB-CA-C	5.49	118.33	110.10
2	E	517	THR	CA-CB-OG1	-5.47	97.50	109.00
1	A	210	ALA	N-CA-CB	5.45	117.72	110.10
1	A	130	GLU	CG-CD-OE2	-5.44	107.42	118.30
1	B	85	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
1	B	45	PHE	CB-CA-C	5.42	121.24	110.40
1	B	191	THR	CA-CB-CG2	5.42	119.98	112.40
1	B	84	PHE	N-CA-CB	-5.42	100.85	110.60
1	C	145	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	100	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	102	MET	CA-CB-CG	5.40	122.48	113.30
2	F	563	ASP	CB-CG-OD2	5.40	123.16	118.30
2	F	621	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	208	ASP	CB-CA-C	5.38	121.16	110.40
1	A	130	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	A	216	ILE	C-N-CA	5.37	135.12	121.70
2	F	595	GLU	CG-CD-OE2	-5.36	107.58	118.30
1	B	216	ILE	C-N-CA	5.34	135.06	121.70
2	E	568	ARG	CD-NE-CZ	-5.34	116.13	123.60
2	E	621	ASP	CB-CA-C	5.33	121.07	110.40
2	F	621	ASP	CB-CA-C	5.33	121.07	110.40
2	F	547	GLY	C-N-CA	5.33	133.50	122.30
2	F	655	VAL	CA-C-O	5.33	131.29	120.10
2	E	514	VAL	C-N-CA	5.33	133.49	122.30
2	D	655	VAL	CA-CB-CG2	5.32	118.88	110.90
1	B	120	ILE	CB-CA-C	5.31	122.21	111.60
1	C	210	ALA	N-CA-CB	5.30	117.52	110.10
2	E	615	THR	CA-C-O	-5.29	108.99	120.10
2	F	532	TYR	CA-C-O	-5.29	109.00	120.10
2	D	615	THR	CA-C-O	-5.29	109.00	120.10
2	D	655	VAL	CA-C-O	5.29	131.20	120.10
2	D	582	PHE	O-C-N	5.26	131.12	122.70
2	D	663	ARG	CD-NE-CZ	5.26	130.97	123.60
1	A	168	TYR	CB-CG-CD1	-5.26	117.84	121.00
2	F	644	LYS	C-N-CA	5.26	134.84	121.70
1	B	208	ASP	CB-CA-C	5.25	120.90	110.40
1	C	114	LEU	CA-CB-CG	5.24	127.34	115.30
2	D	665	LEU	CA-C-O	-5.23	109.12	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	OD1-CG-OD2	-5.23	113.37	123.30
2	F	538	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	118	ALA	CA-C-O	-5.22	109.14	120.10
1	C	85	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	A	45	PHE	CB-CA-C	5.22	120.84	110.40
2	D	621	ASP	CB-CA-C	5.21	120.83	110.40
1	C	118	ALA	CA-C-O	-5.21	109.15	120.10
2	E	563	ASP	CB-CG-OD2	5.21	122.99	118.30
2	E	655	VAL	CA-C-O	5.21	131.03	120.10
2	F	559	ALA	CB-CA-C	5.21	117.91	110.10
1	A	84	PHE	N-CA-CB	-5.20	101.23	110.60
1	B	197	VAL	CA-CB-CG2	5.20	118.70	110.90
1	A	179	VAL	C-N-CA	5.19	134.69	121.70
2	F	562	GLU	CG-CD-OE2	-5.18	107.94	118.30
2	F	615	THR	CA-C-O	-5.18	109.22	120.10
1	A	201	PRO	C-N-CA	5.17	134.64	121.70
2	E	564	TYR	CB-CG-CD2	5.17	124.10	121.00
1	B	98	GLN	CA-CB-CG	5.17	124.78	113.40
2	E	582	PHE	O-C-N	5.17	130.97	122.70
2	E	656	GLU	CG-CD-OE2	-5.17	107.96	118.30
2	D	623	PRO	C-N-CA	5.16	134.60	121.70
2	D	670	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	190	MET	CA-CB-CG	5.16	122.07	113.30
1	C	192	ASN	CB-CA-C	5.14	120.69	110.40
2	F	654	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	C	109	ASP	N-CA-CB	-5.12	101.38	110.60
2	E	663	ARG	CD-NE-CZ	5.11	130.76	123.60
2	F	623	PRO	C-N-CA	5.11	134.48	121.70
1	A	230	GLN	O-C-N	5.11	131.88	123.20
2	E	623	PRO	C-N-CA	5.09	134.44	121.70
2	D	514	VAL	C-N-CA	5.09	133.00	122.30
2	E	621	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	219	ILE	CB-CA-C	5.09	121.78	111.60
1	B	210	ALA	N-CA-CB	5.09	117.22	110.10
2	D	671	GLU	CG-CD-OE2	-5.08	108.13	118.30
1	A	118	ALA	CA-C-O	-5.08	109.44	120.10
1	A	204	LEU	CB-CG-CD1	-5.07	102.38	111.00
2	E	654	TYR	O-C-N	5.07	130.81	122.70
1	C	136	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	C	126	ARG	N-CA-CB	5.06	119.71	110.60
1	A	171	LEU	CB-CG-CD1	5.06	119.60	111.00
1	C	216	ILE	C-N-CA	5.05	134.34	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	179	VAL	C-N-CA	5.05	134.32	121.70
1	A	126	ARG	CB-CG-CD	5.05	124.72	111.60
1	B	127	GLU	CG-CD-OE1	5.04	128.38	118.30
1	C	102	MET	CA-CB-CG	5.04	121.87	113.30
1	C	78	LEU	O-C-N	5.04	130.76	122.70
1	C	208	ASP	CB-CA-C	5.04	120.47	110.40
1	C	138	TYR	CB-CG-CD1	5.03	124.02	121.00
2	F	552	THR	N-CA-CB	5.02	119.84	110.30
1	C	197	VAL	CA-CB-CG2	5.01	118.42	110.90
1	A	126	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	A	39	PRO	N-CA-C	5.00	125.11	112.10

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ALA	Mainchain
1	A	156	THR	Mainchain
1	A	193	THR	Mainchain
1	A	216	ILE	Mainchain
1	B	118	ALA	Mainchain
1	B	156	THR	Mainchain
1	B	193	THR	Mainchain
1	B	216	ILE	Mainchain
1	C	118	ALA	Mainchain
1	C	156	THR	Mainchain
1	C	193	THR	Mainchain
1	C	216	ILE	Mainchain
2	D	532	TYR	Mainchain
2	D	533	VAL	Mainchain
2	D	545	MET	Mainchain
2	D	593	VAL	Mainchain
2	D	666	LYS	Mainchain
2	E	545	MET	Mainchain
2	E	666	LYS	Mainchain
2	F	593	VAL	Mainchain
2	F	666	LYS	Mainchain

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	1593	0	1595	152	0
1	B	1593	0	1595	160	0
1	C	1593	0	1595	154	0
2	D	1337	0	1328	155	0
2	E	1337	0	1329	156	0
2	F	1337	0	1329	153	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	D	32	0	13	9	0
4	E	32	0	13	7	0
4	F	32	0	13	7	0
5	A	63	0	0	7	0
5	B	62	0	0	14	0
5	C	62	0	0	10	0
5	D	36	0	0	9	0
5	E	39	0	0	8	0
5	F	40	0	0	10	0
All	All	9191	0	8810	857	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 48.

All (857) 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:A:40:LEU:HB3	1:A:41:PRO:HD2	1.47	0.97
1:C:211:ILE:HG13	1:C:212:THR:H	1.28	0.97
1:A:211:ILE:HG13	1:A:212:THR:H	1.30	0.96
1:B:211:ILE:HG13	1:B:212:THR:H	1.27	0.96
1:B:40:LEU:HB3	1:B:41:PRO:HD2	1.48	0.94
1:C:40:LEU:HB3	1:C:41:PRO:HD2	1.47	0.93
2:E:535:THR:HG22	2:E:536:VAL:O	1.69	0.92
2:D:535:THR:HG22	2:D:536:VAL:O	1.69	0.91
2:F:535:THR:HG22	2:F:536:VAL:O	1.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:655:VAL:HG23	2:D:668:VAL:HG22	1.52	0.88
2:F:655:VAL:HG23	2:F:668:VAL:HG22	1.55	0.88
1:C:84:PHE:HB3	1:C:198:VAL:HG11	1.53	0.88
2:D:532:TYR:N	4:D:678:GNP:H3'	1.89	0.88
1:C:216:ILE:HG22	1:C:217:ASN:H	1.38	0.87
1:C:212:THR:HG22	1:C:213:LEU:HG	1.57	0.87
1:B:84:PHE:HB3	1:B:198:VAL:HG11	1.56	0.86
1:B:216:ILE:HG22	1:B:217:ASN:H	1.41	0.86
1:C:212:THR:HB	1:C:214:LYS:H	1.40	0.86
1:A:84:PHE:HB3	1:A:198:VAL:HG11	1.57	0.86
1:A:212:THR:HG22	1:A:213:LEU:HG	1.58	0.86
1:A:212:THR:HB	1:A:214:LYS:H	1.41	0.85
2:E:655:VAL:HG23	2:E:668:VAL:HG22	1.57	0.85
2:D:508:VAL:HG22	2:D:579:LEU:HD12	1.59	0.85
1:A:216:ILE:HG22	1:A:217:ASN:H	1.42	0.84
1:B:212:THR:HB	1:B:214:LYS:H	1.41	0.84
2:E:508:VAL:HG22	2:E:579:LEU:HD12	1.58	0.83
2:F:508:VAL:HG22	2:F:579:LEU:HD12	1.59	0.83
2:E:532:TYR:N	4:E:678:GNP:H3'	1.94	0.83
2:E:576:ASP:O	2:E:577:VAL:HB	1.76	0.82
1:B:212:THR:HG22	1:B:213:LEU:HG	1.60	0.82
2:E:620:ARG:O	2:E:626:ILE:HD11	1.79	0.82
2:F:576:ASP:O	2:F:577:VAL:HB	1.79	0.81
1:B:126:ARG:HA	5:B:277:HOH:O	1.80	0.81
1:A:210:ALA:O	1:A:214:LYS:HD2	1.81	0.81
2:D:576:ASP:O	2:D:577:VAL:HB	1.79	0.81
2:F:620:ARG:O	2:F:626:ILE:HD11	1.81	0.81
2:D:620:ARG:O	2:D:626:ILE:HD11	1.82	0.79
1:B:210:ALA:O	1:B:214:LYS:HD2	1.82	0.79
2:F:532:TYR:N	4:F:678:GNP:H3'	1.98	0.79
2:F:532:TYR:O	2:F:533:VAL:HG13	1.83	0.77
1:C:81:GLU:HA	1:C:188:ASN:HA	1.66	0.77
1:A:147:ILE:O	1:A:152:ARG:NH1	2.18	0.76
2:D:532:TYR:O	2:D:533:VAL:HG13	1.84	0.76
1:A:199:PHE:HB3	5:A:281:HOH:O	1.85	0.76
1:A:81:GLU:HA	1:A:188:ASN:HA	1.66	0.76
1:A:37:ARG:N	1:A:38:PRO:HD3	1.99	0.76
1:B:37:ARG:N	1:B:38:PRO:HD3	2.00	0.76
1:B:147:ILE:O	1:B:152:ARG:NH1	2.18	0.75
1:B:197:VAL:HG21	2:E:534:PRO:HG2	1.68	0.75
1:A:212:THR:HG22	1:A:213:LEU:H	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ILE:O	1:C:152:ARG:NH1	2.19	0.75
1:A:132:LEU:HD12	1:A:167:ASN:HD22	1.50	0.75
1:B:181:ILE:HG23	1:B:188:ASN:HD21	1.50	0.75
1:A:217:ASN:HB3	1:A:218:PRO:HD3	1.68	0.75
1:A:181:ILE:HG23	1:A:188:ASN:HD21	1.51	0.75
2:E:617:ILE:O	2:E:620:ARG:HB2	1.87	0.75
1:B:81:GLU:HA	1:B:188:ASN:HA	1.68	0.75
1:B:37:ARG:HD3	1:B:101:ASN:HD21	1.52	0.74
1:A:217:ASN:CB	2:D:536:VAL:HG11	2.18	0.74
2:F:668:VAL:HG23	5:F:213:HOH:O	1.88	0.74
1:C:210:ALA:O	1:C:214:LYS:HD2	1.86	0.74
2:E:532:TYR:C	2:E:533:VAL:HG22	2.09	0.74
1:C:217:ASN:HB3	1:C:218:PRO:HD3	1.70	0.73
1:B:217:ASN:HB3	1:B:218:PRO:HD3	1.71	0.73
1:C:217:ASN:CB	2:F:536:VAL:HG11	2.18	0.73
1:B:202:ASN:HA	5:B:277:HOH:O	1.88	0.72
1:A:51:HIS:HA	1:A:54:GLU:HG2	1.71	0.72
1:B:217:ASN:HB2	2:E:536:VAL:HG11	1.72	0.72
2:D:617:ILE:O	2:D:620:ARG:HB2	1.88	0.72
1:A:198:VAL:HG22	2:D:561:GLN:OE1	1.89	0.72
1:B:217:ASN:CB	2:E:536:VAL:HG11	2.19	0.72
2:F:617:ILE:O	2:F:620:ARG:HB2	1.90	0.72
4:D:678:GNP:O3G	5:D:1:HOH:O	2.08	0.72
1:C:197:VAL:HG21	2:F:534:PRO:HG2	1.71	0.72
1:C:191:THR:HB	2:F:532:TYR:OH	1.90	0.71
1:A:37:ARG:HD3	1:A:101:ASN:HD21	1.55	0.71
1:C:198:VAL:HG22	2:F:561:GLN:OE1	1.90	0.71
1:C:212:THR:HG22	1:C:213:LEU:H	1.55	0.71
2:F:539:ASN:N	2:F:539:ASN:HD22	1.88	0.71
1:B:213:LEU:HD22	5:E:24:HOH:O	1.91	0.71
1:A:217:ASN:HB2	2:D:536:VAL:HG11	1.71	0.71
1:B:132:LEU:HD12	1:B:167:ASN:HD22	1.55	0.71
1:C:141:VAL:HG22	1:C:222:PHE:CD1	2.26	0.70
1:B:198:VAL:HG22	2:E:561:GLN:OE1	1.91	0.70
1:B:212:THR:HG22	1:B:213:LEU:H	1.56	0.70
1:C:37:ARG:N	1:C:38:PRO:HD3	2.03	0.70
1:C:217:ASN:HB2	2:F:536:VAL:HG11	1.72	0.70
2:F:569:PRO:HB3	2:F:604:HIS:NE2	2.05	0.70
1:B:40:LEU:HD23	1:B:101:ASN:HB3	1.73	0.70
1:A:197:VAL:HG21	2:D:534:PRO:HG2	1.72	0.70
1:B:51:HIS:HA	1:B:54:GLU:HG2	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLU:HB3	5:C:245:HOH:O	1.91	0.70
1:A:191:THR:HB	2:D:532:TYR:OH	1.92	0.70
2:E:569:PRO:HB3	2:E:604:HIS:NE2	2.05	0.70
2:E:539:ASN:N	2:E:539:ASN:HD22	1.90	0.70
1:B:94:ARG:HG3	5:B:264:HOH:O	1.92	0.70
1:B:211:ILE:HG13	1:B:212:THR:N	2.06	0.70
2:D:501:PRO:HG3	2:D:550:PRO:HB2	1.74	0.69
2:D:569:PRO:HB3	2:D:604:HIS:NE2	2.07	0.69
1:C:181:ILE:HG23	1:C:188:ASN:HD21	1.56	0.69
1:C:51:HIS:HA	1:C:54:GLU:HG2	1.73	0.69
1:A:44:GLN:HB2	1:A:100:TYR:HB3	1.74	0.69
1:B:141:VAL:HG22	1:B:222:PHE:CD1	2.27	0.69
1:C:44:GLN:HB2	1:C:100:TYR:HB3	1.74	0.69
1:C:37:ARG:HD3	1:C:101:ASN:HD21	1.58	0.69
1:C:132:LEU:HD12	1:C:167:ASN:HD22	1.58	0.69
2:F:501:PRO:HG3	2:F:550:PRO:HB2	1.74	0.69
1:A:108:PHE:HD1	1:A:116:LEU:HD23	1.58	0.68
1:A:141:VAL:HG22	1:A:222:PHE:CD2	2.28	0.68
2:D:539:ASN:N	2:D:539:ASN:HD22	1.89	0.68
2:E:617:ILE:HD11	2:E:656:GLU:HB3	1.75	0.68
1:C:199:PHE:HB3	5:C:288:HOH:O	1.93	0.68
2:F:617:ILE:HD11	2:F:656:GLU:HB3	1.76	0.68
1:B:37:ARG:NH1	1:B:97:GLN:HB3	2.09	0.68
1:C:40:LEU:HD23	1:C:101:ASN:HB3	1.76	0.68
2:F:667:ASN:ND2	5:F:213:HOH:O	2.27	0.68
4:F:678:GNP:O3G	5:F:3:HOH:O	2.10	0.68
1:C:125:LEU:HD11	1:C:174:LEU:HD22	1.75	0.68
2:E:646:ALA:O	2:E:649:LEU:N	2.26	0.68
2:F:646:ALA:O	2:F:649:LEU:N	2.27	0.68
1:C:37:ARG:NH1	1:C:97:GLN:HB3	2.09	0.67
2:E:501:PRO:HG3	2:E:550:PRO:HB2	1.76	0.67
1:A:200:GLY:N	1:A:201:PRO:HD2	2.10	0.67
1:C:200:GLY:N	1:C:201:PRO:HD2	2.09	0.67
1:B:138:TYR:HA	5:B:267:HOH:O	1.94	0.67
1:B:44:GLN:HB2	1:B:100:TYR:HB3	1.76	0.67
1:B:108:PHE:HD1	1:B:116:LEU:HD23	1.58	0.67
1:A:40:LEU:HD23	1:A:101:ASN:HB3	1.75	0.66
1:B:48:SER:OG	1:B:51:HIS:HB2	1.94	0.66
1:C:108:PHE:HD1	1:C:116:LEU:HD23	1.60	0.66
1:B:125:LEU:HD11	1:B:174:LEU:HD22	1.77	0.66
2:E:667:ASN:ND2	5:E:297:HOH:O	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:HD3	1:B:101:ASN:ND2	2.11	0.66
1:B:215:ALA:C	1:B:216:ILE:HD12	2.16	0.66
2:D:633:LYS:HG2	2:D:634:GLN:HE21	1.61	0.66
1:B:188:ASN:O	1:B:189:LYS:HB2	1.96	0.65
1:A:215:ALA:C	1:A:216:ILE:HD12	2.17	0.65
2:D:617:ILE:HD11	2:D:656:GLU:HB3	1.78	0.65
1:C:215:ALA:C	1:C:216:ILE:HD12	2.16	0.65
1:A:40:LEU:HD23	1:A:101:ASN:CB	2.27	0.65
1:C:211:ILE:HG13	1:C:212:THR:N	2.08	0.65
2:F:606:PRO:O	2:F:607:LYS:HB2	1.96	0.65
1:A:37:ARG:HD3	1:A:101:ASN:ND2	2.11	0.65
1:B:212:THR:HG21	1:B:214:LYS:HE3	1.79	0.65
2:E:633:LYS:HG2	2:E:634:GLN:HE21	1.62	0.65
2:E:606:PRO:O	2:E:607:LYS:HB2	1.95	0.65
1:C:212:THR:HG21	1:C:214:LYS:HE3	1.79	0.65
1:C:48:SER:OG	1:C:51:HIS:HB2	1.97	0.65
1:B:169:GLN:HA	1:B:169:GLN:HE21	1.61	0.64
1:B:191:THR:HB	2:E:532:TYR:OH	1.97	0.64
2:D:633:LYS:HG2	2:D:634:GLN:NE2	2.12	0.64
1:C:188:ASN:O	1:C:189:LYS:HB2	1.96	0.64
2:F:633:LYS:HG2	2:F:634:GLN:HE21	1.63	0.64
1:A:188:ASN:O	1:A:189:LYS:HB2	1.97	0.64
2:F:542:VAL:HA	5:F:90:HOH:O	1.98	0.64
2:D:646:ALA:O	2:D:649:LEU:N	2.30	0.64
1:A:37:ARG:NH1	1:A:97:GLN:HB3	2.13	0.64
1:A:217:ASN:CG	2:D:536:VAL:HG11	2.18	0.64
1:C:37:ARG:HD3	1:C:101:ASN:ND2	2.11	0.64
1:C:40:LEU:HD23	1:C:101:ASN:CB	2.28	0.63
2:D:612:LEU:HD23	2:D:654:TYR:HB2	1.80	0.63
1:B:130:GLU:HG3	1:B:131:PRO:HD2	1.81	0.63
1:B:40:LEU:HD23	1:B:101:ASN:CB	2.28	0.63
1:B:78:LEU:HG	5:B:263:HOH:O	1.97	0.63
1:C:217:ASN:CG	2:F:536:VAL:HG11	2.17	0.63
2:E:532:TYR:O	2:E:533:VAL:HG13	1.99	0.63
1:A:169:GLN:HE21	1:A:169:GLN:HA	1.63	0.63
2:D:674:LEU:O	2:D:674:LEU:HD12	1.99	0.63
2:E:661:THR:HG21	2:E:663:ARG:HB3	1.80	0.63
1:B:47:VAL:HG13	1:B:52:LEU:HD21	1.81	0.63
2:E:674:LEU:O	2:E:674:LEU:HD12	1.99	0.63
2:E:532:TYR:O	2:E:533:VAL:HG22	1.98	0.62
1:A:211:ILE:HG13	1:A:212:THR:N	2.09	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:661:THR:CG2	2:E:663:ARG:HB3	2.29	0.62
1:B:126:ARG:HG2	5:B:277:HOH:O	1.98	0.62
2:E:633:LYS:HG2	2:E:634:GLN:NE2	2.14	0.62
1:B:200:GLY:N	1:B:201:PRO:HD2	2.14	0.62
1:C:47:VAL:HG13	1:C:52:LEU:HD21	1.82	0.62
1:B:216:ILE:HD13	2:E:537:PHE:CD1	2.35	0.62
2:D:515:GLY:HA2	4:D:678:GNP:H8	1.82	0.62
2:E:668:VAL:HG23	5:E:297:HOH:O	1.99	0.62
2:F:503:THR:O	2:F:504:ILE:HG13	1.98	0.62
1:C:180:GLN:HG3	5:C:270:HOH:O	2.00	0.62
1:A:47:VAL:HG13	1:A:52:LEU:HD21	1.81	0.62
1:C:179:VAL:HG21	1:C:230:GLN:HG3	1.81	0.62
2:D:503:THR:O	2:D:504:ILE:HG13	1.98	0.62
2:E:668:VAL:HG12	2:E:669:PHE:CD2	2.35	0.62
1:A:125:LEU:HD11	1:A:174:LEU:HD22	1.82	0.62
1:C:169:GLN:HA	1:C:169:GLN:HE21	1.63	0.62
2:E:518:CYS:HB3	2:E:528:PHE:CE2	2.35	0.62
2:F:653:LYS:HD2	2:F:655:VAL:HG12	1.82	0.62
2:F:668:VAL:HG12	2:F:669:PHE:CD2	2.35	0.62
1:C:130:GLU:HG3	1:C:131:PRO:HD2	1.82	0.61
2:D:668:VAL:HG12	2:D:669:PHE:CD2	2.34	0.61
1:C:153:VAL:N	1:C:154:PRO:HD2	2.14	0.61
1:C:216:ILE:HD13	2:F:537:PHE:CD1	2.35	0.61
1:A:153:VAL:N	1:A:154:PRO:HD2	2.15	0.61
2:D:661:THR:CG2	2:D:663:ARG:HB3	2.30	0.61
1:B:217:ASN:CG	2:E:536:VAL:HG11	2.20	0.61
2:F:515:GLY:HA2	4:F:678:GNP:H8	1.81	0.61
2:F:649:LEU:O	2:F:650:LYS:HB2	2.00	0.61
2:D:606:PRO:O	2:D:607:LYS:HB2	1.99	0.61
2:D:653:LYS:HD3	2:D:654:TYR:O	2.01	0.61
2:D:661:THR:HG21	2:D:663:ARG:HB3	1.83	0.61
2:F:653:LYS:HD3	2:F:654:TYR:O	2.01	0.61
2:F:661:THR:HG21	2:F:663:ARG:HB3	1.83	0.61
1:B:104:LEU:HD12	1:B:105:PRO:HD2	1.82	0.61
2:D:535:THR:HG22	2:D:536:VAL:C	2.21	0.61
1:B:99:LYS:NZ	1:B:111:TYR:OH	2.29	0.61
2:F:633:LYS:HG2	2:F:634:GLN:NE2	2.15	0.61
1:B:211:ILE:CG1	1:B:212:THR:H	2.09	0.60
1:C:140:HIS:NE2	1:C:156:THR:OG1	2.34	0.60
2:E:622:ASP:O	2:E:625:THR:OG1	2.19	0.60
1:B:153:VAL:N	1:B:154:PRO:HD2	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:553:LEU:HD22	2:E:673:ILE:HD11	1.83	0.60
2:F:674:LEU:O	2:F:674:LEU:HD12	2.02	0.60
1:C:192:ASN:OD1	1:C:227:LEU:HB3	2.02	0.60
2:E:515:GLY:HA2	4:E:678:GNP:H8	1.82	0.60
1:A:179:VAL:HG21	1:A:230:GLN:HG3	1.83	0.60
2:F:508:VAL:CG2	2:F:579:LEU:HD12	2.31	0.60
1:C:184:HIS:O	1:C:187:GLN:HG2	2.02	0.60
2:D:518:CYS:HB3	2:D:528:PHE:CE2	2.37	0.60
2:E:653:LYS:HD2	2:E:655:VAL:HG12	1.83	0.60
1:B:211:ILE:O	1:B:215:ALA:N	2.34	0.60
1:A:216:ILE:HD13	2:D:537:PHE:CD1	2.36	0.60
2:F:661:THR:CG2	2:F:663:ARG:HB3	2.31	0.60
1:A:52:LEU:O	1:A:56:ASN:HB2	2.02	0.59
1:A:130:GLU:HG3	1:A:131:PRO:HD2	1.84	0.59
1:A:217:ASN:CB	1:A:218:PRO:HD3	2.33	0.59
2:D:542:VAL:HA	5:D:52:HOH:O	2.02	0.59
1:A:83:ILE:HD13	1:A:181:ILE:HD12	1.83	0.59
1:C:78:LEU:HG	5:C:270:HOH:O	2.00	0.59
2:E:653:LYS:HD3	2:E:654:TYR:O	2.02	0.59
1:C:104:LEU:HD12	1:C:105:PRO:HD2	1.84	0.59
1:A:215:ALA:O	1:A:216:ILE:HD12	2.02	0.59
1:C:215:ALA:O	1:C:216:ILE:HD12	2.02	0.59
1:A:104:LEU:HD12	1:A:105:PRO:HD2	1.85	0.59
1:B:184:HIS:O	1:B:187:GLN:HG2	2.03	0.59
2:D:508:VAL:CG2	2:D:579:LEU:HD12	2.32	0.59
1:A:43:GLN:HA	1:A:101:ASN:HA	1.85	0.59
1:C:99:LYS:NZ	1:C:111:TYR:OH	2.29	0.59
1:B:52:LEU:O	1:B:56:ASN:HB2	2.03	0.59
1:A:119:VAL:HG23	1:A:120:ILE:HD13	1.85	0.58
1:C:211:ILE:O	1:C:215:ALA:N	2.36	0.58
1:A:100:TYR:CE2	1:A:106:VAL:HG21	2.38	0.58
1:B:37:ARG:NH1	1:B:45:PHE:HB2	2.18	0.58
2:E:503:THR:O	2:E:504:ILE:HG13	2.03	0.58
2:E:535:THR:HG22	2:E:536:VAL:C	2.22	0.58
2:E:649:LEU:O	2:E:650:LYS:HB2	2.04	0.58
1:A:211:ILE:O	1:A:215:ALA:N	2.35	0.58
1:B:197:VAL:O	2:E:564:TYR:HE2	1.86	0.58
2:F:547:GLY:N	5:F:41:HOH:O	2.33	0.58
1:A:181:ILE:HG23	1:A:188:ASN:ND2	2.18	0.58
1:A:216:ILE:HG22	2:D:536:VAL:HG13	1.84	0.58
2:F:518:CYS:HB3	2:F:528:PHE:CE2	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:OG	1:A:51:HIS:HB2	2.03	0.58
2:E:568:ARG:O	2:E:571:SER:HB2	2.04	0.58
1:A:192:ASN:OD1	1:A:227:LEU:HB3	2.03	0.58
1:C:132:LEU:HA	1:C:167:ASN:ND2	2.19	0.58
1:C:52:LEU:O	1:C:56:ASN:HB2	2.03	0.58
1:B:179:VAL:HG21	1:B:230:GLN:HG3	1.84	0.58
2:F:535:THR:HG22	2:F:536:VAL:C	2.22	0.58
1:C:197:VAL:O	2:F:564:TYR:HE2	1.86	0.58
2:F:587:PRO:HG2	2:F:634:GLN:OE1	2.04	0.58
1:A:184:HIS:O	1:A:187:GLN:HG2	2.03	0.58
1:A:37:ARG:NH1	1:A:45:PHE:HB2	2.19	0.58
1:B:215:ALA:O	1:B:216:ILE:HD12	2.04	0.58
2:E:590:PHE:O	2:E:593:VAL:HB	2.04	0.58
1:B:43:GLN:HA	1:B:101:ASN:HA	1.85	0.57
1:B:192:ASN:OD1	1:B:227:LEU:HB3	2.04	0.57
2:F:612:LEU:HD23	2:F:654:TYR:HB2	1.85	0.57
2:F:655:VAL:CG2	2:F:668:VAL:HG22	2.32	0.57
1:C:213:LEU:HD22	5:F:47:HOH:O	2.04	0.57
1:C:217:ASN:CB	1:C:218:PRO:HD3	2.33	0.57
2:F:590:PHE:O	2:F:593:VAL:HB	2.04	0.57
1:A:197:VAL:O	2:D:564:TYR:HE2	1.87	0.57
2:D:659:ALA:HB2	5:D:274:HOH:O	2.04	0.57
1:A:132:LEU:HA	1:A:167:ASN:ND2	2.19	0.57
1:A:60:GLU:HB3	5:A:245:HOH:O	2.03	0.57
2:D:568:ARG:O	2:D:571:SER:HB2	2.05	0.57
1:B:132:LEU:HA	1:B:167:ASN:ND2	2.20	0.57
1:B:181:ILE:HG23	1:B:188:ASN:ND2	2.19	0.57
1:B:217:ASN:CB	1:B:218:PRO:HD3	2.33	0.57
1:C:43:GLN:HA	1:C:101:ASN:HA	1.87	0.57
2:F:622:ASP:O	2:F:625:THR:OG1	2.21	0.57
2:D:590:PHE:O	2:D:593:VAL:HB	2.05	0.57
1:B:96:VAL:HG13	1:B:106:VAL:HG11	1.87	0.57
1:B:81:GLU:CA	1:B:188:ASN:HA	2.35	0.57
2:D:653:LYS:HD2	2:D:655:VAL:HG12	1.86	0.56
1:A:40:LEU:HB3	1:A:41:PRO:CD	2.30	0.56
1:B:96:VAL:HG13	1:B:106:VAL:CG1	2.35	0.56
1:A:106:VAL:HB	5:A:253:HOH:O	2.04	0.56
2:E:590:PHE:CZ	2:E:645:LEU:HG	2.41	0.56
2:F:597:TRP:HA	2:F:597:TRP:CE3	2.41	0.56
1:A:102:MET:SD	2:E:674:LEU:HD13	2.44	0.56
1:B:100:TYR:CE2	1:B:106:VAL:HG21	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:CA	1:C:188:ASN:HA	2.34	0.56
2:D:509:VAL:HG12	2:D:558:THR:HG21	1.85	0.56
2:E:522:SER:HB3	2:E:665:LEU:HD21	1.87	0.56
1:A:96:VAL:HG13	1:A:106:VAL:HG11	1.87	0.56
2:D:590:PHE:CZ	2:D:645:LEU:HG	2.40	0.56
1:A:157:LEU:HD21	1:A:232:GLU:O	2.05	0.56
1:C:157:LEU:HD21	1:C:232:GLU:O	2.06	0.56
1:C:215:ALA:HB1	2:F:567:LEU:HD22	1.87	0.56
2:F:522:SER:HB3	2:F:665:LEU:HD21	1.86	0.56
1:A:93:VAL:HG13	1:A:120:ILE:CD1	2.35	0.56
1:A:212:THR:HG21	1:A:214:LYS:HE3	1.86	0.56
2:F:610:PHE:O	2:F:652:VAL:HG22	2.06	0.56
2:F:620:ARG:NH2	2:F:656:GLU:OE1	2.39	0.56
2:E:508:VAL:CG2	2:E:579:LEU:HD12	2.32	0.56
1:A:211:ILE:CG1	1:A:212:THR:H	2.13	0.56
2:D:610:PHE:O	2:D:652:VAL:HG22	2.06	0.56
2:D:649:LEU:O	2:D:650:LYS:HB2	2.05	0.56
2:E:509:VAL:HG12	2:E:558:THR:HG21	1.88	0.56
2:E:512:GLY:O	2:E:513:ALA:HB3	2.06	0.56
1:A:99:LYS:NZ	1:A:111:TYR:OH	2.30	0.55
1:C:37:ARG:NH1	1:C:45:PHE:HB2	2.21	0.55
2:D:655:VAL:CG2	2:D:668:VAL:HG22	2.29	0.55
2:F:590:PHE:CZ	2:F:645:LEU:HG	2.41	0.55
1:A:44:GLN:CB	1:A:100:TYR:HB3	2.36	0.55
1:C:216:ILE:O	1:C:218:PRO:HD2	2.06	0.55
1:C:83:ILE:O	1:C:85:ARG:N	2.39	0.55
1:A:216:ILE:CG2	2:D:536:VAL:HG13	2.36	0.55
1:C:217:ASN:ND2	2:F:536:VAL:HG11	2.21	0.55
2:D:522:SER:HB3	2:D:665:LEU:HD21	1.87	0.55
2:D:620:ARG:NH2	2:D:656:GLU:OE1	2.39	0.55
1:C:216:ILE:HG22	2:F:536:VAL:HG13	1.87	0.55
2:F:568:ARG:O	2:F:571:SER:HB2	2.06	0.55
1:A:215:ALA:HB1	2:D:567:LEU:HD22	1.89	0.55
1:A:81:GLU:CA	1:A:188:ASN:HA	2.34	0.55
2:D:646:ALA:O	2:D:647:ARG:C	2.43	0.55
2:E:613:VAL:HA	2:E:655:VAL:O	2.07	0.55
2:F:646:ALA:O	2:F:647:ARG:C	2.44	0.55
1:A:178:LEU:HB3	1:A:195:LEU:HD13	1.88	0.55
1:B:216:ILE:HG22	2:E:536:VAL:HG13	1.87	0.55
2:D:587:PRO:HG2	2:D:634:GLN:OE1	2.06	0.55
1:B:216:ILE:CG2	2:E:536:VAL:HG13	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:HG3	2:E:548:GLY:HA3	1.88	0.55
2:E:655:VAL:CG2	2:E:668:VAL:HG22	2.34	0.55
2:F:544:VAL:HG22	5:F:67:HOH:O	2.06	0.55
1:B:93:VAL:HG13	1:B:120:ILE:CD1	2.36	0.55
1:B:178:LEU:HB3	1:B:195:LEU:HD13	1.87	0.55
1:C:119:VAL:HG23	1:C:120:ILE:HD13	1.89	0.55
2:E:597:TRP:HA	2:E:597:TRP:CE3	2.42	0.55
1:C:144:PHE:CZ	1:C:152:ARG:HD2	2.41	0.55
1:A:94:ARG:NH2	5:A:248:HOH:O	2.40	0.54
1:A:83:ILE:O	1:A:85:ARG:N	2.40	0.54
2:E:573:PRO:HD3	5:E:257:HOH:O	2.07	0.54
1:A:217:ASN:ND2	2:D:536:VAL:HG11	2.23	0.54
2:E:645:LEU:HD13	2:E:649:LEU:HD12	1.90	0.54
2:E:610:PHE:O	2:E:652:VAL:HG22	2.06	0.54
1:C:93:VAL:HG13	1:C:120:ILE:CD1	2.37	0.54
2:D:595:GLU:O	2:D:596:LYS:HB2	2.07	0.54
2:E:665:LEU:HD12	2:E:669:PHE:CE2	2.42	0.54
2:F:639:PRO:HA	2:F:654:TYR:HE2	1.73	0.54
1:C:211:ILE:CG1	1:C:212:THR:H	2.10	0.54
2:E:612:LEU:HD23	2:E:654:TYR:HB2	1.88	0.54
2:F:512:GLY:O	2:F:513:ALA:HB3	2.07	0.54
2:F:509:VAL:HG12	2:F:558:THR:HG21	1.89	0.54
2:E:540:TYR:HB2	2:E:555:LEU:HB2	1.89	0.54
2:E:620:ARG:NH1	2:E:637:ILE:O	2.41	0.54
2:E:653:LYS:HD2	2:E:655:VAL:CG1	2.37	0.54
2:F:613:VAL:HA	2:F:655:VAL:O	2.08	0.54
1:B:44:GLN:CB	1:B:100:TYR:HB3	2.38	0.54
1:C:65:VAL:HG11	1:C:124:PHE:HB2	1.90	0.54
2:D:597:TRP:HA	2:D:597:TRP:CE3	2.43	0.54
2:D:665:LEU:HD12	2:D:669:PHE:CE2	2.43	0.54
2:F:505:LYS:HB3	2:F:575:THR:HA	1.89	0.54
1:A:189:LYS:HD3	2:D:532:TYR:CD1	2.43	0.53
1:B:216:ILE:O	1:B:218:PRO:HD2	2.08	0.53
1:C:44:GLN:CB	1:C:100:TYR:HB3	2.36	0.53
2:D:582:PHE:HE1	2:D:584:VAL:HA	1.73	0.53
2:F:553:LEU:HD22	2:F:673:ILE:HD11	1.90	0.53
1:A:213:LEU:HD22	5:D:81:HOH:O	2.08	0.53
1:B:144:PHE:CZ	1:B:152:ARG:HD2	2.44	0.53
2:D:620:ARG:NH1	2:D:637:ILE:O	2.42	0.53
2:E:649:LEU:C	2:E:650:LYS:HD3	2.28	0.53
2:E:620:ARG:NH2	2:E:656:GLU:OE1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:VAL:HG23	1:B:120:ILE:HD13	1.89	0.53
1:C:40:LEU:HB3	1:C:41:PRO:CD	2.30	0.53
2:E:587:PRO:HG2	2:E:634:GLN:OE1	2.08	0.53
2:D:540:TYR:HB2	2:D:555:LEU:HB2	1.90	0.53
2:E:532:TYR:C	2:E:533:VAL:CG2	2.77	0.53
1:A:70:VAL:O	1:A:74:GLN:HG3	2.08	0.53
1:C:116:LEU:N	1:C:117:PRO:CD	2.72	0.53
2:E:639:PRO:HA	2:E:654:TYR:HE2	1.72	0.53
2:D:582:PHE:CE1	2:D:584:VAL:HA	2.44	0.53
2:D:645:LEU:HD13	2:D:649:LEU:HD12	1.91	0.53
1:B:215:ALA:HB1	2:E:567:LEU:HD22	1.91	0.53
1:B:83:ILE:O	1:B:85:ARG:N	2.42	0.53
2:F:568:ARG:NH2	5:F:279:HOH:O	2.34	0.53
2:D:665:LEU:HD12	2:D:669:PHE:HE2	1.74	0.53
1:A:144:PHE:CZ	1:A:152:ARG:HD2	2.43	0.53
1:C:96:VAL:HG13	1:C:106:VAL:CG1	2.39	0.53
1:C:125:LEU:CD1	1:C:174:LEU:HD22	2.39	0.53
1:C:178:LEU:HB3	1:C:195:LEU:HD13	1.91	0.53
2:F:572:TYR:N	2:F:573:PRO:HD2	2.23	0.53
2:D:505:LYS:HB3	2:D:575:THR:HA	1.91	0.52
1:A:96:VAL:HG13	1:A:106:VAL:CG1	2.38	0.52
1:C:181:ILE:HG23	1:C:188:ASN:ND2	2.23	0.52
2:D:572:TYR:N	2:D:573:PRO:HD2	2.24	0.52
2:D:622:ASP:O	2:D:625:THR:OG1	2.26	0.52
1:A:65:VAL:HG11	1:A:124:PHE:HB2	1.91	0.52
1:A:140:HIS:NE2	1:A:156:THR:OG1	2.39	0.52
1:B:153:VAL:N	1:B:154:PRO:CD	2.73	0.52
1:B:83:ILE:HD12	1:B:84:PHE:CD2	2.44	0.52
1:C:153:VAL:N	1:C:154:PRO:CD	2.72	0.52
2:D:613:VAL:HA	2:D:655:VAL:O	2.08	0.52
1:A:216:ILE:O	1:A:218:PRO:HD2	2.10	0.52
1:B:157:LEU:HD21	1:B:232:GLU:O	2.09	0.52
2:D:516:LYS:HB2	4:D:678:GNP:O1B	2.09	0.52
2:D:553:LEU:HD22	2:D:673:ILE:HD11	1.90	0.52
2:D:561:GLN:HG3	5:D:1:HOH:O	2.09	0.52
2:E:582:PHE:CE1	2:E:584:VAL:HA	2.44	0.52
2:F:645:LEU:HD13	2:F:649:LEU:HD12	1.90	0.52
1:B:70:VAL:O	1:B:74:GLN:HG3	2.09	0.52
2:F:620:ARG:NH1	2:F:637:ILE:O	2.42	0.52
1:B:116:LEU:N	1:B:117:PRO:CD	2.72	0.52
2:D:512:GLY:O	2:D:513:ALA:HB3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:665:LEU:HD12	2:E:669:PHE:HE2	1.74	0.52
2:F:532:TYR:C	2:F:533:VAL:HG22	2.29	0.52
1:C:211:ILE:HB	2:F:570:LEU:CD1	2.40	0.52
2:F:582:PHE:CE1	2:F:584:VAL:HA	2.45	0.52
1:B:40:LEU:HB3	1:B:41:PRO:CD	2.31	0.52
1:A:116:LEU:N	1:A:117:PRO:CD	2.73	0.52
1:B:217:ASN:ND2	2:E:536:VAL:HG11	2.24	0.52
2:D:519:LEU:HD12	5:D:151:HOH:O	2.08	0.52
2:E:582:PHE:HE1	2:E:584:VAL:HA	1.74	0.52
1:B:177:PHE:O	1:B:180:GLN:HG2	2.10	0.52
1:B:65:VAL:HG11	1:B:124:PHE:HB2	1.92	0.52
1:C:107:ASP:C	1:C:109:ASP:H	2.14	0.52
1:C:216:ILE:CG2	1:C:217:ASN:H	2.13	0.52
2:D:503:THR:C	2:D:504:ILE:HG13	2.30	0.52
2:E:595:GLU:O	2:E:596:LYS:HB2	2.10	0.52
2:F:532:TYR:N	2:F:533:VAL:HG22	2.25	0.52
1:A:153:VAL:N	1:A:154:PRO:CD	2.72	0.51
1:C:216:ILE:HG22	1:C:217:ASN:N	2.17	0.51
2:D:532:TYR:C	2:D:533:VAL:HG22	2.30	0.51
2:D:532:TYR:O	2:D:533:VAL:CG1	2.56	0.51
2:F:582:PHE:HE1	2:F:584:VAL:HA	1.75	0.51
2:E:572:TYR:N	2:E:573:PRO:HD2	2.25	0.51
2:F:572:TYR:N	2:F:573:PRO:CD	2.73	0.51
2:F:503:THR:C	2:F:504:ILE:HG13	2.30	0.51
1:C:216:ILE:CG2	2:F:536:VAL:HG13	2.39	0.51
2:F:653:LYS:HD2	2:F:655:VAL:CG1	2.40	0.51
2:F:665:LEU:HD12	2:F:669:PHE:CE2	2.45	0.51
1:C:100:TYR:CE2	1:C:106:VAL:HG21	2.46	0.51
1:C:70:VAL:HG22	1:C:177:PHE:CD2	2.45	0.51
1:A:70:VAL:HG22	1:A:177:PHE:CD2	2.46	0.51
1:B:180:GLN:HG3	5:B:263:HOH:O	2.11	0.51
2:D:595:GLU:O	2:D:596:LYS:CB	2.58	0.51
2:D:639:PRO:HA	2:D:654:TYR:HE2	1.75	0.51
1:B:211:ILE:HB	2:E:570:LEU:CD1	2.41	0.51
2:D:559:ALA:HB3	2:D:564:TYR:CB	2.41	0.51
2:D:568:ARG:N	2:D:569:PRO:CD	2.73	0.51
2:F:516:LYS:HB2	4:F:678:GNP:O1B	2.10	0.51
2:D:508:VAL:HG12	2:D:516:LYS:HG2	1.93	0.51
2:F:508:VAL:HG12	2:F:516:LYS:HG2	1.93	0.51
2:F:595:GLU:O	2:F:596:LYS:HB2	2.10	0.51
2:E:539:ASN:N	2:E:539:ASN:ND2	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:505:LYS:HB3	2:E:575:THR:HA	1.93	0.51
2:E:632:ASN:O	2:E:633:LYS:HD2	2.11	0.51
1:C:189:LYS:HZ3	2:F:532:TYR:HD1	1.58	0.51
1:B:125:LEU:CD1	1:B:174:LEU:HD22	2.41	0.51
1:B:70:VAL:HG22	1:B:177:PHE:CD2	2.46	0.51
1:C:189:LYS:HD3	2:F:532:TYR:CD1	2.46	0.51
2:F:665:LEU:HD12	2:F:669:PHE:HE2	1.76	0.51
2:D:539:ASN:N	2:D:539:ASN:ND2	2.59	0.50
2:D:559:ALA:O	2:D:568:ARG:NH2	2.43	0.50
2:F:532:TYR:O	2:F:533:VAL:CG1	2.56	0.50
2:F:568:ARG:N	2:F:569:PRO:CD	2.74	0.50
1:A:151:GLN:HA	1:A:154:PRO:HG2	1.93	0.50
1:C:70:VAL:O	1:C:74:GLN:HG3	2.10	0.50
1:A:211:ILE:HB	2:D:570:LEU:CD1	2.41	0.50
1:A:133:LEU:O	1:A:134:THR:CB	2.60	0.50
2:D:666:LYS:HB2	5:D:17:HOH:O	2.11	0.50
1:C:157:LEU:HD23	1:C:233:LEU:HA	1.93	0.50
2:E:568:ARG:N	2:E:569:PRO:CD	2.74	0.50
2:F:595:GLU:O	2:F:596:LYS:CB	2.60	0.50
2:F:598:VAL:CB	2:F:599:PRO:HD3	2.42	0.50
1:C:94:ARG:NH2	5:C:247:HOH:O	2.43	0.50
2:F:653:LYS:HG2	2:F:654:TYR:H	1.76	0.50
1:B:63:PRO:O	1:B:67:ARG:HG3	2.12	0.50
2:D:519:LEU:HB3	5:D:274:HOH:O	2.11	0.50
2:E:673:ILE:O	2:E:677:LEU:HG	2.11	0.50
2:D:547:GLY:N	5:D:131:HOH:O	2.38	0.50
2:F:646:ALA:O	2:F:650:LYS:N	2.44	0.50
1:A:216:ILE:HG22	1:A:217:ASN:N	2.21	0.49
1:B:107:ASP:C	1:B:109:ASP:H	2.16	0.49
1:B:142:VAL:HG21	5:B:246:HOH:O	2.12	0.49
1:C:63:PRO:O	1:C:67:ARG:HG3	2.12	0.49
1:C:84:PHE:CD1	1:C:118:ALA:HB1	2.47	0.49
1:C:177:PHE:O	1:C:180:GLN:HG2	2.12	0.49
1:A:45:PHE:HZ	1:A:120:ILE:HG23	1.77	0.49
2:F:559:ALA:O	2:F:568:ARG:NH2	2.43	0.49
1:B:217:ASN:HB3	1:B:218:PRO:CD	2.41	0.49
2:E:523:TYR:HB2	2:E:665:LEU:HD11	1.94	0.49
1:A:107:ASP:C	1:A:109:ASP:H	2.15	0.49
1:B:81:GLU:HA	1:B:188:ASN:CA	2.39	0.49
1:C:189:LYS:HZ3	2:F:532:TYR:HB2	1.76	0.49
1:C:83:ILE:HD12	1:C:84:PHE:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:540:TYR:HB2	2:F:555:LEU:HB2	1.94	0.49
1:A:157:LEU:CD2	1:A:233:LEU:HA	2.42	0.49
2:D:653:LYS:HD2	2:D:655:VAL:CG1	2.42	0.49
1:C:199:PHE:O	1:C:202:ASN:HB2	2.13	0.49
2:E:516:LYS:NZ	4:E:678:GNP:O1G	2.44	0.49
1:A:200:GLY:N	1:A:201:PRO:CD	2.76	0.49
1:A:212:THR:CG2	1:A:213:LEU:H	2.22	0.49
1:B:47:VAL:CG2	1:B:48:SER:N	2.76	0.49
2:F:673:ILE:O	2:F:677:LEU:HG	2.12	0.49
1:A:177:PHE:O	1:A:180:GLN:HG2	2.12	0.49
1:A:84:PHE:CD1	1:A:118:ALA:HB1	2.46	0.49
1:C:133:LEU:O	1:C:134:THR:CB	2.61	0.49
2:D:572:TYR:N	2:D:573:PRO:CD	2.74	0.49
2:E:646:ALA:O	2:E:647:ARG:C	2.50	0.49
1:B:45:PHE:HZ	1:B:120:ILE:HG23	1.77	0.49
1:B:92:VAL:O	1:B:95:GLU:N	2.44	0.49
2:D:649:LEU:C	2:D:650:LYS:HD3	2.33	0.49
2:E:598:VAL:HB	2:E:599:PRO:HD3	1.95	0.49
2:E:564:TYR:HD1	2:E:567:LEU:HD12	1.78	0.48
2:F:501:PRO:HG3	2:F:550:PRO:CB	2.43	0.48
2:D:653:LYS:HG2	2:D:654:TYR:H	1.78	0.48
2:E:601:ILE:HG23	2:E:610:PHE:CE1	2.49	0.48
2:E:503:THR:C	2:E:504:ILE:HG13	2.33	0.48
1:A:157:LEU:HD23	1:A:233:LEU:HA	1.95	0.48
1:B:66:LEU:O	1:B:70:VAL:HB	2.14	0.48
2:D:523:TYR:HB2	2:D:665:LEU:HD11	1.96	0.48
1:A:83:ILE:CD1	1:A:181:ILE:HD12	2.43	0.48
2:D:501:PRO:HG3	2:D:550:PRO:CB	2.43	0.48
2:D:509:VAL:HG12	2:D:558:THR:CG2	2.44	0.48
2:E:539:ASN:HD22	2:E:539:ASN:H	1.61	0.48
1:B:194:ASN:O	1:B:197:VAL:HG23	2.13	0.48
1:B:83:ILE:HD13	1:B:181:ILE:HD12	1.96	0.48
2:D:673:ILE:O	2:D:677:LEU:HG	2.13	0.48
2:E:646:ALA:HA	2:E:651:ALA:HB3	1.95	0.48
2:D:598:VAL:CB	2:D:599:PRO:HD3	2.44	0.48
2:E:572:TYR:N	2:E:573:PRO:CD	2.76	0.48
2:F:519:LEU:HD12	5:F:121:HOH:O	2.13	0.48
1:A:165:GLU:OE2	1:A:169:GLN:OE1	2.31	0.48
1:A:217:ASN:HB3	1:A:218:PRO:CD	2.41	0.48
2:D:646:ALA:O	2:D:650:LYS:N	2.43	0.48
1:A:38:PRO:HA	1:A:39:PRO:HD2	1.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:CD1	1:B:105:PRO:HD2	2.42	0.48
1:C:217:ASN:HB3	1:C:218:PRO:CD	2.42	0.48
1:C:66:LEU:O	1:C:70:VAL:HB	2.14	0.48
2:E:583:SER:N	2:E:589:SER:OG	2.43	0.48
2:E:595:GLU:O	2:E:596:LYS:CB	2.61	0.48
2:E:597:TRP:O	2:E:601:ILE:HB	2.14	0.48
2:E:643:GLU:O	2:E:644:LYS:C	2.52	0.48
2:F:598:VAL:HB	2:F:599:PRO:HD3	1.94	0.48
1:C:45:PHE:HZ	1:C:120:ILE:HG23	1.78	0.48
1:C:194:ASN:HA	1:C:197:VAL:HG23	1.95	0.47
1:C:211:ILE:HG13	2:F:570:LEU:HD13	1.95	0.47
2:D:583:SER:N	2:D:589:SER:OG	2.43	0.47
1:B:211:ILE:HG13	2:E:570:LEU:HD13	1.96	0.47
2:F:622:ASP:HA	2:F:623:PRO:HD2	1.83	0.47
1:B:133:LEU:O	1:B:134:THR:CB	2.62	0.47
1:A:81:GLU:HA	1:A:188:ASN:CA	2.39	0.47
2:E:611:LEU:HD23	2:E:653:LYS:O	2.15	0.47
2:F:596:LYS:HE3	2:F:597:TRP:CZ2	2.49	0.47
2:F:632:ASN:O	2:F:633:LYS:HD2	2.14	0.47
1:B:151:GLN:HA	1:B:154:PRO:HG2	1.96	0.47
1:B:185:SER:O	1:B:189:LYS:HA	2.15	0.47
2:D:643:GLU:O	2:D:644:LYS:C	2.52	0.47
2:D:617:ILE:HD13	2:D:656:GLU:OE1	2.15	0.47
2:E:646:ALA:O	2:E:650:LYS:N	2.47	0.47
2:F:597:TRP:O	2:F:601:ILE:HB	2.14	0.47
1:A:66:LEU:O	1:A:70:VAL:HB	2.14	0.47
1:B:140:HIS:NE2	1:B:156:THR:OG1	2.40	0.47
1:C:104:LEU:CD1	1:C:105:PRO:HD2	2.44	0.47
2:F:539:ASN:N	2:F:539:ASN:ND2	2.57	0.47
2:F:601:ILE:HG23	2:F:610:PHE:CE1	2.49	0.47
2:F:516:LYS:NZ	4:F:678:GNP:O1G	2.46	0.47
1:B:205:TRP:HZ3	5:B:277:HOH:O	1.97	0.47
2:F:569:PRO:HG2	5:F:224:HOH:O	2.13	0.47
1:A:199:PHE:O	1:A:202:ASN:HB2	2.14	0.47
1:B:86:ARG:HG2	5:B:237:HOH:O	2.15	0.47
1:B:37:ARG:HH12	1:B:97:GLN:HB3	1.78	0.47
1:C:151:GLN:HA	1:C:154:PRO:HG2	1.95	0.47
2:D:564:TYR:HD1	2:D:567:LEU:HD12	1.80	0.47
2:D:617:ILE:CD1	2:D:656:GLU:HB3	2.44	0.47
1:B:84:PHE:CD1	1:B:118:ALA:HB1	2.50	0.47
2:D:642:ALA:HB3	2:D:654:TYR:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:653:LYS:HG2	2:E:654:TYR:H	1.79	0.47
2:F:590:PHE:CE1	2:F:645:LEU:HG	2.50	0.47
1:A:83:ILE:HD12	1:A:84:PHE:CD2	2.49	0.47
1:C:200:GLY:N	1:C:201:PRO:CD	2.77	0.47
2:D:596:LYS:HE3	2:D:597:TRP:CZ2	2.50	0.47
2:E:598:VAL:CB	2:E:599:PRO:HD3	2.45	0.47
2:F:564:TYR:HD1	2:F:567:LEU:HD12	1.80	0.47
2:F:583:SER:N	2:F:589:SER:OG	2.47	0.47
1:A:185:SER:O	1:A:189:LYS:HA	2.15	0.47
1:C:113:GLU:O	1:C:114:LEU:HB3	2.14	0.47
1:A:216:ILE:CG1	2:D:567:LEU:HD13	2.44	0.47
2:E:522:SER:HB3	2:E:665:LEU:CD2	2.45	0.47
2:F:539:ASN:HD22	2:F:539:ASN:H	1.59	0.47
1:A:193:THR:HG22	1:A:224:LYS:HD2	1.98	0.46
2:D:539:ASN:H	2:D:539:ASN:HD22	1.60	0.46
2:D:516:LYS:NZ	4:D:678:GNP:O1G	2.45	0.46
2:F:523:TYR:HB2	2:F:665:LEU:HD11	1.97	0.46
1:A:63:PRO:O	1:A:67:ARG:HG3	2.14	0.46
1:B:113:GLU:O	1:B:114:LEU:HB3	2.14	0.46
1:C:96:VAL:HG13	1:C:106:VAL:HG11	1.96	0.46
2:F:649:LEU:C	2:F:650:LYS:HD3	2.35	0.46
1:C:81:GLU:HA	1:C:188:ASN:CA	2.38	0.46
2:D:559:ALA:HB3	2:D:564:TYR:HB3	1.96	0.46
1:B:211:ILE:CG1	2:E:570:LEU:HD13	2.45	0.46
1:B:216:ILE:HG22	1:B:217:ASN:N	2.19	0.46
1:B:38:PRO:HA	1:B:39:PRO:HD2	1.63	0.46
1:B:60:GLU:HB3	5:B:257:HOH:O	2.15	0.46
2:D:597:TRP:O	2:D:601:ILE:HB	2.16	0.46
2:E:559:ALA:HB3	2:E:564:TYR:CB	2.45	0.46
2:E:617:ILE:HD13	2:E:656:GLU:OE1	2.15	0.46
1:B:189:LYS:HD3	2:E:532:TYR:CD1	2.51	0.46
1:B:216:ILE:CG1	2:E:567:LEU:HD13	2.46	0.46
1:C:157:LEU:CD2	1:C:233:LEU:HA	2.45	0.46
1:A:125:LEU:CD1	1:A:174:LEU:HD22	2.45	0.46
1:A:175:THR:O	1:A:179:VAL:HG23	2.15	0.46
1:A:191:THR:HB	2:D:532:TYR:HH	1.77	0.46
2:E:509:VAL:HG12	2:E:558:THR:CG2	2.46	0.46
1:A:189:LYS:NZ	2:D:532:TYR:HD1	2.13	0.46
1:B:133:LEU:CB	1:B:203:LEU:HD13	2.45	0.46
1:B:194:ASN:HA	1:B:197:VAL:HG23	1.97	0.46
1:B:94:ARG:NH2	5:B:247:HOH:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:THR:O	1:C:179:VAL:HG23	2.16	0.46
1:C:194:ASN:O	1:C:197:VAL:HG23	2.16	0.46
2:D:564:TYR:O	2:D:568:ARG:HB2	2.15	0.46
2:E:559:ALA:O	2:E:568:ARG:NH2	2.46	0.46
2:F:564:TYR:O	2:F:568:ARG:HB2	2.15	0.46
1:C:83:ILE:HD13	1:C:181:ILE:HD12	1.96	0.46
2:D:601:ILE:HG23	2:D:610:PHE:CE1	2.50	0.46
2:F:522:SER:HB3	2:F:665:LEU:CD2	2.46	0.46
1:A:113:GLU:O	1:A:114:LEU:HB3	2.15	0.46
1:A:189:LYS:HZ3	2:D:532:TYR:HB2	1.81	0.46
2:E:657:CYS:HA	2:E:664:GLY:HA3	1.98	0.46
2:F:617:ILE:CD1	2:F:656:GLU:HB3	2.45	0.46
1:A:104:LEU:CD1	1:A:105:PRO:HD2	2.45	0.45
1:C:37:ARG:HH12	1:C:97:GLN:CG	2.29	0.45
2:E:594:LYS:HG3	2:E:595:GLU:N	2.31	0.45
1:C:211:ILE:CG1	2:F:570:LEU:HD13	2.46	0.45
2:F:615:THR:HG22	2:F:616:GLN:HG3	1.98	0.45
1:B:141:VAL:HG22	1:B:222:PHE:CG	2.51	0.45
2:D:522:SER:HB3	2:D:665:LEU:CD2	2.45	0.45
2:D:598:VAL:HB	2:D:599:PRO:HD3	1.98	0.45
2:F:509:VAL:HG12	2:F:558:THR:CG2	2.46	0.45
1:A:194:ASN:O	1:A:197:VAL:HG23	2.17	0.45
1:B:86:ARG:NH1	5:B:292:HOH:O	2.50	0.45
1:C:165:GLU:OE2	1:C:169:GLN:OE1	2.34	0.45
2:D:509:VAL:HA	2:D:558:THR:OG1	2.15	0.45
2:D:590:PHE:CE1	2:D:645:LEU:HG	2.50	0.45
2:E:515:GLY:HA2	4:E:678:GNP:C8	2.46	0.45
2:E:542:VAL:HA	5:E:50:HOH:O	2.16	0.45
2:E:642:ALA:HB3	2:E:654:TYR:CE2	2.52	0.45
2:E:666:LYS:HB2	5:E:53:HOH:O	2.16	0.45
2:F:659:ALA:HB3	4:F:678:GNP:O6	2.16	0.45
1:A:72:TYR:O	1:A:75:ALA:HB3	2.17	0.45
2:D:532:TYR:O	2:D:532:TYR:CD2	2.70	0.45
1:C:216:ILE:CG1	2:F:567:LEU:HD13	2.47	0.45
1:B:157:LEU:CD2	1:B:233:LEU:HA	2.46	0.45
1:B:157:LEU:HD23	1:B:233:LEU:HA	1.99	0.45
1:C:185:SER:O	1:C:189:LYS:HA	2.16	0.45
2:D:611:LEU:HD23	2:D:653:LYS:O	2.17	0.45
2:F:533:VAL:H	2:F:534:PRO:HD3	1.82	0.45
1:B:116:LEU:N	1:B:117:PRO:HD3	2.31	0.45
1:C:62:ILE:HA	1:C:63:PRO:HD3	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:590:PHE:CE1	2:E:645:LEU:HG	2.52	0.45
2:E:650:LYS:N	2:E:650:LYS:HD3	2.32	0.45
1:C:116:LEU:O	1:C:120:ILE:HG12	2.17	0.45
2:F:559:ALA:HB3	2:F:564:TYR:CB	2.47	0.45
2:E:532:TYR:O	2:E:533:VAL:CG2	2.65	0.44
2:F:611:LEU:HD23	2:F:653:LYS:O	2.17	0.44
1:C:106:VAL:HB	5:C:240:HOH:O	2.17	0.44
1:A:40:LEU:HD23	1:A:101:ASN:HB2	1.98	0.44
1:B:93:VAL:HG13	1:B:120:ILE:HD11	1.99	0.44
2:D:622:ASP:HA	2:D:623:PRO:HD2	1.87	0.44
2:F:539:ASN:H	2:F:539:ASN:ND2	2.15	0.44
2:F:642:ALA:HB3	2:F:654:TYR:CE2	2.53	0.44
1:C:150:SER:HA	5:C:272:HOH:O	2.17	0.44
2:E:532:TYR:O	2:E:533:VAL:CG1	2.65	0.44
2:E:615:THR:HG22	2:E:616:GLN:HG3	2.00	0.44
2:E:617:ILE:CD1	2:E:656:GLU:HB3	2.46	0.44
1:B:181:ILE:CG2	1:B:188:ASN:HD21	2.24	0.44
1:A:189:LYS:NZ	2:D:532:TYR:CD1	2.85	0.44
2:E:521:ILE:HG22	2:E:527:LYS:O	2.17	0.44
2:E:596:LYS:HE3	2:E:597:TRP:CZ2	2.53	0.44
2:E:661:THR:O	2:E:662:GLN:HB2	2.18	0.44
1:A:86:ARG:HG2	5:A:236:HOH:O	2.17	0.44
1:B:165:GLU:OE2	1:B:169:GLN:OE1	2.35	0.44
2:D:515:GLY:HA2	4:D:678:GNP:C8	2.47	0.44
2:D:632:ASN:O	2:D:633:LYS:HD2	2.17	0.44
2:E:622:ASP:HA	2:E:623:PRO:HD2	1.82	0.44
1:C:191:THR:CB	2:F:532:TYR:OH	2.63	0.44
1:A:138:TYR:HB3	1:A:139:PRO:HD3	1.99	0.44
2:D:594:LYS:HB3	2:D:649:LEU:HD11	1.99	0.44
2:E:564:TYR:O	2:E:568:ARG:HB2	2.17	0.44
1:A:47:VAL:CG2	1:A:48:SER:N	2.81	0.44
2:F:509:VAL:HA	2:F:558:THR:OG1	2.17	0.44
2:F:584:VAL:CG1	2:F:620:ARG:NH1	2.81	0.44
1:A:79:THR:O	1:A:187:GLN:HG3	2.17	0.43
1:A:93:VAL:HG13	1:A:120:ILE:HD11	1.99	0.43
1:A:181:ILE:CG2	1:A:188:ASN:HD21	2.25	0.43
2:E:509:VAL:HA	2:E:558:THR:OG1	2.17	0.43
2:E:561:GLN:HG3	5:E:2:HOH:O	2.18	0.43
2:E:506:CYS:SG	2:E:579:LEU:HG	2.58	0.43
2:F:532:TYR:CD2	2:F:532:TYR:C	2.91	0.43
1:A:212:THR:HG22	1:A:213:LEU:N	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:CB	1:A:41:PRO:HD2	2.33	0.43
1:C:167:ASN:O	1:C:171:LEU:HB2	2.18	0.43
1:C:93:VAL:HG13	1:C:120:ILE:HD11	1.99	0.43
2:E:568:ARG:N	2:E:569:PRO:HD3	2.33	0.43
1:A:141:VAL:HG22	1:A:222:PHE:CG	2.52	0.43
1:A:194:ASN:HA	1:A:197:VAL:HG23	1.99	0.43
1:B:79:THR:O	1:B:187:GLN:HG3	2.18	0.43
1:C:212:THR:CG2	1:C:213:LEU:H	2.26	0.43
2:D:568:ARG:N	2:D:569:PRO:HD3	2.33	0.43
1:B:138:TYR:HB3	1:B:139:PRO:HD3	1.99	0.43
1:B:175:THR:O	1:B:179:VAL:HG23	2.18	0.43
1:C:169:GLN:NE2	1:C:172:ARG:HH21	2.17	0.43
1:C:218:PRO:HD2	5:C:276:HOH:O	2.19	0.43
1:C:72:TYR:O	1:C:75:ALA:HB3	2.18	0.43
2:D:501:PRO:CG	2:D:550:PRO:HB2	2.46	0.43
2:F:515:GLY:HA2	4:F:678:GNP:C8	2.47	0.43
2:F:568:ARG:N	2:F:569:PRO:HD3	2.34	0.43
2:F:646:ALA:HA	2:F:651:ALA:HB3	2.00	0.43
2:F:617:ILE:HD13	2:F:656:GLU:OE1	2.18	0.43
1:C:104:LEU:CG	1:C:105:PRO:HD2	2.49	0.43
1:C:95:GLU:O	1:C:96:VAL:C	2.56	0.43
1:A:189:LYS:HD3	2:D:532:TYR:CE1	2.53	0.43
2:E:547:GLY:N	5:E:60:HOH:O	2.42	0.43
1:A:37:ARG:HH12	1:A:97:GLN:HB3	1.82	0.43
1:C:212:THR:HG22	1:C:213:LEU:N	2.29	0.43
2:D:532:TYR:O	2:D:533:VAL:CB	2.66	0.43
1:A:191:THR:CB	2:D:532:TYR:OH	2.66	0.43
1:B:167:ASN:O	1:B:171:LEU:HB2	2.19	0.43
1:C:49:LEU:HA	1:C:52:LEU:HD12	2.01	0.43
2:D:539:ASN:H	2:D:539:ASN:ND2	2.16	0.43
2:D:615:THR:HG22	2:D:616:GLN:HG3	2.00	0.43
1:A:169:GLN:NE2	1:A:172:ARG:HH21	2.17	0.43
1:A:218:PRO:HD2	5:A:274:HOH:O	2.18	0.43
1:C:37:ARG:HH12	1:C:97:GLN:HB3	1.80	0.43
1:B:189:LYS:NZ	2:E:532:TYR:HD1	2.17	0.43
2:E:576:ASP:O	2:E:577:VAL:CB	2.56	0.43
2:E:532:TYR:O	2:E:533:VAL:CB	2.66	0.42
2:E:584:VAL:CG1	2:E:620:ARG:NH1	2.82	0.42
2:E:517:THR:HB	4:E:678:GNP:O1A	2.19	0.42
1:B:199:PHE:O	1:B:202:ASN:HB2	2.18	0.42
1:C:83:ILE:HG13	1:C:83:ILE:H	1.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:516:LYS:HB2	4:E:678:GNP:O1B	2.19	0.42
2:F:532:TYR:O	2:F:533:VAL:CB	2.67	0.42
1:C:138:TYR:HB3	1:C:139:PRO:HD3	2.01	0.42
1:C:40:LEU:HD23	1:C:101:ASN:HB2	2.00	0.42
2:F:599:PRO:O	2:F:603:HIS:HB3	2.19	0.42
2:F:643:GLU:O	2:F:644:LYS:C	2.57	0.42
2:D:584:VAL:CG1	2:D:620:ARG:NH1	2.82	0.42
2:E:507:VAL:HB	2:E:556:PHE:HB2	2.00	0.42
1:C:189:LYS:HD3	2:F:532:TYR:HD1	1.84	0.42
2:F:521:ILE:HG22	2:F:527:LYS:O	2.18	0.42
2:F:532:TYR:O	2:F:532:TYR:CD2	2.72	0.42
1:A:211:ILE:CG1	2:D:570:LEU:HD13	2.50	0.42
1:C:92:VAL:O	1:C:95:GLU:N	2.44	0.42
1:A:70:VAL:HG22	1:A:177:PHE:CE2	2.55	0.42
1:B:169:GLN:NE2	1:B:172:ARG:HH21	2.17	0.42
2:E:638:THR:HA	2:E:639:PRO:HD3	1.90	0.42
2:F:608:THR:HA	2:F:609:PRO:HD2	1.64	0.42
1:A:189:LYS:HD3	2:D:532:TYR:HD1	1.83	0.42
1:C:140:HIS:CE1	1:C:222:PHE:HE1	2.38	0.42
1:C:126:ARG:CG	1:C:202:ASN:OD1	2.67	0.42
1:C:211:ILE:CG1	1:C:212:THR:N	2.76	0.42
2:D:522:SER:O	2:D:526:ASN:HA	2.20	0.42
2:D:521:ILE:HG22	2:D:527:LYS:O	2.19	0.42
2:D:532:TYR:O	2:D:533:VAL:HG22	2.19	0.42
1:B:189:LYS:HZ3	2:E:532:TYR:HB2	1.85	0.42
2:E:659:ALA:HB3	4:E:678:GNP:O6	2.20	0.42
1:B:193:THR:HG22	1:B:224:LYS:HD2	2.01	0.42
2:D:599:PRO:O	2:D:603:HIS:HB3	2.20	0.42
2:D:659:ALA:HB3	4:D:678:GNP:O6	2.20	0.42
2:E:599:PRO:O	2:E:603:HIS:HB3	2.20	0.42
1:B:169:GLN:CD	1:B:172:ARG:HH21	2.23	0.42
1:C:116:LEU:N	1:C:117:PRO:HD3	2.35	0.42
1:C:133:LEU:CB	1:C:203:LEU:HD13	2.50	0.42
2:D:598:VAL:HG21	2:D:649:LEU:HD13	2.01	0.42
1:B:104:LEU:CG	1:B:105:PRO:HD2	2.50	0.41
1:C:141:VAL:HG22	1:C:222:PHE:CG	2.54	0.41
1:A:216:ILE:HG13	2:D:567:LEU:HD13	2.02	0.41
2:F:661:THR:O	2:F:662:GLN:HB2	2.20	0.41
1:A:133:LEU:CB	1:A:203:LEU:HD13	2.51	0.41
1:C:79:THR:O	1:C:187:GLN:HG3	2.19	0.41
2:E:611:LEU:HA	2:E:611:LEU:HD23	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:O	1:A:171:LEU:HB2	2.20	0.41
1:A:211:ILE:HG13	2:D:570:LEU:HD13	2.02	0.41
1:B:70:VAL:HG22	1:B:177:PHE:CE2	2.54	0.41
1:B:72:TYR:O	1:B:75:ALA:HB3	2.19	0.41
2:D:585:VAL:O	2:D:629:LEU:HD22	2.21	0.41
1:B:217:ASN:ND2	2:E:536:VAL:HG21	2.35	0.41
2:E:594:LYS:HB3	2:E:649:LEU:HD11	2.01	0.41
1:C:38:PRO:HA	1:C:39:PRO:HD2	1.62	0.41
2:E:564:TYR:CD1	2:E:567:LEU:HD12	2.54	0.41
2:F:501:PRO:CG	2:F:550:PRO:HB2	2.47	0.41
2:F:584:VAL:HG13	2:F:620:ARG:NH1	2.35	0.41
1:A:140:HIS:CE1	1:A:222:PHE:HE2	2.39	0.41
1:C:207:LYS:HG3	5:C:239:HOH:O	2.20	0.41
1:C:217:ASN:ND2	2:F:536:VAL:HG21	2.35	0.41
2:D:507:VAL:HB	2:D:556:PHE:HB2	2.02	0.41
2:D:584:VAL:HG13	2:D:620:ARG:NH1	2.36	0.41
2:E:559:ALA:HB3	2:E:564:TYR:HB3	2.01	0.41
2:F:654:TYR:OH	2:F:656:GLU:OE2	2.36	0.41
1:B:140:HIS:CE1	1:B:156:THR:HG1	2.35	0.41
1:B:191:THR:HB	2:E:532:TYR:HH	1.84	0.41
2:D:650:LYS:HD3	2:D:650:LYS:N	2.36	0.41
2:D:516:LYS:HB2	4:D:678:GNP:O2B	2.20	0.41
2:E:508:VAL:HG12	2:E:516:LYS:HG2	2.03	0.41
1:B:197:VAL:CG2	2:E:534:PRO:HG2	2.45	0.41
2:F:594:LYS:HB3	2:F:649:LEU:HD11	2.01	0.41
2:F:643:GLU:OE2	2:F:654:TYR:HB3	2.21	0.41
1:B:189:LYS:HZ3	2:E:532:TYR:HD1	1.62	0.41
1:B:83:ILE:H	1:B:83:ILE:HG13	1.74	0.41
1:C:132:LEU:HB3	5:C:278:HOH:O	2.21	0.41
2:E:532:TYR:O	2:E:532:TYR:CD2	2.73	0.41
1:B:95:GLU:O	1:B:96:VAL:C	2.59	0.41
1:C:169:GLN:CD	1:C:172:ARG:HH21	2.24	0.41
2:D:657:CYS:HA	2:D:664:GLY:HA3	2.02	0.41
2:E:572:TYR:H	2:E:573:PRO:HD2	1.85	0.41
2:F:501:PRO:O	2:F:502:GLN:C	2.59	0.41
2:F:638:THR:HA	2:F:639:PRO:HD3	1.89	0.41
1:B:218:PRO:HD2	5:B:275:HOH:O	2.21	0.41
2:D:646:ALA:HA	2:D:651:ALA:HB3	2.03	0.41
1:C:189:LYS:NZ	2:F:532:TYR:HD1	2.17	0.41
1:A:104:LEU:CG	1:A:105:PRO:HD2	2.50	0.41
1:B:222:PHE:CE2	1:B:226:LEU:HD11	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:HA	1:B:63:PRO:HD3	1.83	0.41
1:B:81:GLU:HA	1:B:188:ASN:CB	2.51	0.41
2:D:564:TYR:CD1	2:D:567:LEU:HD12	2.55	0.41
2:F:511:ASP:O	2:F:514:VAL:HG13	2.20	0.41
2:F:507:VAL:HB	2:F:556:PHE:HB2	2.02	0.41
1:B:140:HIS:CE1	1:B:222:PHE:HE1	2.39	0.41
1:A:189:LYS:NZ	2:D:532:TYR:HB2	2.35	0.41
2:E:501:PRO:HG3	2:E:550:PRO:CB	2.45	0.41
2:E:606:PRO:O	2:E:607:LYS:CB	2.68	0.41
2:F:585:VAL:O	2:F:629:LEU:HD22	2.21	0.41
1:A:95:GLU:O	1:A:96:VAL:C	2.58	0.40
1:B:44:GLN:CG	1:B:100:TYR:HB3	2.51	0.40
2:D:661:THR:O	2:D:662:GLN:HB2	2.21	0.40
2:D:517:THR:HB	4:D:678:GNP:O1A	2.22	0.40
2:E:608:THR:HA	2:E:609:PRO:HD2	1.61	0.40
2:F:572:TYR:H	2:F:573:PRO:HD2	1.85	0.40
1:A:49:LEU:HA	1:A:52:LEU:HD12	2.03	0.40
1:B:96:VAL:CG1	1:B:106:VAL:HG11	2.52	0.40
1:C:189:LYS:CE	2:F:532:TYR:HD1	2.35	0.40
1:A:44:GLN:CG	1:A:100:TYR:HB3	2.50	0.40
1:B:37:ARG:HH12	1:B:97:GLN:CG	2.35	0.40
1:B:56:ASN:HA	1:B:57:PRO:HD2	1.89	0.40
1:B:45:PHE:CD1	1:B:97:GLN:HG2	2.57	0.40
2:D:532:TYR:C	2:D:532:TYR:CD2	2.94	0.40
2:D:611:LEU:HD23	2:D:611:LEU:HA	1.77	0.40
2:E:585:VAL:O	2:E:629:LEU:HD22	2.22	0.40
1:A:86:ARG:NH1	5:A:267:HOH:O	2.54	0.40
1:B:200:GLY:N	1:B:201:PRO:CD	2.80	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	197/199 (99%)	157 (80%)	29 (15%)	11 (6%)	2	3
1	B	197/199 (99%)	157 (80%)	29 (15%)	11 (6%)	2	3
1	C	197/199 (99%)	159 (81%)	26 (13%)	12 (6%)	1	2
2	D	170/177 (96%)	137 (81%)	21 (12%)	12 (7%)	1	1
2	E	170/177 (96%)	136 (80%)	22 (13%)	12 (7%)	1	1
2	F	170/177 (96%)	136 (80%)	22 (13%)	12 (7%)	1	1
All	All	1101/1128 (98%)	882 (80%)	149 (14%)	70 (6%)	1	2

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ALA
1	A	210	ALA
1	A	211	ILE
1	A	216	ILE
1	A	217	ASN
2	D	533	VAL
2	D	577	VAL
2	D	596	LYS
1	B	209	ALA
1	B	210	ALA
1	B	211	ILE
1	B	216	ILE
1	B	217	ASN
2	E	533	VAL
2	E	577	VAL
2	E	596	LYS
1	C	209	ALA
1	C	210	ALA
1	C	211	ILE
1	C	216	ILE
1	C	217	ASN
2	F	533	VAL
2	F	577	VAL
2	F	596	LYS
1	A	84	PHE
2	D	502	GLN
2	D	546	ILE
2	D	633	LYS
1	B	84	PHE
2	E	502	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	546	ILE
2	E	633	LYS
1	C	84	PHE
2	F	502	GLN
2	F	546	ILE
2	F	548	GLY
2	F	633	LYS
1	A	75	ALA
2	D	607	LYS
2	D	646	ALA
1	B	75	ALA
2	E	548	GLY
2	E	607	LYS
2	E	609	PRO
2	E	623	PRO
2	E	646	ALA
1	C	75	ALA
2	F	607	LYS
2	F	646	ALA
1	A	114	LEU
1	A	212	THR
2	D	609	PRO
2	D	623	PRO
1	B	114	LEU
1	C	114	LEU
2	F	609	PRO
2	F	623	PRO
2	D	548	GLY
1	B	129	PRO
1	B	212	THR
1	C	129	PRO
1	C	212	THR
1	A	129	PRO
2	E	536	VAL
2	F	536	VAL
1	A	39	PRO
2	D	536	VAL
1	B	39	PRO
1	C	39	PRO
1	C	164	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/180 (97%)	143 (82%)	32 (18%)	1	4
1	B	175/180 (97%)	141 (81%)	34 (19%)	1	3
1	C	175/180 (97%)	139 (79%)	36 (21%)	1	3
2	D	147/157 (94%)	102 (69%)	45 (31%)	0	0
2	E	147/157 (94%)	102 (69%)	45 (31%)	0	0
2	F	147/157 (94%)	100 (68%)	47 (32%)	0	0
All	All	966/1011 (96%)	727 (75%)	239 (25%)	0	2

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	40	LEU
1	A	43	GLN
1	A	47	VAL
1	A	53	GLN
1	A	64	ILE
1	A	68	GLU
1	A	78	LEU
1	A	80	THR
1	A	81	GLU
1	A	83	ILE
1	A	86	ARG
1	A	90	THR
1	A	94	ARG
1	A	102	MET
1	A	112	ASN
1	A	121	LEU
1	A	137	LEU
1	A	142	VAL
1	A	146	ASN
1	A	147	ILE
1	A	151	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	159	VAL
1	A	161	GLN
1	A	169	GLN
1	A	171	LEU
1	A	180	GLN
1	A	181	ILE
1	A	187	GLN
1	A	190	MET
1	A	197	VAL
1	A	213	LEU
2	D	505	LYS
2	D	507	VAL
2	D	509	VAL
2	D	511	ASP
2	D	516	LYS
2	D	519	LEU
2	D	522	SER
2	D	527	LYS
2	D	533	VAL
2	D	539	ASN
2	D	557	ASP
2	D	563	ASP
2	D	567	LEU
2	D	568	ARG
2	D	574	GLN
2	D	576	ASP
2	D	579	LEU
2	D	584	VAL
2	D	589	SER
2	D	591	GLU
2	D	594	LYS
2	D	595	GLU
2	D	596	LYS
2	D	601	ILE
2	D	603	HIS
2	D	607	LYS
2	D	611	LEU
2	D	612	LEU
2	D	617	ILE
2	D	620	ARG
2	D	623	PRO
2	D	633	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	635	LYS
2	D	640	GLU
2	D	641	THR
2	D	643	GLU
2	D	645	LEU
2	D	647	ARG
2	D	648	ASP
2	D	650	LYS
2	D	663	ARG
2	D	666	LYS
2	D	667	ASN
2	D	668	VAL
2	D	677	LEU
1	B	37	ARG
1	B	40	LEU
1	B	43	GLN
1	B	47	VAL
1	B	53	GLN
1	B	64	ILE
1	B	68	GLU
1	B	78	LEU
1	B	80	THR
1	B	81	GLU
1	B	83	ILE
1	B	86	ARG
1	B	90	THR
1	B	94	ARG
1	B	102	MET
1	B	112	ASN
1	B	121	LEU
1	B	137	LEU
1	B	142	VAL
1	B	146	ASN
1	B	147	ILE
1	B	151	GLN
1	B	159	VAL
1	B	161	GLN
1	B	169	GLN
1	B	171	LEU
1	B	180	GLN
1	B	181	ILE
1	B	187	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	189	LYS
1	B	190	MET
1	B	197	VAL
1	B	213	LEU
1	B	229	HIS
2	E	505	LYS
2	E	507	VAL
2	E	509	VAL
2	E	511	ASP
2	E	516	LYS
2	E	519	LEU
2	E	522	SER
2	E	527	LYS
2	E	533	VAL
2	E	539	ASN
2	E	557	ASP
2	E	563	ASP
2	E	566	ARG
2	E	567	LEU
2	E	574	GLN
2	E	576	ASP
2	E	579	LEU
2	E	584	VAL
2	E	589	SER
2	E	591	GLU
2	E	594	LYS
2	E	595	GLU
2	E	596	LYS
2	E	601	ILE
2	E	603	HIS
2	E	607	LYS
2	E	611	LEU
2	E	612	LEU
2	E	617	ILE
2	E	620	ARG
2	E	623	PRO
2	E	633	LYS
2	E	635	LYS
2	E	640	GLU
2	E	641	THR
2	E	643	GLU
2	E	645	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	647	ARG
2	E	648	ASP
2	E	650	LYS
2	E	663	ARG
2	E	666	LYS
2	E	667	ASN
2	E	668	VAL
2	E	677	LEU
1	C	37	ARG
1	C	40	LEU
1	C	43	GLN
1	C	47	VAL
1	C	53	GLN
1	C	64	ILE
1	C	68	GLU
1	C	78	LEU
1	C	80	THR
1	C	81	GLU
1	C	83	ILE
1	C	86	ARG
1	C	90	THR
1	C	94	ARG
1	C	102	MET
1	C	112	ASN
1	C	121	LEU
1	C	137	LEU
1	C	142	VAL
1	C	146	ASN
1	C	147	ILE
1	C	151	GLN
1	C	159	VAL
1	C	161	GLN
1	C	162	THR
1	C	169	GLN
1	C	171	LEU
1	C	180	GLN
1	C	181	ILE
1	C	187	GLN
1	C	189	LYS
1	C	190	MET
1	C	197	VAL
1	C	212	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	213	LEU
1	C	229	HIS
2	F	505	LYS
2	F	507	VAL
2	F	509	VAL
2	F	511	ASP
2	F	516	LYS
2	F	519	LEU
2	F	522	SER
2	F	527	LYS
2	F	533	VAL
2	F	539	ASN
2	F	557	ASP
2	F	563	ASP
2	F	566	ARG
2	F	567	LEU
2	F	568	ARG
2	F	574	GLN
2	F	576	ASP
2	F	579	LEU
2	F	584	VAL
2	F	589	SER
2	F	591	GLU
2	F	594	LYS
2	F	595	GLU
2	F	596	LYS
2	F	601	ILE
2	F	603	HIS
2	F	607	LYS
2	F	611	LEU
2	F	612	LEU
2	F	617	ILE
2	F	620	ARG
2	F	623	PRO
2	F	633	LYS
2	F	635	LYS
2	F	640	GLU
2	F	641	THR
2	F	643	GLU
2	F	645	LEU
2	F	647	ARG
2	F	648	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	650	LYS
2	F	653	LYS
2	F	663	ARG
2	F	666	LYS
2	F	667	ASN
2	F	668	VAL
2	F	677	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	146	ASN
1	A	167	ASN
1	A	169	GLN
1	A	230	GLN
2	D	539	ASN
2	D	592	ASN
2	D	634	GLN
1	B	110	GLN
1	B	146	ASN
1	B	167	ASN
1	B	169	GLN
1	B	230	GLN
2	E	539	ASN
2	E	592	ASN
2	E	634	GLN
2	E	667	ASN
1	C	110	GLN
1	C	146	ASN
1	C	167	ASN
1	C	169	GLN
1	C	230	GLN
2	F	539	ASN
2	F	592	ASN
2	F	667	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
4	GNP	F	678	3	28,34,34	4.02	15 (53%)	30,54,54	2.68	13 (43%)
4	GNP	D	678	3	28,34,34	3.77	11 (39%)	30,54,54	2.87	16 (53%)
4	GNP	E	678	3	28,34,34	3.74	13 (46%)	30,54,54	2.79	14 (46%)

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
4	GNP	F	678	3	-	11/17/38/38	0/3/3/3
4	GNP	D	678	3	-	11/17/38/38	0/3/3/3
4	GNP	E	678	3	-	11/17/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	678	GNP	C4-N9	-9.19	1.35	1.47
4	F	678	GNP	PB-O2B	-9.02	1.32	1.56
4	E	678	GNP	C4-N9	-8.91	1.35	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	678	GNP	C4-N9	-8.80	1.36	1.47
4	D	678	GNP	PB-O2B	-8.54	1.33	1.56
4	F	678	GNP	PG-O1G	8.49	1.59	1.46
4	E	678	GNP	PB-O2B	-8.28	1.34	1.56
4	F	678	GNP	C5-C6	-7.25	1.40	1.52
4	D	678	GNP	C5-C6	-6.77	1.41	1.52
4	E	678	GNP	PG-O1G	6.73	1.56	1.46
4	E	678	GNP	C5-C6	-6.72	1.41	1.52
4	D	678	GNP	O6-C6	6.50	1.36	1.23
4	D	678	GNP	PG-O1G	6.36	1.56	1.46
4	E	678	GNP	O6-C6	6.36	1.36	1.23
4	F	678	GNP	O6-C6	6.21	1.35	1.23
4	D	678	GNP	PB-N3B	5.59	1.78	1.63
4	F	678	GNP	PB-N3B	5.51	1.77	1.63
4	E	678	GNP	PB-N3B	5.47	1.77	1.63
4	F	678	GNP	PG-O2G	-4.95	1.43	1.56
4	D	678	GNP	PG-O2G	-4.67	1.44	1.56
4	F	678	GNP	O3'-C3'	4.22	1.52	1.43
4	E	678	GNP	PG-O2G	-4.17	1.45	1.56
4	D	678	GNP	PB-O3A	-4.04	1.54	1.59
4	E	678	GNP	O3'-C3'	3.91	1.52	1.43
4	D	678	GNP	O3'-C3'	3.63	1.51	1.43
4	E	678	GNP	PB-O3A	-2.96	1.55	1.59
4	F	678	GNP	PB-O3A	-2.67	1.55	1.59
4	E	678	GNP	C2'-C3'	2.46	1.60	1.53
4	F	678	GNP	C2'-C3'	2.39	1.59	1.53
4	F	678	GNP	PB-O1B	2.30	1.49	1.46
4	D	678	GNP	C2'-C3'	2.25	1.59	1.53
4	E	678	GNP	O2'-C2'	2.21	1.48	1.43
4	F	678	GNP	O2'-C2'	2.18	1.48	1.43
4	E	678	GNP	O4'-C1'	2.18	1.47	1.42
4	F	678	GNP	O4'-C1'	2.15	1.47	1.42
4	D	678	GNP	C2'-C1'	2.14	1.60	1.53
4	F	678	GNP	C2'-C1'	2.09	1.60	1.53
4	E	678	GNP	C2'-C1'	2.07	1.60	1.53
4	F	678	GNP	C5'-C4'	-2.03	1.45	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	678	GNP	C5-C6-N1	7.82	127.83	118.19
4	D	678	GNP	C5-C6-N1	7.70	127.68	118.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	678	GNP	C5-C6-N1	7.37	127.27	118.19
4	D	678	GNP	O3'-C3'-C4'	-5.13	96.21	111.05
4	D	678	GNP	O1G-PG-N3B	-4.93	104.50	111.77
4	E	678	GNP	O3'-C3'-C4'	-4.84	97.06	111.05
4	F	678	GNP	O3'-C3'-C4'	-4.76	97.29	111.05
4	E	678	GNP	O1G-PG-N3B	-4.66	104.91	111.77
4	F	678	GNP	O3'-C3'-C2'	-4.36	97.73	111.82
4	F	678	GNP	O1G-PG-N3B	-4.32	105.41	111.77
4	D	678	GNP	O3G-PG-O1G	-4.16	102.99	113.45
4	D	678	GNP	O3'-C3'-C2'	-4.10	98.57	111.82
4	E	678	GNP	O6-C6-C5	-4.04	111.61	119.86
4	E	678	GNP	O3'-C3'-C2'	-4.04	98.75	111.82
4	E	678	GNP	C2'-C3'-C4'	3.94	110.29	102.64
4	D	678	GNP	C2'-C3'-C4'	3.94	110.29	102.64
4	F	678	GNP	O3G-PG-O1G	-3.61	104.38	113.45
4	F	678	GNP	C2'-C3'-C4'	3.56	109.55	102.64
4	F	678	GNP	O6-C6-C5	-3.49	112.75	119.86
4	E	678	GNP	O3G-PG-O1G	-3.43	104.84	113.45
4	D	678	GNP	O6-C6-C5	-3.31	113.11	119.86
4	D	678	GNP	C4'-O4'-C1'	3.22	116.59	109.47
4	E	678	GNP	C4'-O4'-C1'	3.21	116.55	109.47
4	E	678	GNP	O2'-C2'-C1'	-3.17	99.42	110.02
4	D	678	GNP	O2'-C2'-C1'	-3.03	99.89	110.02
4	F	678	GNP	O2'-C2'-C1'	-3.01	99.95	110.02
4	F	678	GNP	C4'-O4'-C1'	2.98	116.04	109.47
4	D	678	GNP	O3G-PG-O2G	2.79	115.06	107.64
4	D	678	GNP	O2B-PB-O3A	2.71	113.67	104.64
4	F	678	GNP	O2G-PG-O1G	-2.66	106.77	113.45
4	E	678	GNP	O4'-C4'-C3'	-2.65	99.87	105.11
4	D	678	GNP	O6-C6-N1	-2.61	119.19	122.69
4	E	678	GNP	O2G-PG-O1G	-2.55	107.04	113.45
4	D	678	GNP	O4'-C4'-C3'	-2.53	100.10	105.11
4	F	678	GNP	O2A-PA-O1A	2.45	124.38	112.24
4	E	678	GNP	O2A-PA-O1A	2.34	123.83	112.24
4	E	678	GNP	O3G-PG-O2G	2.31	113.80	107.64
4	D	678	GNP	O2G-PG-O1G	-2.29	107.69	113.45
4	D	678	GNP	O2A-PA-O1A	2.25	123.38	112.24
4	E	678	GNP	O3A-PB-N3B	2.24	112.80	106.59
4	F	678	GNP	O4'-C4'-C3'	-2.24	100.69	105.11
4	D	678	GNP	O3A-PB-N3B	2.08	112.37	106.59
4	F	678	GNP	O6-C6-N1	-2.06	119.93	122.69

There are no chirality outliers.

All (33) torsion outliers are listed below:

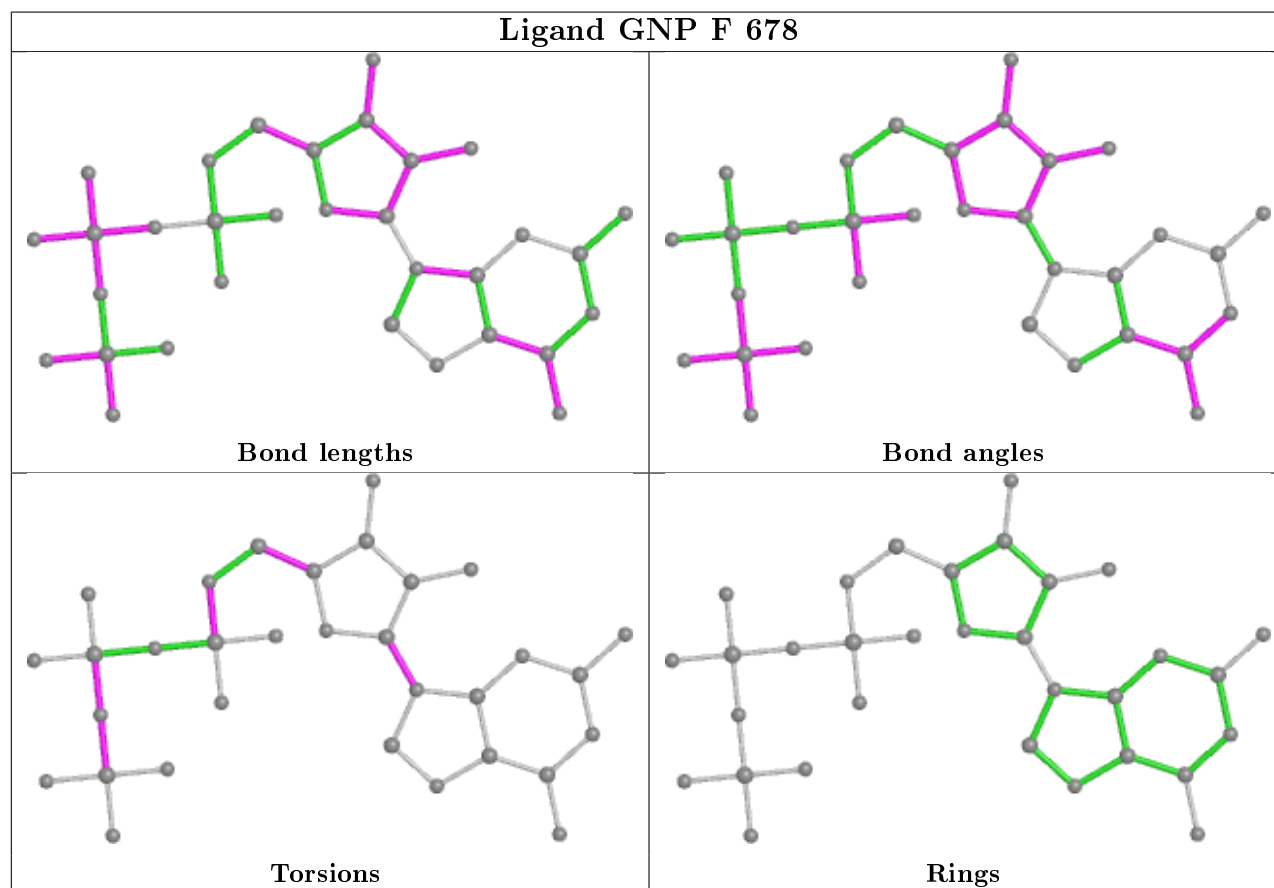
Mol	Chain	Res	Type	Atoms
4	F	678	GNP	PB-N3B-PG-O1G
4	F	678	GNP	PG-N3B-PB-O1B
4	F	678	GNP	PG-N3B-PB-O3A
4	F	678	GNP	C5'-O5'-PA-O2A
4	F	678	GNP	O4'-C4'-C5'-O5'
4	F	678	GNP	O4'-C1'-N9-C4
4	F	678	GNP	C2'-C1'-N9-C8
4	F	678	GNP	C2'-C1'-N9-C4
4	E	678	GNP	PB-N3B-PG-O1G
4	E	678	GNP	PG-N3B-PB-O1B
4	E	678	GNP	PG-N3B-PB-O3A
4	E	678	GNP	C5'-O5'-PA-O2A
4	E	678	GNP	O4'-C4'-C5'-O5'
4	E	678	GNP	O4'-C1'-N9-C4
4	E	678	GNP	C2'-C1'-N9-C8
4	E	678	GNP	C2'-C1'-N9-C4
4	D	678	GNP	PB-N3B-PG-O1G
4	D	678	GNP	PG-N3B-PB-O1B
4	D	678	GNP	PG-N3B-PB-O3A
4	D	678	GNP	C5'-O5'-PA-O2A
4	D	678	GNP	O4'-C4'-C5'-O5'
4	D	678	GNP	O4'-C1'-N9-C4
4	D	678	GNP	C2'-C1'-N9-C8
4	D	678	GNP	C2'-C1'-N9-C4
4	F	678	GNP	C3'-C4'-C5'-O5'
4	E	678	GNP	C3'-C4'-C5'-O5'
4	D	678	GNP	C3'-C4'-C5'-O5'
4	F	678	GNP	C5'-O5'-PA-O3A
4	E	678	GNP	C5'-O5'-PA-O3A
4	D	678	GNP	C5'-O5'-PA-O3A
4	F	678	GNP	C5'-O5'-PA-O1A
4	E	678	GNP	C5'-O5'-PA-O1A
4	D	678	GNP	C5'-O5'-PA-O1A

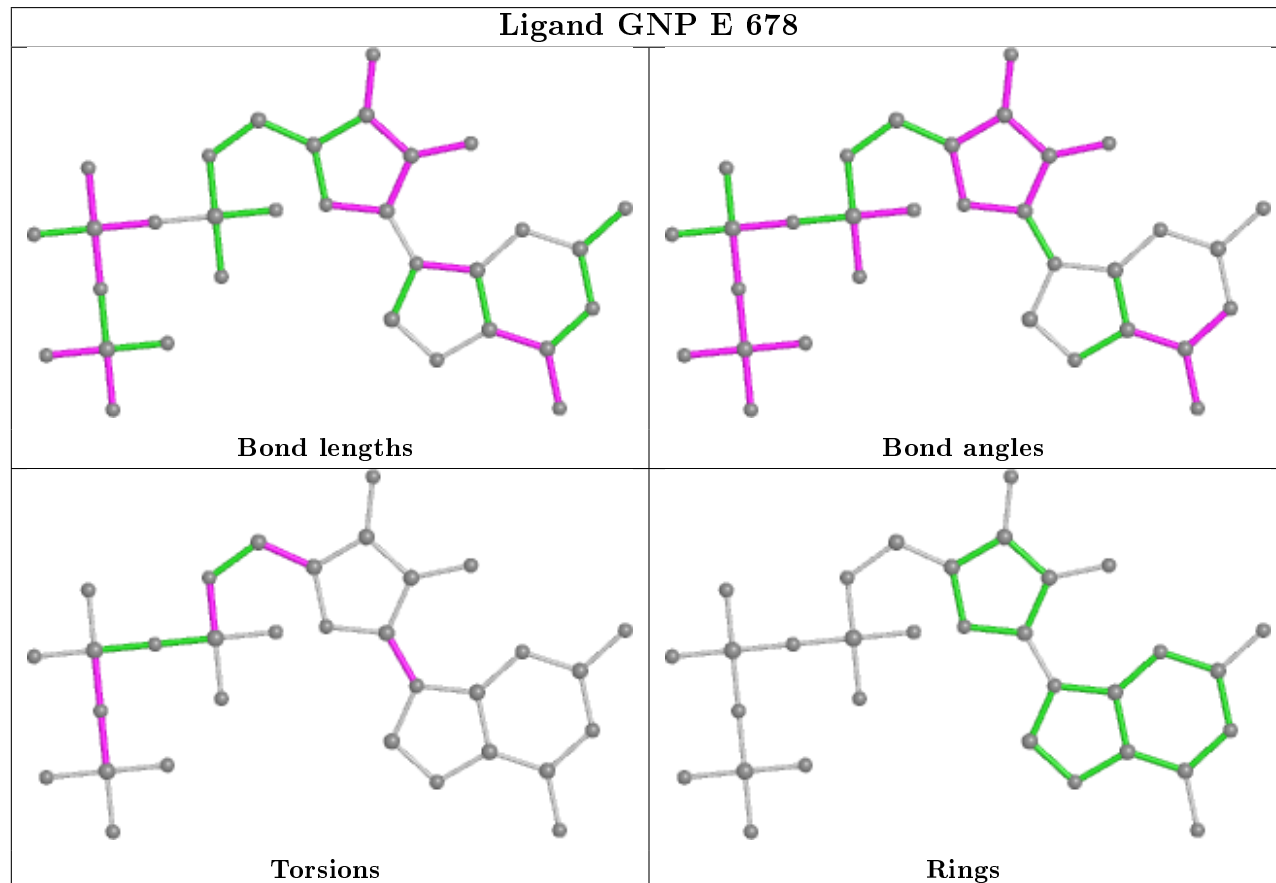
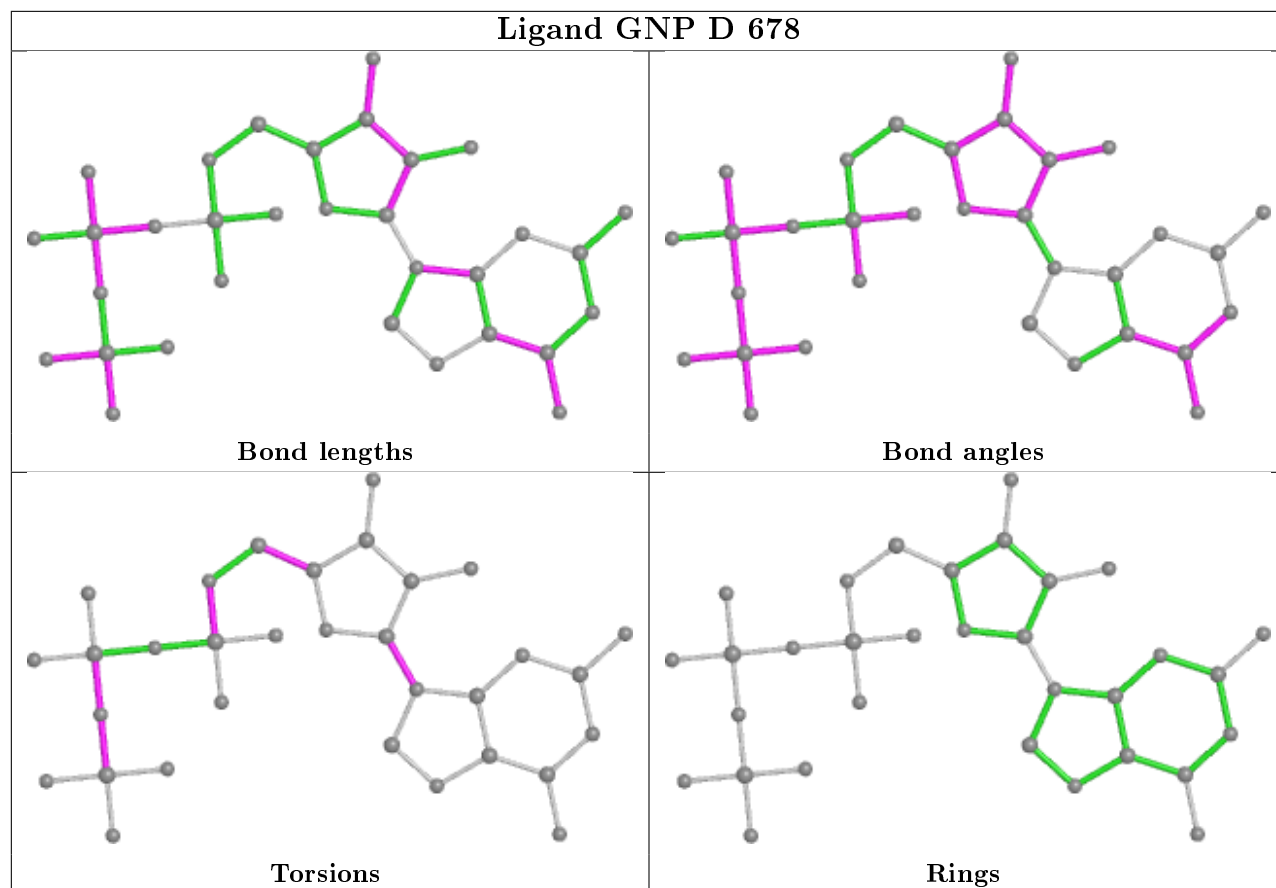
There are no ring outliers.

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	678	GNP	7	0
4	D	678	GNP	9	0
4	E	678	GNP	7	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 than 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.





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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.