



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:08 AM UTC

PDB ID : 1Y9E / pdb_00001y9e
Title : Crystal structure of Bacillus subtilis protein yhfP with NAD bound
Authors : Min, T.; Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-12-15
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

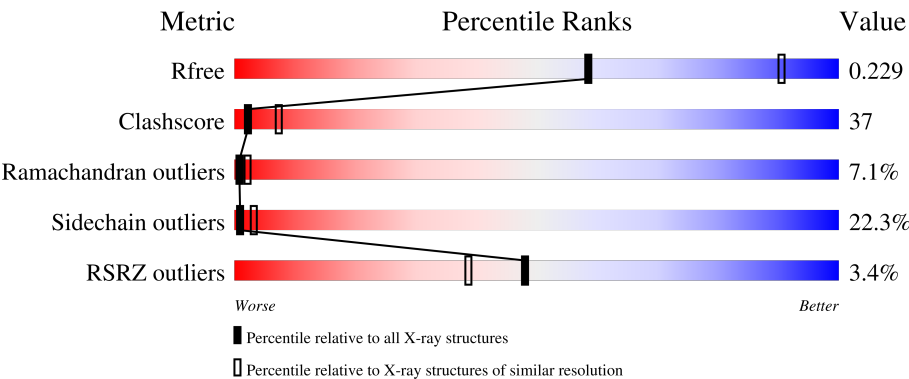
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



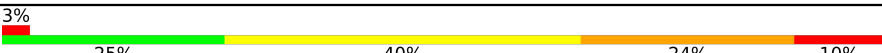
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	330	3% 30%33%26%10%
1	B	330	3% 27%37%23%13%
1	C	330	5% 24%42%25%10%
1	D	330	4% 25%38%25%11%
1	E	330	2% 27%38%24%10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	330	

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
2	NAD	A	1255	-	X	-	-
2	NAD	B	2255	-	X	-	-
2	NAD	C	3255	-	X	-	-
2	NAD	D	4255	-	X	-	-
2	NAD	E	5255	-	X	-	-
2	NAD	F	6255	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14982 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 hypothetical protein yhfP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	Se	0	0	0
			2429	1529	414	481	1	4			
1	B	329	Total	C	N	O	S	Se	0	0	0
			2421	1525	406	485	1	4			
1	C	329	Total	C	N	O	S	Se	0	0	0
			2412	1516	408	483	1	4			
1	D	329	Total	C	N	O	S	Se	0	0	0
			2431	1527	414	485	1	4			
1	E	329	Total	C	N	O	S	Se	0	0	0
			2433	1531	414	483	1	4			
1	F	329	Total	C	N	O	S	Se	0	0	0
			2437	1533	414	485	1	4			

There are 24 discrepancies between the modelled and reference sequences:

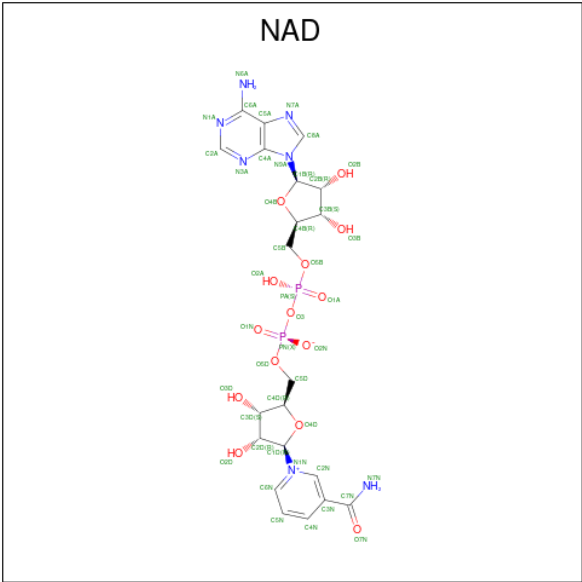
Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MSE	MET	modified residue	UNP O07615
A	170	MSE	MET	modified residue	UNP O07615
A	278	MSE	MET	modified residue	UNP O07615
A	288	MSE	MET	modified residue	UNP O07615
B	126	MSE	MET	modified residue	UNP O07615
B	170	MSE	MET	modified residue	UNP O07615
B	278	MSE	MET	modified residue	UNP O07615
B	288	MSE	MET	modified residue	UNP O07615
C	126	MSE	MET	modified residue	UNP O07615
C	170	MSE	MET	modified residue	UNP O07615
C	278	MSE	MET	modified residue	UNP O07615
C	288	MSE	MET	modified residue	UNP O07615
D	126	MSE	MET	modified residue	UNP O07615
D	170	MSE	MET	modified residue	UNP O07615
D	278	MSE	MET	modified residue	UNP O07615
D	288	MSE	MET	modified residue	UNP O07615
E	126	MSE	MET	modified residue	UNP O07615

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	170	MSE	MET	modified residue	UNP O07615
E	278	MSE	MET	modified residue	UNP O07615
E	288	MSE	MET	modified residue	UNP O07615
F	126	MSE	MET	modified residue	UNP O07615
F	170	MSE	MET	modified residue	UNP O07615
F	278	MSE	MET	modified residue	UNP O07615
F	288	MSE	MET	modified residue	UNP O07615

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			11	6	5		
2	B	1	Total	C	N	0	0
			11	6	5		
2	C	1	Total	C	N	0	0
			11	6	5		
2	D	1	Total	C	N	0	0
			11	6	5		
2	E	1	Total	C	N	0	0
			11	6	5		
2	F	1	Total	C	N	0	0
			11	6	5		

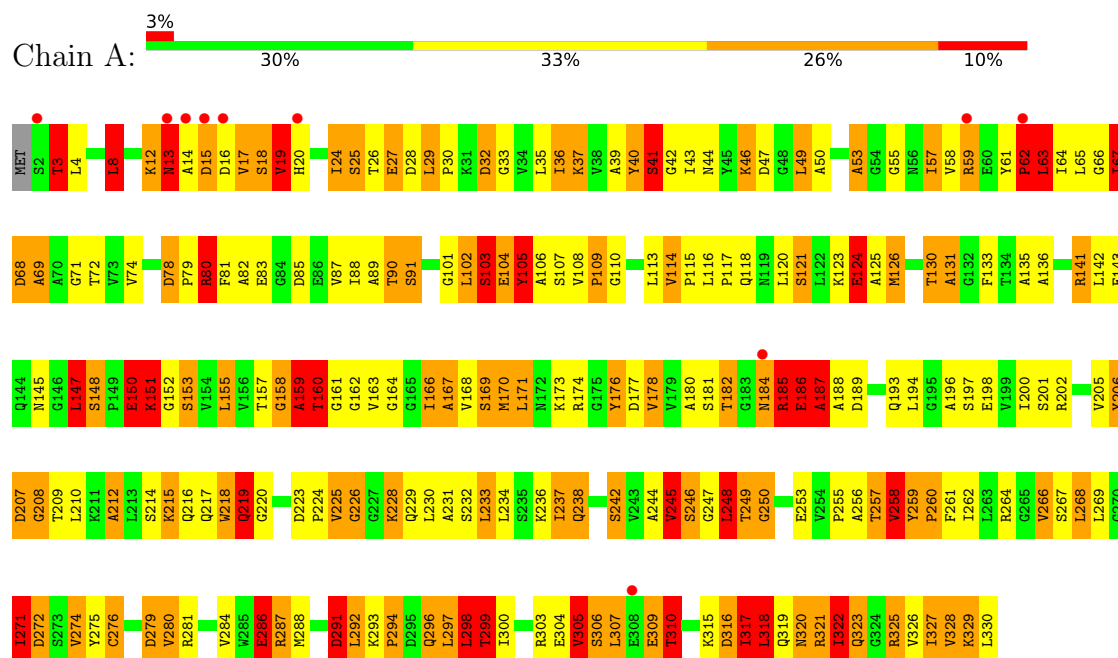
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total 65	O 65	0	0
3	B	56	Total 56	O 56	0	0
3	C	57	Total 57	O 57	0	0
3	D	53	Total 53	O 53	0	0
3	E	60	Total 60	O 60	0	0
3	F	62	Total 62	O 62	0	0

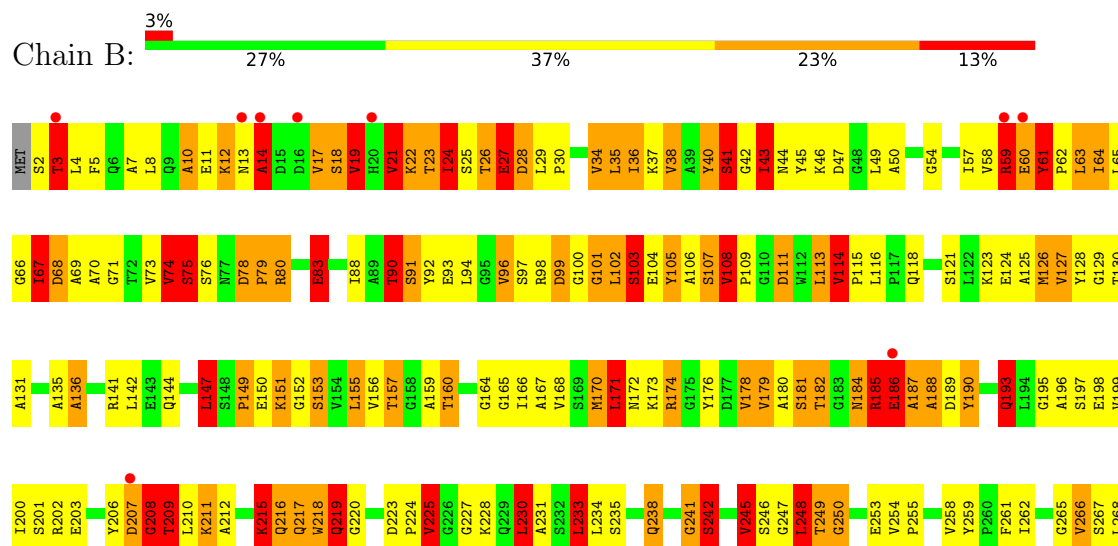
3 Residue-property plots [i](#)

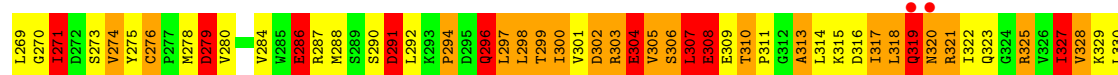
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

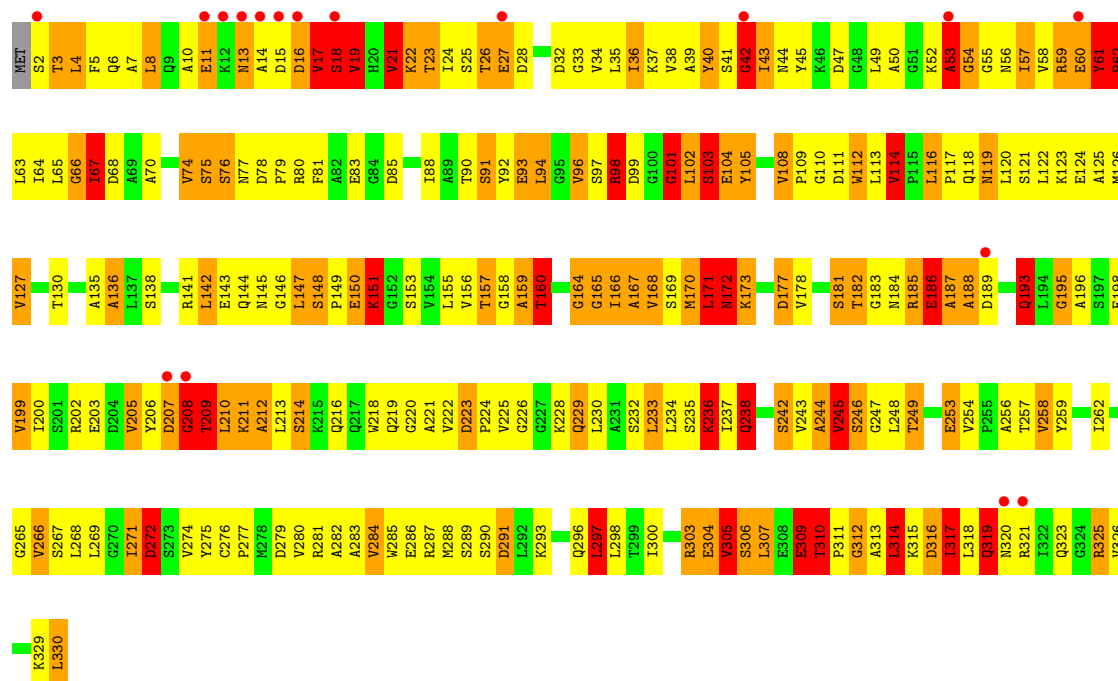
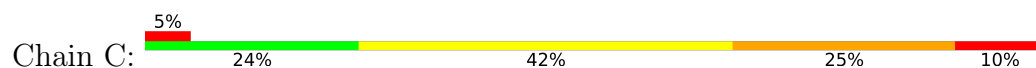


• Molecule 1: hypothetical protein yhfP

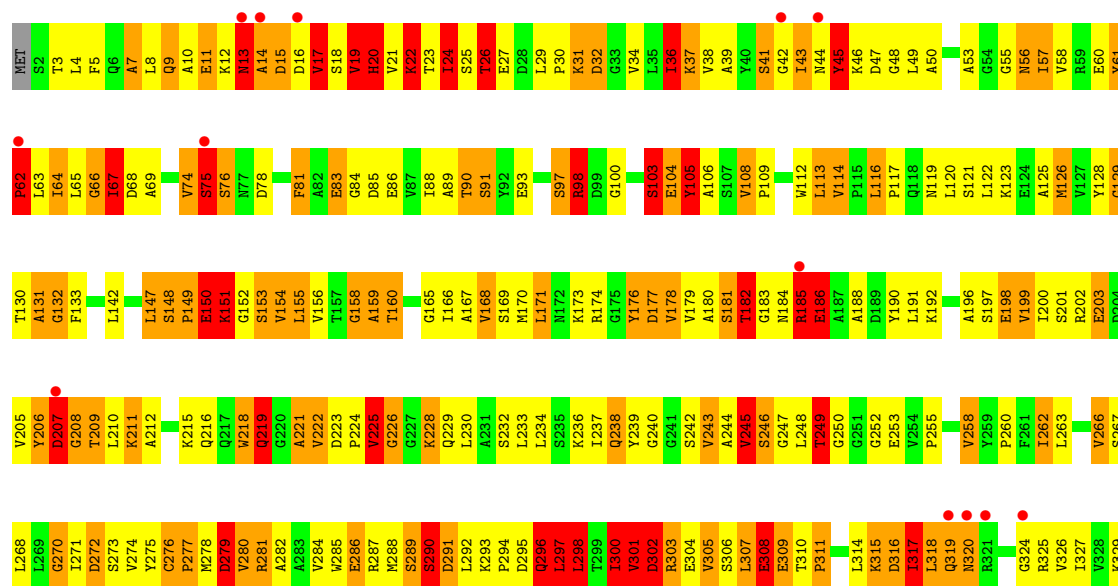
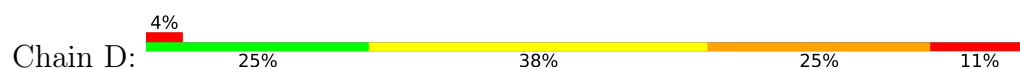




• Molecule 1: hypothetical protein yhfP

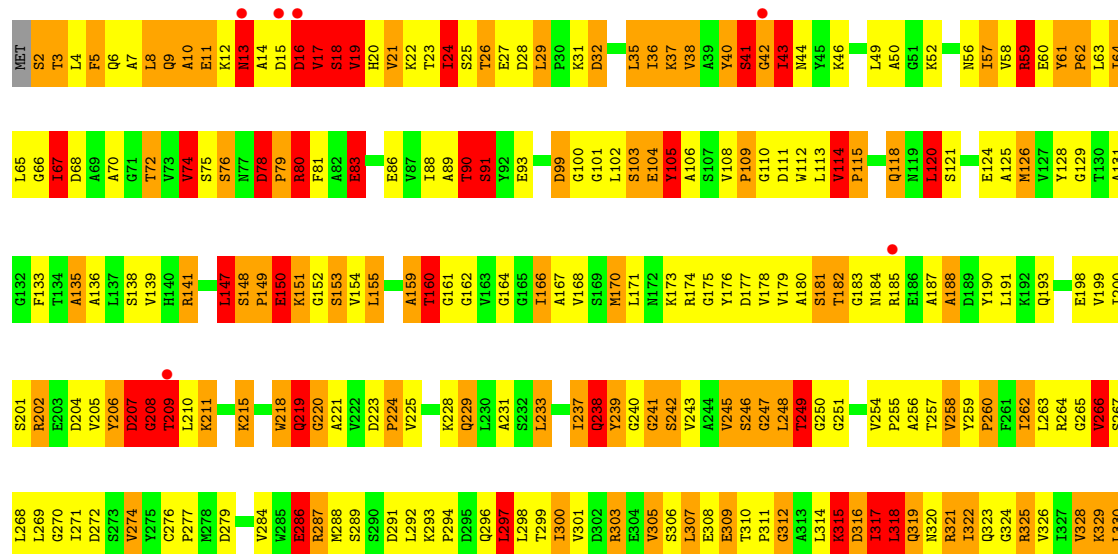
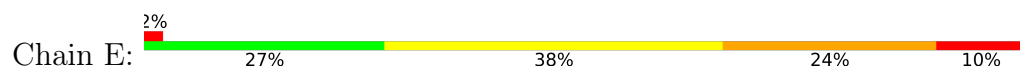


• Molecule 1: hypothetical protein yhfP

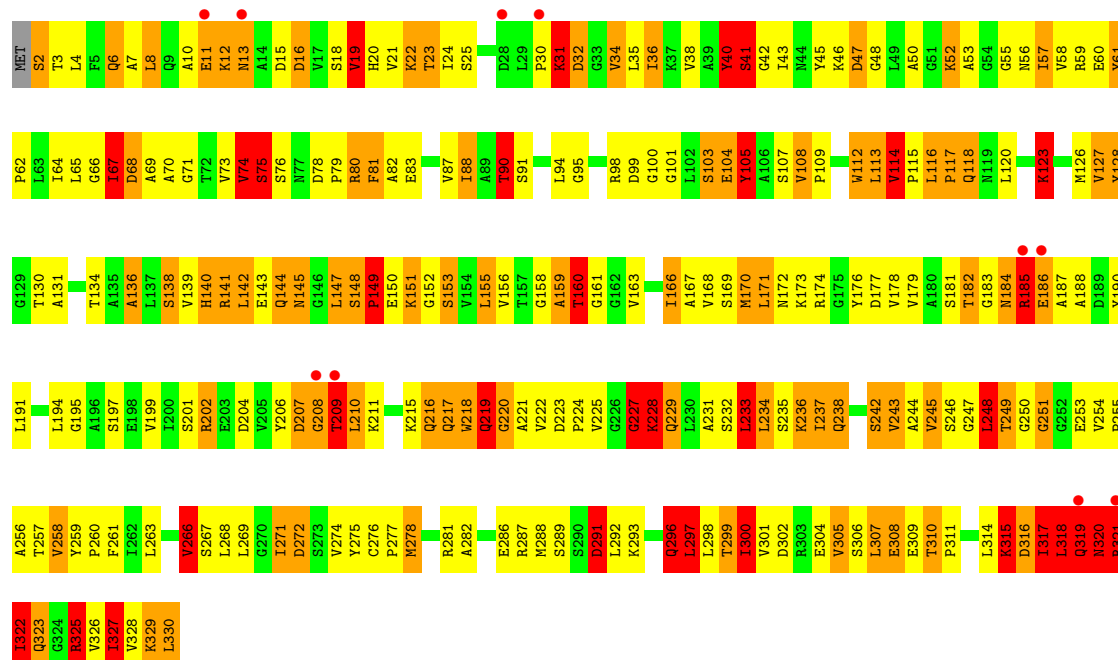
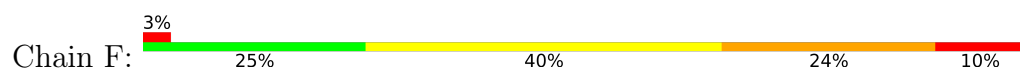


L330

• Molecule 1: hypothetical protein yhfP



• Molecule 1: hypothetical protein yhfP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.27Å 136.92Å 167.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.98-2.80) 94.1 (19.98-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.233 0.225 , 0.229	Depositor DCC
R_{free} test set	4706 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14982	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2.63	160/2461 (6.5%)	2.47	161/3333 (4.8%)
1	B	2.59	143/2453 (5.8%)	2.32	132/3325 (4.0%)
1	C	2.53	129/2444 (5.3%)	2.33	139/3315 (4.2%)
1	D	2.49	124/2463 (5.0%)	2.30	148/3335 (4.4%)
1	E	2.64	155/2465 (6.3%)	2.38	139/3338 (4.2%)
1	F	2.73	164/2469 (6.6%)	2.42	178/3343 (5.3%)
All	All	2.60	875/14755 (5.9%)	2.37	897/19989 (4.5%)

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	9
1	B	0	9
1	C	1	8
1	D	1	5
1	E	0	5
1	F	0	4
All	All	2	40

All (875) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	209	THR	CA-CB	22.83	1.92	1.53
1	F	105	TYR	N-CA	16.84	1.68	1.46
1	B	114	VAL	CA-CB	15.23	1.66	1.54
1	C	151	LYS	C-O	14.27	1.42	1.24
1	E	67	ILE	CA-CB	14.14	1.73	1.54
1	F	170	MSE	SE-CE	-13.75	1.54	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	SER	N-CA	13.21	1.63	1.46
1	E	160	THR	N-CA	12.99	1.62	1.46
1	E	105	TYR	N-CA	12.61	1.62	1.46
1	A	238	GLN	CG-CD	12.32	1.82	1.52
1	C	303	ARG	CA-C	12.31	1.69	1.52
1	E	238	GLN	CD-NE2	12.22	1.58	1.33
1	F	67	ILE	CA-CB	12.21	1.71	1.54
1	F	238	GLN	CD-NE2	12.06	1.58	1.33
1	A	151	LYS	C-O	11.98	1.39	1.24
1	C	258	VAL	CA-C	11.87	1.67	1.52
1	D	108	VAL	CA-C	11.80	1.62	1.53
1	B	248	LEU	CG-CD1	11.51	1.90	1.52
1	B	75	SER	CA-C	11.44	1.68	1.52
1	A	298	LEU	CG-CD1	11.37	1.90	1.52
1	A	160	THR	CA-CB	11.26	1.72	1.53
1	B	160	THR	N-CA	11.21	1.60	1.46
1	F	75	SER	N-CA	11.20	1.60	1.46
1	B	160	THR	CA-CB	11.19	1.72	1.53
1	C	177	ASP	CA-C	-10.90	1.39	1.52
1	A	328	VAL	CA-CB	-10.88	1.41	1.54
1	C	208	GLY	CA-C	10.87	1.67	1.51
1	B	159	ALA	N-CA	10.86	1.61	1.45
1	D	198	GLU	CG-CD	10.84	1.79	1.52
1	C	4	LEU	CA-C	10.80	1.65	1.52
1	D	151	LYS	C-O	10.66	1.38	1.24
1	A	131	ALA	CA-C	-10.63	1.36	1.53
1	B	238	GLN	CD-NE2	10.63	1.55	1.33
1	B	286	GLU	CG-CD	10.57	1.78	1.52
1	A	63	LEU	N-CA	10.55	1.59	1.45
1	E	319	GLN	CG-CD	10.45	1.78	1.52
1	A	160	THR	N-CA	10.35	1.59	1.46
1	C	249	THR	C-O	10.34	1.37	1.24
1	F	151	LYS	C-O	10.21	1.37	1.24
1	C	207	ASP	CB-CG	10.21	1.77	1.52
1	F	3	THR	N-CA	10.18	1.58	1.46
1	F	209	THR	CA-C	10.14	1.66	1.52
1	D	225	VAL	CA-CB	10.12	1.68	1.54
1	E	246	SER	N-CA	9.96	1.59	1.46
1	C	42	GLY	C-O	9.96	1.37	1.23
1	D	219	GLN	N-CA	9.89	1.58	1.46
1	B	327	ILE	CA-CB	-9.87	1.42	1.54
1	E	209	THR	CA-CB	-9.87	1.36	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	160	THR	N-CA	9.82	1.58	1.46
1	A	41	SER	C-O	9.80	1.36	1.24
1	D	16	ASP	CA-C	9.77	1.65	1.52
1	B	215	LYS	CB-CG	9.77	1.81	1.52
1	E	21	VAL	CA-CB	-9.73	1.41	1.54
1	E	62	PRO	N-CA	9.69	1.59	1.47
1	A	317	ILE	N-CA	9.68	1.58	1.46
1	E	199	VAL	C-O	-9.61	1.14	1.24
1	F	185	ARG	N-CA	9.57	1.58	1.45
1	F	293	LYS	C-O	9.56	1.36	1.24
1	E	286	GLU	CD-OE1	9.56	1.43	1.25
1	A	286	GLU	CG-CD	9.45	1.75	1.52
1	F	160	THR	CA-CB	9.39	1.69	1.53
1	A	19	VAL	CA-CB	9.37	1.67	1.54
1	B	159	ALA	CA-CB	-9.37	1.39	1.53
1	E	83	GLU	CG-CD	9.32	1.75	1.52
1	D	286	GLU	CG-CD	9.27	1.75	1.52
1	F	179	VAL	CA-C	-9.25	1.41	1.52
1	F	266	VAL	CA-CB	9.25	1.63	1.54
1	B	180	ALA	N-CA	9.22	1.57	1.46
1	A	288	MSE	SE-CE	-9.21	1.67	1.95
1	E	208	GLY	N-CA	9.20	1.58	1.45
1	A	19	VAL	N-CA	9.18	1.57	1.46
1	E	59	ARG	CG-CD	9.18	1.79	1.52
1	C	114	VAL	CA-C	-9.15	1.44	1.52
1	A	266	VAL	CA-CB	9.14	1.64	1.54
1	A	143	GLU	C-O	-9.14	1.12	1.24
1	F	202	ARG	NE-CZ	9.12	1.43	1.33
1	C	303	ARG	N-CA	9.09	1.57	1.46
1	A	322	ILE	CG1-CD1	9.08	1.87	1.51
1	D	244	ALA	CA-CB	-9.08	1.40	1.53
1	E	255	PRO	N-CA	-9.03	1.40	1.47
1	D	57	ILE	CA-CB	-9.02	1.42	1.54
1	E	300	ILE	CA-CB	9.00	1.64	1.54
1	A	168	VAL	CA-CB	8.97	1.65	1.54
1	D	225	VAL	CB-CG2	8.95	1.82	1.52
1	C	200	ILE	CA-C	-8.95	1.42	1.52
1	B	301	VAL	CA-C	-8.92	1.41	1.52
1	B	106	ALA	CA-CB	8.91	1.68	1.53
1	E	149	PRO	C-O	-8.87	1.12	1.24
1	E	177	ASP	C-O	8.86	1.34	1.24
1	C	114	VAL	C-O	-8.83	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	GLY	C-O	8.77	1.31	1.23
1	E	17	VAL	CA-CB	8.74	1.66	1.54
1	B	207	ASP	C-O	8.74	1.34	1.24
1	F	149	PRO	C-O	-8.69	1.12	1.24
1	B	116	LEU	C-O	-8.66	1.12	1.24
1	C	160	THR	CA-CB	8.63	1.68	1.53
1	F	65	LEU	C-O	8.57	1.35	1.23
1	D	97	SER	N-CA	-8.54	1.36	1.46
1	A	268	LEU	CA-C	8.51	1.63	1.52
1	F	271	ILE	C-O	-8.50	1.14	1.24
1	B	245	VAL	CA-CB	-8.48	1.43	1.54
1	F	322	ILE	C-O	-8.47	1.15	1.24
1	B	235	SER	C-O	8.46	1.36	1.24
1	F	296	GLN	C-O	8.44	1.34	1.24
1	A	89	ALA	CA-CB	8.37	1.68	1.53
1	D	106	ALA	CA-CB	-8.37	1.40	1.53
1	E	153	SER	N-CA	8.35	1.56	1.46
1	B	118	GLN	C-O	-8.33	1.14	1.24
1	D	105	TYR	N-CA	8.32	1.56	1.46
1	A	67	ILE	N-CA	8.31	1.56	1.46
1	E	42	GLY	C-O	8.30	1.35	1.23
1	A	327	ILE	CA-CB	-8.30	1.44	1.54
1	C	238	GLN	CD-NE2	8.27	1.50	1.33
1	C	207	ASP	CA-C	-8.25	1.41	1.52
1	F	257	THR	CA-C	-8.24	1.44	1.53
1	D	279	ASP	CB-CG	-8.23	1.31	1.52
1	F	136	ALA	CA-CB	-8.23	1.40	1.53
1	C	237	ILE	CA-CB	8.22	1.64	1.54
1	A	170	MSE	SE-CE	-8.22	1.70	1.95
1	F	76	SER	C-O	8.21	1.34	1.24
1	D	7	ALA	CA-CB	-8.20	1.39	1.53
1	F	254	VAL	CA-CB	-8.16	1.43	1.54
1	E	43	ILE	CA-CB	-8.13	1.44	1.53
1	B	99	ASP	C-O	-8.10	1.13	1.23
1	D	207	ASP	C-O	8.10	1.34	1.24
1	B	43	ILE	C-O	-8.08	1.14	1.24
1	E	219	GLN	CA-C	-8.08	1.42	1.52
1	D	301	VAL	CA-CB	8.08	1.65	1.54
1	D	149	PRO	N-CA	8.07	1.56	1.47
1	E	109	PRO	C-O	-8.06	1.14	1.23
1	F	71	GLY	C-O	-8.06	1.17	1.24
1	C	19	VAL	CA-CB	8.05	1.65	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	39	ALA	N-CA	8.05	1.56	1.46
1	C	96	VAL	CA-CB	8.04	1.65	1.54
1	B	305	VAL	CA-CB	8.03	1.63	1.55
1	E	32	ASP	CA-C	8.02	1.62	1.52
1	D	81	PHE	CA-C	-8.00	1.43	1.52
1	A	159	ALA	N-CA	7.98	1.56	1.46
1	B	246	SER	C-O	-7.95	1.15	1.24
1	C	282	ALA	C-O	7.94	1.33	1.24
1	D	188	ALA	CA-CB	7.94	1.66	1.53
1	D	36	ILE	CA-CB	7.94	1.63	1.54
1	B	105	TYR	N-CA	7.92	1.56	1.46
1	E	262	ILE	C-O	-7.91	1.13	1.24
1	C	214	SER	CA-C	-7.90	1.42	1.53
1	F	329	LYS	CE-NZ	7.90	1.73	1.49
1	E	5	PHE	C-O	7.88	1.33	1.23
1	F	186	GLU	CG-CD	7.84	1.71	1.52
1	A	121	SER	C-O	7.84	1.34	1.23
1	E	184	ASN	CA-C	-7.83	1.43	1.52
1	A	78	ASP	N-CA	-7.82	1.35	1.46
1	F	202	ARG	C-O	7.82	1.33	1.24
1	B	14	ALA	N-CA	7.82	1.56	1.46
1	A	326	VAL	CA-CB	-7.79	1.45	1.54
1	E	167	ALA	CA-CB	-7.79	1.41	1.53
1	F	67	ILE	N-CA	7.79	1.56	1.46
1	C	244	ALA	C-O	7.78	1.32	1.24
1	F	249	THR	N-CA	7.75	1.57	1.46
1	C	167	ALA	CA-CB	-7.74	1.41	1.53
1	C	309	GLU	CA-C	7.74	1.63	1.52
1	E	269	LEU	C-O	-7.73	1.14	1.24
1	F	322	ILE	CA-CB	7.71	1.64	1.54
1	B	303	ARG	CB-CG	7.70	1.75	1.52
1	E	219	GLN	N-CA	7.69	1.56	1.46
1	A	58	VAL	CA-CB	-7.68	1.44	1.53
1	E	168	VAL	CA-CB	7.67	1.63	1.54
1	C	85	ASP	CA-C	7.65	1.62	1.52
1	A	37	LYS	CA-CB	7.65	1.62	1.52
1	A	3	THR	CA-C	7.64	1.62	1.52
1	A	83	GLU	N-CA	7.64	1.56	1.46
1	B	207	ASP	CA-C	-7.64	1.42	1.52
1	A	24	ILE	CG1-CD1	7.63	1.81	1.51
1	B	174	ARG	C-O	7.62	1.33	1.24
1	C	130	THR	CA-CB	7.60	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	PHE	CA-C	-7.60	1.43	1.52
1	C	60	GLU	N-CA	7.59	1.55	1.45
1	B	96	VAL	CA-C	7.58	1.62	1.52
1	A	182	THR	C-O	-7.58	1.14	1.23
1	C	3	THR	CA-CB	7.58	1.64	1.53
1	A	102	LEU	CA-C	7.57	1.61	1.53
1	A	169	SER	CA-C	-7.56	1.43	1.52
1	A	219	GLN	N-CA	7.55	1.55	1.46
1	F	206	TYR	N-CA	7.54	1.55	1.46
1	D	58	VAL	CA-CB	-7.52	1.45	1.54
1	F	202	ARG	CD-NE	7.52	1.56	1.46
1	A	187	ALA	N-CA	7.52	1.55	1.46
1	A	49	LEU	N-CA	7.51	1.55	1.46
1	E	38	VAL	C-O	-7.51	1.15	1.24
1	D	238	GLN	CD-NE2	7.50	1.49	1.33
1	E	135	ALA	CA-CB	-7.46	1.41	1.53
1	F	148	SER	C-O	7.45	1.32	1.24
1	D	47	ASP	CA-C	7.44	1.62	1.52
1	D	186	GLU	CG-CD	7.44	1.70	1.52
1	E	83	GLU	C-O	-7.43	1.14	1.23
1	F	168	VAL	C-O	-7.43	1.15	1.24
1	E	88	ILE	CA-CB	-7.40	1.45	1.54
1	B	173	LYS	C-O	-7.39	1.15	1.24
1	C	210	LEU	N-CA	7.39	1.54	1.45
1	D	148	SER	CA-C	7.39	1.59	1.52
1	D	203	GLU	CG-CD	7.38	1.70	1.52
1	D	91	SER	CA-C	-7.38	1.42	1.52
1	F	207	ASP	C-O	7.37	1.33	1.24
1	C	104	GLU	N-CA	7.37	1.55	1.46
1	F	45	TYR	C-O	7.37	1.32	1.24
1	A	310	THR	C-O	-7.32	1.17	1.24
1	D	179	VAL	CA-CB	7.32	1.62	1.54
1	C	105	TYR	N-CA	7.31	1.55	1.46
1	B	58	VAL	CA-C	-7.31	1.44	1.52
1	B	196	ALA	CA-CB	-7.30	1.41	1.53
1	B	83	GLU	CG-CD	7.29	1.70	1.52
1	E	161	GLY	C-O	7.28	1.32	1.23
1	B	215	LYS	CG-CD	7.28	1.74	1.52
1	C	116	LEU	C-O	-7.27	1.15	1.24
1	F	21	VAL	CA-C	-7.26	1.46	1.53
1	D	26	THR	CB-CG2	7.25	1.76	1.52
1	B	207	ASP	CB-CG	7.25	1.70	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	ALA	CA-CB	7.25	1.65	1.53
1	B	88	ILE	C-O	-7.25	1.16	1.24
1	D	296	GLN	CA-C	7.25	1.62	1.52
1	B	231	ALA	C-O	7.24	1.32	1.24
1	A	321	ARG	CD-NE	7.24	1.56	1.46
1	B	91	SER	CA-C	-7.23	1.43	1.52
1	C	237	ILE	C-O	7.20	1.32	1.24
1	B	126	MSE	SE-CE	-7.19	1.73	1.95
1	C	220	GLY	N-CA	7.16	1.52	1.45
1	A	105	TYR	N-CA	7.15	1.55	1.46
1	B	219	GLN	N-CA	7.15	1.55	1.46
1	F	315	LYS	CD-CE	7.15	1.74	1.52
1	E	162	GLY	C-O	7.15	1.33	1.23
1	F	195	GLY	C-O	-7.15	1.15	1.24
1	C	254	VAL	C-O	7.13	1.30	1.23
1	F	304	GLU	C-O	-7.12	1.15	1.24
1	E	229	GLN	CD-NE2	7.12	1.48	1.33
1	A	238	GLN	CA-C	7.11	1.62	1.52
1	F	257	THR	C-O	-7.10	1.16	1.24
1	A	322	ILE	N-CA	7.08	1.54	1.46
1	B	22	LYS	CA-CB	7.08	1.65	1.53
1	E	99	ASP	C-O	-7.06	1.15	1.23
1	E	59	ARG	CB-CG	7.05	1.73	1.52
1	C	258	VAL	CA-CB	-7.05	1.44	1.54
1	C	143	GLU	C-O	-7.04	1.15	1.24
1	D	84	GLY	C-O	-7.04	1.14	1.24
1	F	128	TYR	CA-CB	-7.04	1.44	1.53
1	D	150	GLU	CA-C	-7.01	1.43	1.52
1	F	40	TYR	CZ-OH	7.00	1.52	1.38
1	B	208	GLY	CA-C	6.98	1.61	1.51
1	D	150	GLU	N-CA	6.98	1.55	1.46
1	F	317	ILE	N-CA	6.98	1.55	1.46
1	B	182	THR	CA-C	-6.97	1.44	1.52
1	E	239	TYR	CA-CB	6.96	1.64	1.53
1	B	59	ARG	CA-C	6.95	1.62	1.52
1	F	292	LEU	C-O	-6.95	1.14	1.24
1	F	67	ILE	CG1-CD1	6.94	1.78	1.51
1	F	276	CYS	C-O	-6.94	1.15	1.24
1	E	151	LYS	C-O	6.94	1.34	1.24
1	F	46	LYS	CA-C	6.90	1.62	1.52
1	F	228	LYS	CE-NZ	6.89	1.70	1.49
1	B	265	GLY	C-O	-6.88	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	300	ILE	CA-C	6.88	1.61	1.52
1	D	226	GLY	N-CA	6.88	1.53	1.45
1	B	3	THR	CB-CG2	6.87	1.75	1.52
1	E	245	VAL	CA-CB	-6.85	1.45	1.54
1	C	34	VAL	C-O	-6.85	1.16	1.24
1	C	155	LEU	CA-C	-6.83	1.44	1.52
1	F	117	PRO	N-CA	6.83	1.55	1.47
1	A	126	MSE	SE-CE	-6.82	1.75	1.95
1	F	278	MSE	SE-CE	6.80	2.15	1.95
1	F	301	VAL	CA-CB	6.80	1.62	1.54
1	F	301	VAL	CA-C	-6.79	1.45	1.52
1	F	225	VAL	CA-CB	6.79	1.62	1.54
1	A	53	ALA	CA-CB	6.79	1.65	1.53
1	E	318	LEU	N-CA	6.78	1.54	1.46
1	A	136	ALA	CA-CB	6.77	1.64	1.53
1	C	221	ALA	CA-C	-6.75	1.44	1.52
1	E	115	PRO	C-O	-6.75	1.15	1.23
1	E	67	ILE	N-CA	6.74	1.54	1.46
1	A	19	VAL	CA-C	6.73	1.61	1.52
1	C	8	LEU	CA-C	6.73	1.61	1.52
1	F	21	VAL	C-O	-6.73	1.14	1.23
1	A	41	SER	N-CA	-6.73	1.37	1.46
1	A	247	GLY	N-CA	6.72	1.52	1.45
1	F	329	LYS	CD-CE	6.72	1.72	1.52
1	A	62	PRO	C-N	6.71	1.42	1.33
1	B	62	PRO	N-CA	6.71	1.55	1.47
1	A	280	VAL	CA-CB	6.71	1.63	1.54
1	C	102	LEU	CA-C	6.71	1.61	1.53
1	C	212	ALA	C-O	6.71	1.32	1.24
1	F	304	GLU	CA-C	-6.71	1.44	1.52
1	F	249	THR	C-O	6.67	1.33	1.23
1	B	43	ILE	CA-CB	6.66	1.62	1.53
1	C	121	SER	N-CA	6.66	1.54	1.45
1	A	142	LEU	CA-C	-6.64	1.44	1.52
1	B	319	GLN	CA-CB	6.64	1.64	1.53
1	C	160	THR	N-CA	6.64	1.54	1.46
1	E	321	ARG	CA-C	6.64	1.63	1.52
1	D	253	GLU	CG-CD	6.63	1.68	1.52
1	B	241	GLY	C-O	-6.63	1.15	1.23
1	F	274	VAL	C-O	-6.62	1.16	1.24
1	A	57	ILE	CA-CB	-6.62	1.45	1.54
1	C	296	GLN	C-O	6.62	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	VAL	CA-C	-6.62	1.46	1.52
1	F	116	LEU	N-CA	6.61	1.56	1.46
1	A	115	PRO	CA-C	6.61	1.61	1.52
1	E	251	GLY	N-CA	6.60	1.51	1.45
1	E	59	ARG	NE-CZ	6.60	1.40	1.33
1	F	318	LEU	N-CA	6.59	1.54	1.46
1	B	254	VAL	N-CA	-6.59	1.40	1.46
1	E	326	VAL	C-O	6.58	1.31	1.24
1	B	296	GLN	C-O	6.57	1.32	1.24
1	C	189	ASP	N-CA	6.55	1.54	1.46
1	A	103	SER	CA-C	-6.55	1.44	1.52
1	A	321	ARG	NE-CZ	6.55	1.40	1.33
1	E	56	ASN	CG-OD1	6.55	1.35	1.23
1	D	9	GLN	C-O	-6.55	1.16	1.24
1	B	195	GLY	N-CA	6.54	1.54	1.45
1	E	44	ASN	CB-CG	6.52	1.68	1.52
1	B	38	VAL	N-CA	-6.52	1.38	1.46
1	F	208	GLY	C-O	6.52	1.32	1.23
1	C	271	ILE	CA-CB	-6.51	1.45	1.53
1	B	286	GLU	CB-CG	6.51	1.72	1.52
1	B	40	TYR	CA-CB	-6.51	1.45	1.53
1	A	225	VAL	C-O	-6.51	1.14	1.24
1	C	171	LEU	C-O	6.51	1.31	1.24
1	F	286	GLU	CG-CD	6.50	1.68	1.52
1	D	280	VAL	CA-CB	6.50	1.61	1.54
1	E	301	VAL	CA-CB	-6.50	1.46	1.54
1	D	62	PRO	N-CA	-6.49	1.39	1.47
1	D	317	ILE	CA-CB	6.49	1.61	1.54
1	B	207	ASP	C-N	6.49	1.43	1.33
1	B	170	MSE	SE-CE	-6.49	1.75	1.95
1	F	249	THR	CB-CG2	6.49	1.74	1.52
1	E	40	TYR	C-O	-6.48	1.17	1.24
1	A	178	VAL	CA-CB	-6.48	1.46	1.54
1	D	88	ILE	N-CA	-6.48	1.38	1.46
1	D	114	VAL	CA-CB	6.46	1.62	1.54
1	A	27	GLU	C-O	-6.45	1.15	1.24
1	C	199	VAL	N-CA	6.45	1.53	1.46
1	C	3	THR	N-CA	6.45	1.53	1.46
1	E	274	VAL	CA-CB	-6.44	1.46	1.54
1	C	304	GLU	C-O	-6.43	1.15	1.23
1	B	199	VAL	CA-CB	-6.43	1.46	1.54
1	B	24	ILE	CB-CG2	6.42	1.73	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	ALA	N-CA	6.42	1.54	1.45
1	B	136	ALA	CA-CB	-6.42	1.42	1.53
1	E	323	GLN	CG-CD	6.42	1.68	1.52
1	F	166	ILE	CB-CG2	6.41	1.73	1.52
1	D	211	LYS	C-O	6.40	1.31	1.23
1	D	286	GLU	N-CA	6.39	1.54	1.46
1	E	59	ARG	C-O	-6.39	1.15	1.24
1	E	154	VAL	C-O	-6.39	1.17	1.24
1	A	123	LYS	CD-CE	6.38	1.71	1.52
1	E	180	ALA	N-CA	6.38	1.53	1.46
1	A	82	ALA	CA-CB	-6.38	1.41	1.53
1	A	223	ASP	C-O	-6.38	1.16	1.24
1	C	209	THR	CA-C	6.38	1.61	1.52
1	D	286	GLU	CD-OE2	6.37	1.37	1.25
1	D	215	LYS	CG-CD	6.37	1.71	1.52
1	A	212	ALA	CA-C	6.37	1.61	1.52
1	B	188	ALA	CA-CB	-6.36	1.43	1.53
1	D	277	PRO	CA-C	-6.36	1.45	1.52
1	B	179	VAL	N-CA	6.35	1.54	1.46
1	E	148	SER	C-O	6.35	1.32	1.24
1	C	253	GLU	CA-C	-6.35	1.44	1.52
1	D	151	LYS	N-CA	6.35	1.54	1.46
1	B	114	VAL	CA-C	-6.34	1.48	1.52
1	D	278	MSE	C-O	-6.34	1.16	1.24
1	B	215	LYS	CA-CB	6.33	1.63	1.53
1	A	306	SER	CA-C	6.33	1.60	1.52
1	A	271	ILE	CG1-CD1	-6.33	1.27	1.51
1	B	106	ALA	C-O	6.32	1.31	1.23
1	C	40	TYR	CA-CB	-6.32	1.43	1.53
1	E	10	ALA	CA-CB	-6.32	1.42	1.53
1	C	242	SER	N-CA	6.32	1.54	1.46
1	E	286	GLU	CD-OE2	6.31	1.37	1.25
1	E	209	THR	N-CA	-6.29	1.38	1.46
1	D	117	PRO	CA-C	6.29	1.60	1.52
1	A	180	ALA	CA-CB	-6.28	1.44	1.53
1	F	234	LEU	C-O	-6.28	1.16	1.24
1	F	57	ILE	CA-CB	-6.28	1.46	1.54
1	F	123	LYS	CA-C	6.28	1.61	1.52
1	F	228	LYS	CG-CD	6.27	1.71	1.52
1	C	102	LEU	N-CA	6.26	1.55	1.46
1	B	298	LEU	CA-C	6.25	1.61	1.52
1	B	135	ALA	N-CA	6.25	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	19	VAL	CA-CB	6.25	1.62	1.54
1	F	282	ALA	N-CA	6.25	1.54	1.46
1	F	19	VAL	N-CA	6.24	1.54	1.46
1	C	213	LEU	N-CA	6.23	1.53	1.46
1	E	205	VAL	C-O	-6.22	1.16	1.24
1	C	258	VAL	CB-CG2	-6.22	1.32	1.52
1	B	22	LYS	CB-CG	6.22	1.71	1.52
1	B	151	LYS	C-O	6.22	1.32	1.23
1	C	94	LEU	CG-CD1	6.21	1.73	1.52
1	D	13	ASN	CB-CG	6.20	1.67	1.52
1	F	10	ALA	CA-CB	-6.20	1.42	1.53
1	A	72	THR	CA-CB	-6.19	1.43	1.53
1	C	283	ALA	CA-CB	-6.19	1.43	1.53
1	F	322	ILE	CG1-CD1	6.19	1.75	1.51
1	C	198	GLU	CD-OE1	6.18	1.37	1.25
1	E	329	LYS	C-O	-6.18	1.16	1.24
1	E	40	TYR	CA-C	-6.18	1.46	1.53
1	D	153	SER	C-O	-6.18	1.16	1.23
1	D	42	GLY	N-CA	6.18	1.51	1.44
1	C	212	ALA	CA-C	6.17	1.61	1.52
1	E	3	THR	N-CA	6.17	1.53	1.45
1	D	126	MSE	SE-CE	-6.17	1.76	1.95
1	B	79	PRO	C-O	6.17	1.32	1.24
1	B	250	GLY	N-CA	6.17	1.53	1.45
1	D	315	LYS	C-O	-6.16	1.17	1.24
1	D	156	VAL	C-O	-6.16	1.17	1.24
1	A	258	VAL	CB-CG2	-6.16	1.32	1.52
1	D	278	MSE	SE-CE	-6.15	1.76	1.95
1	E	321	ARG	NE-CZ	6.15	1.39	1.33
1	A	206	TYR	N-CA	-6.15	1.38	1.46
1	C	186	GLU	C-O	6.14	1.31	1.24
1	E	309	GLU	CA-C	6.14	1.60	1.52
1	B	130	THR	C-O	-6.13	1.16	1.24
1	F	315	LYS	CE-NZ	6.13	1.67	1.49
1	B	157	THR	N-CA	6.12	1.53	1.45
1	C	112	TRP	C-O	6.12	1.32	1.24
1	F	184	ASN	CA-C	-6.12	1.45	1.53
1	A	329	LYS	C-O	-6.12	1.16	1.23
1	A	257	THR	C-O	-6.11	1.16	1.24
1	A	63	LEU	C-O	-6.11	1.16	1.23
1	D	45	TYR	CE1-CZ	6.11	1.52	1.38
1	E	70	ALA	CA-CB	-6.10	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	188	ALA	N-CA	6.10	1.54	1.46
1	B	17	VAL	N-CA	6.09	1.53	1.46
1	B	105	TYR	CA-C	6.09	1.60	1.52
1	D	308	GLU	C-O	6.08	1.31	1.24
1	E	287	ARG	N-CA	-6.08	1.39	1.46
1	E	76	SER	CA-CB	6.08	1.62	1.53
1	C	10	ALA	CA-CB	-6.08	1.44	1.53
1	E	79	PRO	C-O	6.08	1.31	1.24
1	C	232	SER	C-O	6.08	1.31	1.24
1	E	160	THR	CA-CB	6.07	1.63	1.53
1	C	213	LEU	CA-C	6.06	1.59	1.52
1	D	180	ALA	N-CA	6.06	1.53	1.46
1	C	57	ILE	CA-CB	-6.05	1.46	1.54
1	B	317	ILE	CA-CB	6.05	1.61	1.54
1	A	202	ARG	NE-CZ	6.05	1.39	1.33
1	F	268	LEU	C-O	6.04	1.30	1.24
1	A	259	TYR	N-CA	-6.04	1.37	1.46
1	D	103	SER	C-O	-6.04	1.16	1.23
1	E	249	THR	CA-C	-6.04	1.46	1.53
1	E	147	LEU	N-CA	-6.03	1.38	1.46
1	A	141	ARG	CA-CB	-6.02	1.44	1.53
1	D	98	ARG	CZ-NH2	6.02	1.41	1.33
1	E	59	ARG	CD-NE	6.02	1.54	1.46
1	D	149	PRO	C-O	-6.01	1.17	1.23
1	E	131	ALA	CA-CB	-6.01	1.43	1.53
1	F	41	SER	N-CA	-6.00	1.38	1.46
1	F	58	VAL	CA-CB	-6.00	1.47	1.54
1	A	207	ASP	N-CA	6.00	1.53	1.46
1	B	108	VAL	CB-CG2	-6.00	1.32	1.52
1	F	52	LYS	N-CA	-6.00	1.39	1.46
1	C	17	VAL	CA-CB	5.99	1.62	1.54
1	D	243	VAL	C-O	5.99	1.29	1.24
1	A	275	TYR	N-CA	-5.98	1.39	1.46
1	D	249	THR	CB-CG2	5.98	1.72	1.52
1	C	279	ASP	CG-OD2	5.98	1.36	1.25
1	F	188	ALA	C-O	5.97	1.30	1.24
1	B	284	VAL	C-O	-5.97	1.17	1.24
1	E	257	THR	CA-C	-5.97	1.45	1.52
1	A	182	THR	CA-C	-5.97	1.45	1.52
1	E	81	PHE	CA-C	-5.97	1.45	1.52
1	C	164	GLY	N-CA	5.96	1.53	1.45
1	E	141	ARG	CZ-NH1	-5.96	1.24	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	LEU	N-CA	-5.96	1.39	1.46
1	A	288	MSE	CA-C	-5.96	1.44	1.52
1	D	215	LYS	CD-CE	5.96	1.70	1.52
1	E	83	GLU	N-CA	5.96	1.53	1.46
1	A	106	ALA	CA-C	5.96	1.59	1.52
1	F	172	ASN	N-CA	-5.96	1.39	1.46
1	E	167	ALA	N-CA	-5.95	1.39	1.46
1	E	182	THR	CB-CG2	5.95	1.72	1.52
1	D	255	PRO	N-CA	5.94	1.54	1.47
1	D	237	ILE	C-O	5.93	1.32	1.24
1	F	143	GLU	C-O	-5.93	1.16	1.24
1	F	293	LYS	N-CA	-5.92	1.39	1.46
1	E	62	PRO	C-O	-5.92	1.17	1.23
1	E	40	TYR	N-CA	-5.91	1.38	1.46
1	B	22	LYS	N-CA	5.91	1.53	1.46
1	B	230	LEU	N-CA	-5.90	1.38	1.46
1	E	56	ASN	CB-CG	5.90	1.66	1.52
1	B	186	GLU	CG-CD	5.90	1.66	1.52
1	A	259	TYR	CA-CB	-5.90	1.44	1.53
1	D	97	SER	C-O	-5.89	1.18	1.24
1	D	21	VAL	C-O	-5.89	1.17	1.24
1	A	223	ASP	N-CA	5.88	1.53	1.46
1	A	248	LEU	N-CA	5.88	1.53	1.46
1	F	118	GLN	CG-CD	5.88	1.66	1.52
1	F	263	LEU	C-O	5.88	1.31	1.24
1	F	243	VAL	N-CA	5.88	1.53	1.46
1	E	263	LEU	CA-C	-5.87	1.45	1.52
1	A	194	LEU	C-O	-5.87	1.16	1.24
1	B	130	THR	CA-CB	-5.87	1.43	1.53
1	A	180	ALA	C-O	-5.87	1.16	1.24
1	F	222	VAL	N-CA	-5.87	1.39	1.46
1	E	159	ALA	CA-CB	-5.86	1.43	1.53
1	B	207	ASP	CG-OD1	5.86	1.36	1.25
1	B	321	ARG	CA-C	5.86	1.60	1.52
1	D	16	ASP	CA-CB	5.86	1.62	1.53
1	B	144	GLN	CA-C	5.85	1.60	1.52
1	C	249	THR	CB-CG2	5.85	1.71	1.52
1	F	159	ALA	N-CA	5.85	1.53	1.46
1	E	56	ASN	N-CA	-5.85	1.38	1.46
1	E	57	ILE	C-O	-5.84	1.17	1.23
1	E	229	GLN	CA-CB	-5.84	1.43	1.53
1	E	57	ILE	CA-CB	-5.84	1.49	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	PRO	N-CA	5.84	1.54	1.47
1	D	45	TYR	CE2-CZ	5.83	1.52	1.38
1	A	218	TRP	C-N	-5.83	1.25	1.33
1	F	112	TRP	C-O	5.82	1.31	1.24
1	F	31	LYS	CB-CG	5.82	1.70	1.52
1	E	307	LEU	C-O	5.82	1.30	1.24
1	E	184	ASN	CG-OD1	-5.81	1.12	1.23
1	B	212	ALA	C-O	-5.81	1.17	1.24
1	A	166	ILE	C-O	5.80	1.31	1.24
1	A	210	LEU	CG-CD1	5.80	1.71	1.52
1	D	240	GLY	C-O	-5.80	1.15	1.23
1	F	163	VAL	N-CA	-5.80	1.39	1.46
1	A	121	SER	CA-CB	-5.80	1.43	1.53
1	A	37	LYS	CD-CE	5.80	1.69	1.52
1	A	37	LYS	CE-NZ	5.80	1.66	1.49
1	A	148	SER	C-O	5.79	1.30	1.24
1	D	258	VAL	CB-CG2	-5.79	1.33	1.52
1	B	310	THR	CA-CB	5.79	1.61	1.53
1	C	254	VAL	CA-C	5.79	1.59	1.52
1	D	151	LYS	CD-CE	5.79	1.69	1.52
1	B	189	ASP	CA-C	-5.79	1.45	1.52
1	E	99	ASP	CA-C	-5.79	1.45	1.52
1	E	228	LYS	CD-CE	5.79	1.69	1.52
1	C	66	GLY	C-O	5.78	1.31	1.23
1	C	223	ASP	C-N	-5.78	1.28	1.34
1	D	242	SER	CA-C	-5.77	1.45	1.52
1	C	245	VAL	CB-CG2	-5.77	1.33	1.52
1	A	87	VAL	CA-C	5.76	1.59	1.52
1	E	29	LEU	N-CA	5.76	1.53	1.45
1	B	209	THR	CA-CB	5.76	1.63	1.53
1	D	108	VAL	N-CA	-5.75	1.41	1.46
1	B	41	SER	C-O	5.74	1.31	1.24
1	D	105	TYR	CA-C	5.73	1.60	1.52
1	E	61	TYR	C-O	5.73	1.31	1.24
1	C	67	ILE	CA-CB	5.73	1.62	1.54
1	F	11	GLU	C-O	-5.72	1.16	1.23
1	B	210	LEU	CG-CD1	5.72	1.71	1.52
1	A	148	SER	CA-C	5.72	1.58	1.52
1	E	322	ILE	CA-CB	5.72	1.61	1.54
1	F	53	ALA	C-O	5.72	1.30	1.23
1	A	145	ASN	N-CA	-5.71	1.39	1.46
1	E	233	LEU	CA-C	5.71	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	VAL	C-O	5.71	1.30	1.24
1	A	236	LYS	CA-C	5.71	1.60	1.52
1	A	294	PRO	N-CA	-5.70	1.40	1.46
1	B	153	SER	C-O	-5.70	1.16	1.23
1	F	209	THR	CB-CG2	5.70	1.71	1.52
1	C	208	GLY	N-CA	5.70	1.53	1.45
1	B	40	TYR	C-O	-5.69	1.17	1.24
1	B	59	ARG	CG-CD	5.69	1.69	1.52
1	F	4	LEU	C-O	5.69	1.30	1.23
1	A	200	ILE	CA-C	-5.69	1.46	1.53
1	A	135	ALA	CA-C	5.68	1.60	1.52
1	C	170	MSE	CG-SE	-5.67	1.78	1.95
1	E	62	PRO	CB-CG	5.67	1.78	1.49
1	D	267	SER	C-O	5.67	1.30	1.23
1	C	182	THR	CA-C	-5.66	1.45	1.52
1	B	208	GLY	C-O	5.66	1.31	1.23
1	B	267	SER	C-O	5.66	1.30	1.23
1	A	17	VAL	N-CA	5.66	1.53	1.46
1	C	136	ALA	CA-CB	-5.66	1.44	1.53
1	E	206	TYR	N-CA	5.65	1.53	1.46
1	B	3	THR	CA-CB	5.65	1.63	1.53
1	F	138	SER	N-CA	-5.65	1.39	1.46
1	F	321	ARG	CG-CD	5.64	1.69	1.52
1	D	64	ILE	N-CA	5.63	1.53	1.46
1	A	196	ALA	CA-C	5.63	1.60	1.52
1	D	298	LEU	CG-CD1	5.63	1.71	1.52
1	A	83	GLU	CG-CD	5.62	1.66	1.52
1	F	168	VAL	CA-CB	-5.62	1.48	1.54
1	A	215	LYS	CG-CD	5.62	1.69	1.52
1	A	257	THR	CA-C	-5.62	1.45	1.52
1	E	56	ASN	CG-ND2	5.62	1.45	1.33
1	F	254	VAL	N-CA	-5.62	1.39	1.46
1	F	238	GLN	CB-CG	-5.62	1.35	1.52
1	A	228	LYS	CE-NZ	5.61	1.66	1.49
1	D	24	ILE	C-O	5.61	1.29	1.23
1	E	276	CYS	C-O	-5.61	1.17	1.24
1	C	3	THR	CB-CG2	5.61	1.71	1.52
1	D	216	GLN	C-O	-5.60	1.17	1.24
1	D	151	LYS	CA-C	5.60	1.60	1.52
1	E	262	ILE	N-CA	-5.60	1.39	1.46
1	F	301	VAL	N-CA	5.60	1.52	1.46
1	A	320	ASN	C-O	-5.60	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	81	PHE	N-CA	5.60	1.52	1.45
1	B	90	THR	N-CA	-5.60	1.39	1.46
1	D	219	GLN	C-O	-5.60	1.17	1.24
1	E	24	ILE	CA-CB	5.59	1.62	1.54
1	F	326	VAL	CA-CB	-5.59	1.47	1.54
1	D	210	LEU	N-CA	5.59	1.53	1.45
1	D	236	LYS	CA-C	5.59	1.60	1.52
1	A	53	ALA	CA-C	5.59	1.60	1.52
1	D	113	LEU	CA-C	-5.58	1.45	1.52
1	E	256	ALA	N-CA	5.58	1.53	1.46
1	C	165	GLY	C-O	5.58	1.30	1.23
1	F	99	ASP	CA-C	5.58	1.59	1.52
1	D	166	ILE	CA-CB	5.57	1.61	1.54
1	C	207	ASP	CG-OD1	5.57	1.35	1.25
1	F	160	THR	CA-C	-5.57	1.45	1.52
1	B	34	VAL	N-CA	-5.57	1.39	1.46
1	B	271	ILE	CA-C	5.57	1.59	1.52
1	D	275	TYR	N-CA	5.56	1.52	1.46
1	E	118	GLN	CG-CD	5.56	1.66	1.52
1	F	74	VAL	CA-CB	5.56	1.62	1.54
1	D	19	VAL	CA-CB	5.56	1.62	1.54
1	D	37	LYS	C-O	5.55	1.30	1.23
1	B	68	ASP	CA-C	-5.55	1.45	1.52
1	B	303	ARG	CG-CD	5.55	1.69	1.52
1	F	319	GLN	CG-CD	5.55	1.66	1.52
1	C	58	VAL	C-O	-5.54	1.18	1.24
1	E	21	VAL	C-O	-5.53	1.17	1.24
1	B	61	TYR	CA-C	-5.52	1.45	1.52
1	F	55	GLY	C-O	5.52	1.31	1.23
1	F	83	GLU	CA-C	-5.52	1.45	1.52
1	F	219	GLN	N-CA	5.51	1.53	1.46
1	F	177	ASP	CG-OD1	5.50	1.35	1.25
1	F	215	LYS	CG-CD	5.50	1.69	1.52
1	F	325	ARG	CZ-NH2	5.50	1.40	1.33
1	A	287	ARG	CZ-NH1	-5.50	1.25	1.32
1	C	210	LEU	C-O	-5.50	1.16	1.23
1	E	8	LEU	C-O	-5.50	1.17	1.24
1	C	196	ALA	CA-CB	-5.49	1.44	1.53
1	C	11	GLU	N-CA	5.49	1.52	1.46
1	C	149	PRO	C-O	-5.49	1.15	1.23
1	E	36	ILE	C-O	-5.49	1.18	1.24
1	E	225	VAL	CB-CG1	-5.49	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	201	SER	N-CA	5.48	1.52	1.45
1	A	147	LEU	N-CA	-5.47	1.39	1.46
1	F	296	GLN	CA-C	-5.47	1.45	1.52
1	F	320	ASN	CA-C	5.47	1.60	1.52
1	C	101	GLY	C-O	-5.47	1.16	1.23
1	C	272	ASP	CA-C	-5.47	1.46	1.52
1	F	325	ARG	CB-CG	5.46	1.68	1.52
1	A	176	TYR	N-CA	5.46	1.53	1.45
1	F	161	GLY	C-O	5.46	1.29	1.23
1	F	43	ILE	N-CA	5.46	1.53	1.46
1	A	133	PHE	N-CA	-5.45	1.39	1.46
1	B	80	ARG	C-O	-5.45	1.17	1.24
1	F	90	THR	CA-C	-5.45	1.45	1.52
1	F	231	ALA	CA-C	-5.44	1.45	1.52
1	B	187	ALA	C-O	-5.44	1.16	1.24
1	B	294	PRO	N-CA	-5.44	1.40	1.47
1	F	208	GLY	N-CA	5.44	1.53	1.45
1	F	245	VAL	C-O	5.44	1.31	1.24
1	A	189	ASP	CG-OD2	5.43	1.35	1.25
1	C	198	GLU	CA-C	5.43	1.59	1.52
1	A	81	PHE	C-O	-5.43	1.17	1.23
1	E	76	SER	N-CA	5.43	1.52	1.46
1	B	249	THR	CB-CG2	5.42	1.70	1.52
1	C	27	GLU	CG-CD	5.42	1.65	1.52
1	A	50	ALA	CA-CB	-5.42	1.45	1.53
1	F	145	ASN	C-O	-5.42	1.16	1.23
1	F	327	ILE	CA-CB	-5.42	1.46	1.55
1	A	113	LEU	N-CA	5.42	1.52	1.46
1	C	62	PRO	CB-CG	5.41	1.76	1.49
1	B	108	VAL	CA-CB	-5.41	1.47	1.54
1	E	41	SER	C-O	5.41	1.30	1.24
1	A	36	ILE	CA-C	-5.41	1.46	1.52
1	A	106	ALA	C-O	5.40	1.30	1.23
1	C	281	ARG	N-CA	5.40	1.52	1.46
1	E	126	MSE	CG-SE	-5.40	1.79	1.95
1	E	19	VAL	N-CA	5.40	1.53	1.46
1	F	127	VAL	C-O	-5.40	1.17	1.24
1	D	63	LEU	N-CA	5.40	1.52	1.45
1	D	176	TYR	N-CA	5.40	1.52	1.45
1	C	198	GLU	CD-OE2	5.39	1.35	1.25
1	A	294	PRO	C-O	-5.39	1.17	1.23
1	E	210	LEU	CA-C	-5.39	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	248	LEU	C-O	-5.39	1.17	1.24
1	B	242	SER	C-O	5.38	1.30	1.23
1	B	144	GLN	CD-OE1	5.38	1.33	1.23
1	E	205	VAL	N-CA	-5.38	1.40	1.46
1	E	207	ASP	CA-C	-5.38	1.45	1.52
1	F	114	VAL	CA-CB	5.38	1.60	1.54
1	E	266	VAL	CA-CB	5.37	1.64	1.55
1	A	39	ALA	N-CA	5.37	1.53	1.46
1	B	26	THR	CA-CB	-5.36	1.44	1.53
1	C	27	GLU	CB-CG	5.36	1.68	1.52
1	C	235	SER	N-CA	5.36	1.53	1.46
1	E	220	GLY	C-O	-5.36	1.17	1.24
1	A	163	VAL	N-CA	-5.36	1.40	1.46
1	B	104	GLU	N-CA	5.35	1.52	1.45
1	C	17	VAL	CA-C	5.35	1.59	1.52
1	A	229	GLN	CA-CB	-5.35	1.45	1.53
1	E	277	PRO	C-O	5.35	1.30	1.23
1	C	238	GLN	CA-C	5.35	1.60	1.53
1	A	102	LEU	C-O	5.34	1.29	1.23
1	E	178	VAL	CA-CB	-5.34	1.47	1.54
1	C	42	GLY	N-CA	5.34	1.53	1.45
1	B	216	GLN	CD-NE2	5.34	1.44	1.33
1	A	238	GLN	CA-CB	5.33	1.62	1.53
1	A	268	LEU	N-CA	-5.33	1.39	1.46
1	C	32	ASP	N-CA	5.33	1.53	1.46
1	A	118	GLN	CG-CD	5.33	1.65	1.52
1	F	227	GLY	C-O	-5.33	1.16	1.23
1	A	107	SER	N-CA	-5.33	1.40	1.46
1	E	223	ASP	C-O	-5.33	1.18	1.24
1	D	228	LYS	CA-C	5.32	1.59	1.52
1	E	43	ILE	C-O	-5.32	1.17	1.23
1	A	256	ALA	C-O	-5.32	1.17	1.23
1	A	260	PRO	CA-C	5.32	1.59	1.52
1	B	92	TYR	C-O	-5.32	1.19	1.24
1	C	77	ASN	CG-ND2	5.31	1.44	1.33
1	B	147	LEU	C-O	5.31	1.30	1.23
1	E	170	MSE	CG-SE	-5.31	1.79	1.95
1	F	6	GLN	N-CA	5.31	1.52	1.45
1	E	31	LYS	CB-CG	5.30	1.68	1.52
1	D	302	ASP	CA-C	5.30	1.59	1.52
1	A	225	VAL	N-CA	-5.30	1.39	1.46
1	F	243	VAL	CA-C	-5.30	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	149	PRO	CA-C	-5.29	1.45	1.52
1	F	187	ALA	C-O	-5.29	1.17	1.24
1	E	2	SER	CA-C	5.29	1.64	1.52
1	C	266	VAL	CA-CB	5.29	1.60	1.54
1	A	269	LEU	C-O	5.28	1.30	1.24
1	B	212	ALA	CA-C	5.28	1.59	1.52
1	F	220	GLY	N-CA	5.28	1.51	1.45
1	A	113	LEU	C-O	-5.28	1.17	1.23
1	A	214	SER	CA-CB	-5.28	1.45	1.53
1	B	28	ASP	CA-C	5.28	1.59	1.52
1	E	135	ALA	C-O	5.28	1.30	1.24
1	D	66	GLY	C-O	5.27	1.31	1.23
1	B	121	SER	C-O	5.27	1.31	1.23
1	B	41	SER	CA-C	-5.27	1.45	1.52
1	D	186	GLU	CA-CB	5.26	1.61	1.53
1	D	117	PRO	N-CA	-5.26	1.40	1.47
1	D	108	VAL	CA-CB	5.26	1.61	1.53
1	C	195	GLY	CA-C	5.25	1.59	1.51
1	B	11	GLU	CA-C	5.25	1.58	1.52
1	C	23	THR	CA-C	-5.25	1.46	1.52
1	C	276	CYS	CA-C	5.25	1.58	1.53
1	D	159	ALA	CA-CB	5.24	1.62	1.53
1	E	322	ILE	N-CA	5.24	1.52	1.46
1	F	50	ALA	CA-CB	-5.24	1.44	1.53
1	F	105	TYR	CA-C	5.24	1.59	1.52
1	E	68	ASP	C-O	-5.24	1.17	1.24
1	B	201	SER	N-CA	5.24	1.52	1.45
1	E	319	GLN	CB-CG	5.24	1.68	1.52
1	C	168	VAL	CA-CB	-5.23	1.48	1.54
1	C	200	ILE	C-O	-5.23	1.17	1.23
1	C	172	ASN	C-O	5.22	1.30	1.24
1	E	40	TYR	CA-CB	-5.22	1.46	1.54
1	F	134	THR	CA-CB	-5.22	1.45	1.53
1	A	167	ALA	CA-CB	-5.22	1.45	1.53
1	B	313	ALA	CA-C	5.22	1.59	1.52
1	E	279	ASP	CA-C	-5.21	1.46	1.52
1	A	182	THR	CB-OG1	5.21	1.52	1.43
1	D	178	VAL	N-CA	5.21	1.52	1.46
1	E	43	ILE	CA-C	5.21	1.59	1.52
1	E	250	GLY	C-O	-5.21	1.16	1.23
1	F	83	GLU	CD-OE1	5.20	1.35	1.25
1	F	223	ASP	CA-C	5.20	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	GLY	N-CA	5.20	1.52	1.45
1	C	202	ARG	NE-CZ	5.20	1.38	1.33
1	F	300	ILE	C-N	5.20	1.39	1.33
1	C	259	TYR	C-N	5.19	1.40	1.34
1	C	208	GLY	C-O	5.19	1.30	1.23
1	B	266	VAL	CB-CG2	-5.18	1.35	1.52
1	C	146	GLY	CA-C	-5.18	1.44	1.51
1	B	5	PHE	CA-C	-5.18	1.46	1.52
1	B	254	VAL	CA-CB	5.18	1.59	1.54
1	A	279	ASP	CB-CG	-5.17	1.39	1.52
1	A	69	ALA	C-O	-5.17	1.17	1.23
1	D	13	ASN	N-CA	5.17	1.52	1.46
1	F	128	TYR	C-O	-5.17	1.19	1.23
1	A	79	PRO	C-O	5.16	1.30	1.24
1	F	229	GLN	CD-NE2	5.16	1.44	1.33
1	E	198	GLU	CD-OE2	5.15	1.35	1.25
1	A	114	VAL	CA-C	-5.14	1.49	1.52
1	E	254	VAL	N-CA	-5.14	1.40	1.46
1	D	215	LYS	CA-C	5.14	1.59	1.52
1	B	90	THR	CA-CB	-5.14	1.45	1.53
1	C	170	MSE	C-O	5.14	1.30	1.24
1	B	103	SER	C-O	-5.14	1.16	1.23
1	F	70	ALA	CA-C	-5.13	1.47	1.52
1	F	2	SER	C-N	5.13	1.40	1.33
1	A	182	THR	N-CA	5.13	1.52	1.45
1	A	258	VAL	C-O	5.12	1.30	1.24
1	D	239	TYR	C-O	-5.12	1.17	1.23
1	C	269	LEU	N-CA	5.12	1.52	1.46
1	E	110	GLY	N-CA	5.12	1.52	1.45
1	D	228	LYS	N-CA	5.11	1.52	1.46
1	A	317	ILE	CA-C	-5.11	1.46	1.52
1	C	246	SER	CA-C	-5.11	1.45	1.52
1	D	89	ALA	CA-C	5.11	1.58	1.52
1	D	289	SER	CA-C	-5.11	1.46	1.52
1	C	205	VAL	CA-CB	5.11	1.61	1.54
1	D	182	THR	N-CA	5.11	1.52	1.45
1	D	190	TYR	N-CA	-5.11	1.40	1.46
1	F	320	ASN	N-CA	5.11	1.52	1.46
1	D	212	ALA	CA-CB	-5.10	1.45	1.53
1	F	2	SER	CA-C	5.10	1.63	1.52
1	E	246	SER	CA-C	5.10	1.59	1.52
1	F	256	ALA	CA-C	-5.10	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	83	GLU	CA-CB	5.09	1.61	1.53
1	A	4	LEU	CG-CD1	5.09	1.69	1.52
1	A	205	VAL	CA-CB	5.09	1.60	1.54
1	C	166	ILE	CA-CB	-5.09	1.48	1.54
1	A	118	GLN	CA-C	-5.09	1.45	1.52
1	A	317	ILE	CA-CB	5.09	1.61	1.54
1	B	123	LYS	C-O	5.09	1.30	1.24
1	A	85	ASP	CG-OD2	5.08	1.35	1.25
1	D	198	GLU	CD-OE1	5.08	1.35	1.25
1	F	43	ILE	CG1-CD1	-5.08	1.31	1.51
1	F	94	LEU	CA-C	5.08	1.59	1.52
1	A	27	GLU	CG-CD	5.08	1.64	1.52
1	C	236	LYS	CA-C	5.08	1.59	1.52
1	D	177	ASP	C-O	5.08	1.30	1.24
1	D	280	VAL	N-CA	-5.08	1.40	1.46
1	F	219	GLN	CA-C	-5.08	1.46	1.52
1	A	142	LEU	C-O	-5.08	1.18	1.24
1	A	291	ASP	CB-CG	-5.08	1.39	1.52
1	B	12	LYS	CA-C	-5.08	1.46	1.52
1	F	80	ARG	C-O	-5.08	1.17	1.24
1	B	308	GLU	N-CA	5.07	1.52	1.46
1	F	191	LEU	C-O	5.07	1.30	1.24
1	A	109	PRO	N-CA	-5.07	1.40	1.47
1	E	64	ILE	CA-CB	5.07	1.60	1.54
1	A	276	CYS	CA-C	5.07	1.58	1.53
1	C	203	GLU	N-CA	5.07	1.52	1.46
1	E	289	SER	CA-C	5.07	1.60	1.52
1	E	321	ARG	CA-CB	5.07	1.62	1.53
1	B	211	LYS	C-O	5.07	1.30	1.23
1	B	309	GLU	CD-OE2	5.07	1.34	1.25
1	F	118	GLN	CD-OE1	5.06	1.33	1.23
1	B	40	TYR	C-N	-5.06	1.26	1.33
1	D	103	SER	CA-C	-5.06	1.46	1.52
1	F	140	HIS	CA-CB	-5.06	1.45	1.53
1	F	216	GLN	CA-C	-5.06	1.46	1.52
1	F	236	LYS	CA-CB	-5.06	1.46	1.53
1	A	148	SER	N-CA	-5.06	1.39	1.46
1	B	218	TRP	C-O	5.06	1.30	1.24
1	D	311	PRO	CA-C	5.06	1.59	1.52
1	C	105	TYR	CA-C	5.05	1.59	1.52
1	E	264	ARG	CZ-NH1	5.05	1.39	1.32
1	E	89	ALA	CA-CB	-5.05	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	224	PRO	C-O	5.05	1.30	1.24
1	D	282	ALA	CA-CB	5.05	1.61	1.53
1	F	202	ARG	CZ-NH1	5.05	1.39	1.32
1	B	328	VAL	C-O	-5.05	1.18	1.24
1	C	259	TYR	C-O	5.04	1.30	1.24
1	F	275	TYR	C-O	-5.04	1.17	1.24
1	F	308	GLU	CA-C	5.04	1.60	1.52
1	E	215	LYS	CG-CD	5.03	1.67	1.52
1	B	296	GLN	N-CA	5.03	1.52	1.46
1	E	324	GLY	CA-C	5.03	1.58	1.51
1	A	177	ASP	C-O	5.03	1.30	1.24
1	B	73	VAL	CA-C	5.02	1.59	1.52
1	E	86	GLU	CA-C	-5.02	1.46	1.52
1	D	62	PRO	CG-CD	5.02	1.67	1.50
1	D	17	VAL	N-CA	5.02	1.52	1.46
1	B	71	GLY	N-CA	5.02	1.51	1.45
1	A	121	SER	CA-C	5.01	1.59	1.53
1	B	291	ASP	CA-C	5.01	1.59	1.52
1	B	153	SER	CA-C	-5.01	1.46	1.53
1	E	259	TYR	CA-CB	-5.01	1.47	1.53
1	C	85	ASP	CG-OD1	5.01	1.34	1.25
1	F	31	LYS	N-CA	5.01	1.52	1.46
1	A	3	THR	CA-CB	5.01	1.64	1.54
1	A	18	SER	N-CA	-5.01	1.40	1.46
1	B	27	GLU	CG-CD	5.01	1.64	1.52
1	F	99	ASP	CG-OD2	5.01	1.34	1.25
1	F	13	ASN	C-O	5.00	1.29	1.24
1	A	181	SER	C-O	-5.00	1.18	1.24
1	E	231	ALA	CA-CB	-5.00	1.45	1.53

All (897) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ASP	CA-C-N	22.02	141.80	119.56
1	B	223	ASP	C-N-CA	22.02	141.80	119.56
1	A	61	TYR	C-N-CD	-21.88	72.47	120.60
1	A	61	TYR	CA-C-N	19.28	173.28	127.00
1	A	61	TYR	C-N-CA	19.28	173.28	127.00
1	E	61	TYR	CA-C-N	-17.65	101.37	119.90
1	E	61	TYR	C-N-CA	-17.65	101.37	119.90
1	C	150	GLU	N-CA-C	-14.52	98.06	114.62
1	C	61	TYR	CA-C-N	-14.48	101.74	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	TYR	C-N-CA	-14.48	101.74	119.84
1	E	78	ASP	CA-C-N	13.60	136.84	119.84
1	E	78	ASP	C-N-CA	13.60	136.84	119.84
1	A	41	SER	N-CA-C	13.38	139.30	110.80
1	C	245	VAL	CB-CA-C	-13.15	94.61	110.91
1	C	61	TYR	N-CA-C	12.81	138.13	109.81
1	A	63	LEU	N-CA-C	12.77	128.51	110.50
1	F	242	SER	N-CA-C	12.48	127.74	109.14
1	A	327	ILE	CB-CA-C	-12.29	93.37	111.68
1	C	116	LEU	CA-C-N	-12.04	108.65	120.21
1	C	116	LEU	C-N-CA	-12.04	108.65	120.21
1	A	114	VAL	CA-C-N	-11.97	107.76	119.85
1	A	114	VAL	C-N-CA	-11.97	107.76	119.85
1	B	61	TYR	CA-C-N	-11.91	104.95	119.84
1	B	61	TYR	C-N-CA	-11.91	104.95	119.84
1	A	116	LEU	CA-C-N	-11.70	108.45	120.03
1	A	116	LEU	C-N-CA	-11.70	108.45	120.03
1	E	319	GLN	N-CA-C	-11.31	99.69	113.15
1	F	131	ALA	N-CA-C	-11.24	94.65	110.50
1	B	41	SER	N-CA-C	11.13	134.50	110.80
1	F	301	VAL	CB-CA-C	-11.12	98.07	111.08
1	D	42	GLY	N-CA-C	-11.06	92.32	111.57
1	F	293	LYS	CA-C-O	10.96	126.41	119.29
1	F	74	VAL	O-C-N	-10.95	111.39	123.10
1	A	245	VAL	CB-CA-C	-10.87	97.02	111.15
1	F	144	GLN	N-CA-C	-10.85	99.50	113.17
1	E	183	GLY	CA-C-N	-10.55	105.88	122.87
1	E	183	GLY	C-N-CA	-10.55	105.88	122.87
1	A	238	GLN	CA-CB-CG	10.44	134.98	114.10
1	C	40	TYR	N-CA-C	10.34	123.69	108.60
1	F	202	ARG	N-CA-C	-10.30	100.06	111.28
1	E	61	TYR	N-CA-C	10.22	132.40	109.81
1	A	15	ASP	N-CA-C	10.08	126.01	112.30
1	A	40	TYR	N-CA-C	10.08	124.16	109.14
1	C	223	ASP	CA-C-N	10.07	131.24	120.47
1	C	223	ASP	C-N-CA	10.07	131.24	120.47
1	A	104	GLU	N-CA-C	-9.96	97.39	110.43
1	C	168	VAL	CB-CA-C	-9.93	98.73	112.14
1	C	165	GLY	N-CA-C	-9.90	100.50	112.49
1	D	279	ASP	N-CA-CB	-9.85	93.84	110.49
1	A	325	ARG	NE-CZ-NH1	-9.84	111.66	121.50
1	B	182	THR	CA-C-N	9.83	132.42	120.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	THR	C-N-CA	9.83	132.42	120.14
1	E	41	SER	N-CA-C	9.81	131.71	110.80
1	B	245	VAL	CB-CA-C	-9.80	96.52	111.31
1	B	50	ALA	N-CA-C	-9.76	101.12	113.23
1	F	327	ILE	CB-CG1-CD1	-9.75	93.32	113.80
1	C	269	LEU	CA-C-N	9.69	129.70	120.98
1	C	269	LEU	C-N-CA	9.69	129.70	120.98
1	B	207	ASP	O-C-N	9.68	135.47	122.59
1	E	104	GLU	N-CA-C	-9.64	93.54	109.07
1	D	61	TYR	CA-C-N	9.61	131.85	119.84
1	D	61	TYR	C-N-CA	9.61	131.85	119.84
1	F	325	ARG	NE-CZ-NH1	-9.56	111.94	121.50
1	B	315	LYS	N-CA-C	-9.51	101.24	113.12
1	F	316	ASP	N-CA-C	9.49	122.83	111.82
1	C	74	VAL	CB-CA-C	-9.45	101.69	111.23
1	D	258	VAL	N-CA-C	-9.40	102.42	113.42
1	B	61	TYR	N-CA-C	9.39	130.56	109.81
1	D	303	ARG	N-CA-C	9.35	123.67	108.99
1	B	108	VAL	CA-C-N	-9.34	109.65	120.11
1	B	108	VAL	C-N-CA	-9.34	109.65	120.11
1	F	41	SER	N-CA-CB	-9.34	94.71	110.49
1	F	34	VAL	N-CA-C	-9.32	95.06	108.48
1	A	280	VAL	N-CA-C	-9.31	99.22	112.35
1	A	218	TRP	CA-C-N	-9.25	103.87	121.54
1	A	218	TRP	C-N-CA	-9.25	103.87	121.54
1	D	249	THR	N-CA-C	-9.17	98.32	110.24
1	A	228	LYS	N-CA-C	-9.16	100.69	112.23
1	F	42	GLY	CA-C-N	-9.15	111.22	123.12
1	F	42	GLY	C-N-CA	-9.15	111.22	123.12
1	B	41	SER	CB-CA-C	-9.15	92.22	110.42
1	F	245	VAL	CB-CA-C	-9.14	98.68	111.21
1	B	266	VAL	CB-CA-C	9.07	121.57	111.59
1	A	136	ALA	N-CA-C	-9.05	101.37	111.14
1	E	50	ALA	N-CA-C	-9.04	101.51	112.54
1	E	113	LEU	CA-C-N	-9.03	114.73	123.04
1	E	113	LEU	C-N-CA	-9.03	114.73	123.04
1	D	276	CYS	CA-C-N	9.03	129.59	119.92
1	D	276	CYS	C-N-CA	9.03	129.59	119.92
1	E	207	ASP	CA-C-N	8.91	138.87	121.41
1	E	207	ASP	C-N-CA	8.91	138.87	121.41
1	C	185	ARG	N-CA-C	-8.90	98.77	110.43
1	E	246	SER	N-CA-C	8.87	129.69	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ILE	CB-CA-C	-8.83	100.28	110.96
1	C	207	ASP	N-CA-C	-8.82	92.02	110.80
1	C	148	SER	CA-C-N	-8.81	110.02	121.91
1	C	148	SER	C-N-CA	-8.81	110.02	121.91
1	E	59	ARG	CG-CD-NE	8.75	131.25	112.00
1	B	105	TYR	N-CA-C	8.73	129.39	110.80
1	D	218	TRP	CA-C-N	-8.72	104.88	121.54
1	D	218	TRP	C-N-CA	-8.72	104.88	121.54
1	C	33	GLY	N-CA-C	8.71	126.18	111.98
1	D	62	PRO	N-CA-C	-8.69	94.57	112.47
1	E	114	VAL	N-CA-C	8.69	118.30	108.05
1	B	41	SER	O-C-N	8.68	134.13	122.59
1	D	42	GLY	CA-C-N	8.67	137.30	121.70
1	D	42	GLY	C-N-CA	8.67	137.30	121.70
1	F	131	ALA	CA-C-N	-8.66	104.44	121.41
1	F	131	ALA	C-N-CA	-8.66	104.44	121.41
1	F	171	LEU	CA-C-N	-8.62	108.05	120.29
1	F	171	LEU	C-N-CA	-8.62	108.05	120.29
1	E	43	ILE	N-CA-C	8.62	121.17	107.73
1	F	75	SER	N-CA-C	8.60	129.11	110.80
1	D	198	GLU	N-CA-C	-8.60	95.50	108.99
1	C	254	VAL	CA-C-N	-8.58	109.11	119.84
1	C	254	VAL	C-N-CA	-8.58	109.11	119.84
1	F	288	MSE	N-CA-C	-8.52	102.78	113.01
1	E	141	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	D	41	SER	CA-C-N	8.51	130.04	122.47
1	D	41	SER	C-N-CA	8.51	130.04	122.47
1	E	210	LEU	CB-CA-C	-8.45	99.05	110.79
1	F	317	ILE	N-CA-C	-8.43	91.82	109.34
1	C	209	THR	CB-CA-C	8.41	127.16	110.42
1	C	183	GLY	CA-C-N	-8.36	110.40	122.94
1	C	183	GLY	C-N-CA	-8.36	110.40	122.94
1	F	41	SER	N-CA-C	8.32	128.53	110.80
1	D	246	SER	N-CA-C	8.30	128.48	110.80
1	C	170	MSE	N-CA-C	-8.27	102.34	111.36
1	F	68	ASP	N-CA-C	8.26	122.36	109.07
1	F	326	VAL	CA-C-N	-8.21	110.92	122.34
1	F	326	VAL	C-N-CA	-8.21	110.92	122.34
1	F	258	VAL	N-CA-C	-8.21	92.27	109.34
1	C	247	GLY	CA-C-N	8.17	135.51	122.11
1	C	247	GLY	C-N-CA	8.17	135.51	122.11
1	F	152	GLY	N-CA-C	8.07	122.43	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	207	ASP	CA-C-O	8.06	132.04	120.51
1	E	300	ILE	N-CA-C	-8.05	104.65	113.43
1	D	207	ASP	CA-C-N	8.05	137.18	121.41
1	D	207	ASP	C-N-CA	8.05	137.18	121.41
1	F	104	GLU	CA-C-N	-8.02	106.23	121.54
1	F	104	GLU	C-N-CA	-8.02	106.23	121.54
1	B	171	LEU	N-CA-C	-8.00	102.64	111.36
1	F	104	GLU	O-C-N	-8.00	112.58	122.82
1	A	19	VAL	N-CA-C	7.99	125.97	109.34
1	D	9	GLN	N-CA-C	7.99	121.44	108.41
1	E	74	VAL	CB-CA-C	-7.99	101.87	111.94
1	E	315	LYS	N-CA-C	-7.99	104.05	113.88
1	A	169	SER	CB-CA-C	-7.97	97.31	110.85
1	E	16	ASP	CA-C-N	-7.96	107.63	121.97
1	E	16	ASP	C-N-CA	-7.96	107.63	121.97
1	C	127	VAL	CB-CA-C	-7.96	99.82	112.16
1	A	178	VAL	CB-CA-C	7.93	122.16	110.98
1	F	41	SER	CA-C-N	7.92	136.93	121.41
1	F	41	SER	C-N-CA	7.92	136.93	121.41
1	E	72	THR	N-CA-C	-7.90	95.40	108.76
1	A	317	ILE	N-CA-CB	7.89	124.25	111.23
1	C	74	VAL	N-CA-C	-7.88	94.53	106.42
1	F	276	CYS	CA-C-N	-7.87	112.59	120.31
1	F	276	CYS	C-N-CA	-7.87	112.59	120.31
1	D	97	SER	N-CA-C	-7.87	105.65	114.62
1	B	41	SER	CA-C-N	7.87	136.83	121.41
1	B	41	SER	C-N-CA	7.87	136.83	121.41
1	E	238	GLN	CG-CD-NE2	7.85	128.18	116.40
1	F	139	VAL	N-CA-C	-7.84	102.80	110.72
1	F	321	ARG	N-CA-C	-7.83	104.67	112.97
1	E	120	LEU	CA-CB-CG	7.82	143.66	116.30
1	E	219	GLN	N-CA-CB	7.78	123.64	110.49
1	E	205	VAL	N-CA-C	-7.77	105.59	112.12
1	C	119	ASN	N-CA-C	-7.77	102.01	112.26
1	D	316	ASP	N-CA-C	7.76	119.74	111.28
1	F	300	ILE	CG1-CB-CG2	-7.75	87.46	110.70
1	D	191	LEU	N-CA-C	7.74	120.47	111.02
1	D	42	GLY	O-C-N	-7.74	116.56	123.29
1	A	171	LEU	N-CA-C	-7.73	102.48	112.23
1	F	127	VAL	N-CA-C	-7.73	101.39	111.05
1	C	280	VAL	N-CA-C	7.70	118.47	110.62
1	A	130	THR	CA-C-N	-7.70	111.38	123.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	THR	C-N-CA	-7.70	111.38	123.24
1	F	11	GLU	CA-CB-CG	-7.68	98.73	114.10
1	B	67	ILE	N-CA-CB	7.67	123.89	111.23
1	D	182	THR	CB-CA-C	-7.66	93.59	110.67
1	C	101	GLY	CA-C-N	-7.65	111.43	122.68
1	C	101	GLY	C-N-CA	-7.65	111.43	122.68
1	F	159	ALA	CA-C-N	-7.65	106.92	121.54
1	F	159	ALA	C-N-CA	-7.65	106.92	121.54
1	F	169	SER	N-CA-C	7.63	127.05	110.80
1	C	102	LEU	CB-CA-C	-7.63	100.35	112.09
1	A	306	SER	CA-CB-OG	-7.62	95.85	111.10
1	A	219	GLN	CB-CG-CD	7.57	125.47	112.60
1	A	67	ILE	N-CA-CB	7.56	123.70	111.23
1	E	41	SER	N-CA-CB	-7.55	97.73	110.49
1	E	168	VAL	N-CA-C	-7.54	103.18	110.42
1	E	207	ASP	O-C-N	7.51	132.58	122.59
1	C	214	SER	N-CA-C	-7.51	98.88	109.69
1	F	257	THR	N-CA-CB	7.48	118.16	108.96
1	E	67	ILE	N-CA-CB	7.48	123.57	111.23
1	F	199	VAL	N-CA-C	7.47	118.57	108.11
1	D	219	GLN	N-CA-CB	7.46	123.10	110.49
1	C	104	GLU	N-CA-C	-7.45	100.56	110.24
1	A	291	ASP	N-CA-CB	-7.44	97.91	110.49
1	F	67	ILE	N-CA-CB	7.40	123.44	111.23
1	E	209	THR	CA-CB-OG1	-7.37	98.54	109.60
1	A	55	GLY	N-CA-C	-7.35	102.83	113.86
1	A	284	VAL	CA-C-N	-7.35	109.70	120.28
1	A	284	VAL	C-N-CA	-7.35	109.70	120.28
1	A	113	LEU	CA-C-N	-7.34	116.94	123.33
1	A	113	LEU	C-N-CA	-7.34	116.94	123.33
1	E	210	LEU	N-CA-C	7.34	120.39	107.61
1	E	3	THR	N-CA-C	7.34	120.61	109.23
1	E	184	ASN	N-CA-C	7.34	121.62	109.95
1	C	265	GLY	N-CA-C	-7.33	103.80	115.08
1	C	36	ILE	CB-CA-C	-7.30	99.75	110.62
1	A	24	ILE	CB-CA-C	7.27	121.59	110.55
1	E	56	ASN	CA-C-N	-7.25	115.87	122.97
1	E	56	ASN	C-N-CA	-7.25	115.87	122.97
1	C	98	ARG	NE-CZ-NH2	7.22	125.70	119.20
1	D	116	LEU	CA-C-N	-7.21	112.21	119.92
1	D	116	LEU	C-N-CA	-7.21	112.21	119.92
1	C	235	SER	N-CA-C	7.20	121.51	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	GLN	CB-CG-CD	7.20	124.83	112.60
1	E	120	LEU	CB-CG-CD1	-7.18	89.15	110.70
1	C	304	GLU	N-CA-C	-7.17	100.87	110.55
1	A	245	VAL	N-CA-C	7.17	118.35	108.89
1	B	23	THR	CB-CA-C	-7.14	99.36	110.78
1	C	149	PRO	CA-C-O	-7.14	116.03	121.31
1	C	181	SER	CB-CA-C	-7.12	97.51	109.48
1	F	10	ALA	N-CA-C	-7.12	98.12	109.59
1	B	273	SER	N-CA-C	-7.11	104.74	113.41
1	B	308	GLU	N-CA-CB	7.11	120.68	110.16
1	A	218	TRP	N-CA-C	7.10	125.93	110.80
1	B	182	THR	CB-CA-C	-7.10	94.82	109.94
1	F	259	TYR	N-CA-C	7.09	122.13	112.55
1	B	83	GLU	CA-C-N	-7.08	109.94	122.97
1	B	83	GLU	C-N-CA	-7.08	109.94	122.97
1	D	131	ALA	CA-C-O	-7.08	113.20	120.84
1	F	43	ILE	N-CA-C	7.07	118.05	107.80
1	B	303	ARG	N-CA-C	7.05	117.90	108.38
1	F	275	TYR	N-CA-C	7.04	120.74	112.72
1	C	74	VAL	N-CA-CB	-7.03	105.62	112.65
1	A	148	SER	N-CA-CB	-7.03	99.22	111.17
1	A	259	TYR	CA-C-N	-7.03	111.19	118.85
1	A	259	TYR	C-N-CA	-7.03	111.19	118.85
1	E	238	GLN	CG-CD-OE1	-7.02	106.76	120.80
1	E	202	ARG	CG-CD-NE	-7.02	96.56	112.00
1	C	259	TYR	CA-C-N	-7.01	111.76	119.19
1	C	259	TYR	C-N-CA	-7.01	111.76	119.19
1	C	317	ILE	CB-CA-C	-7.00	99.81	111.29
1	F	68	ASP	CB-CA-C	-6.99	97.63	109.72
1	F	16	ASP	N-CA-C	6.98	121.04	108.48
1	C	213	LEU	N-CA-C	6.97	120.30	109.07
1	B	299	THR	CA-C-N	-6.97	111.70	122.09
1	B	299	THR	C-N-CA	-6.97	111.70	122.09
1	B	279	ASP	N-CA-CB	-6.96	98.72	110.49
1	D	286	GLU	N-CA-CB	6.96	120.94	110.22
1	B	249	THR	O-C-N	-6.96	114.26	122.89
1	A	210	LEU	CB-CG-CD2	-6.95	89.84	110.70
1	D	23	THR	CA-C-N	-6.94	114.84	122.27
1	D	23	THR	C-N-CA	-6.94	114.84	122.27
1	D	132	GLY	N-CA-C	-6.94	96.73	113.18
1	F	75	SER	CB-CA-C	-6.94	96.61	110.42
1	F	153	SER	CA-C-O	-6.94	113.39	121.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH1	-6.93	114.57	121.50
1	C	40	TYR	CB-CA-C	-6.93	97.59	111.17
1	F	254	VAL	CA-C-N	-6.92	111.19	119.84
1	F	254	VAL	C-N-CA	-6.92	111.19	119.84
1	D	16	ASP	CB-CA-C	6.91	120.23	109.03
1	E	59	ARG	CB-CG-CD	6.91	127.19	111.30
1	D	67	ILE	N-CA-CB	6.88	122.58	111.23
1	B	212	ALA	N-CA-C	6.87	118.77	111.28
1	D	10	ALA	N-CA-C	6.87	119.04	109.15
1	F	74	VAL	N-CA-CB	-6.86	100.19	111.44
1	F	142	LEU	N-CA-C	-6.86	103.59	112.23
1	F	87	VAL	N-CA-C	6.85	118.80	108.80
1	D	154	VAL	CB-CA-C	-6.84	100.50	110.63
1	A	16	ASP	N-CA-C	6.84	125.38	110.80
1	B	238	GLN	CG-CD-NE2	6.83	126.64	116.40
1	E	211	LYS	CB-CA-C	-6.81	96.91	109.37
1	F	243	VAL	CA-C-N	-6.80	113.46	123.11
1	F	243	VAL	C-N-CA	-6.80	113.46	123.11
1	B	193	GLN	N-CA-CB	-6.78	100.23	110.07
1	D	17	VAL	CA-C-N	-6.78	114.37	122.44
1	D	17	VAL	C-N-CA	-6.78	114.37	122.44
1	E	178	VAL	CB-CA-C	-6.77	101.44	110.98
1	A	103	SER	CB-CA-C	-6.75	99.08	110.43
1	C	50	ALA	N-CA-C	-6.75	104.31	112.54
1	C	34	VAL	N-CA-C	-6.74	98.03	107.80
1	B	215	LYS	CA-CB-CG	6.74	127.57	114.10
1	D	221	ALA	N-CA-C	-6.73	97.28	108.32
1	D	309	GLU	N-CA-C	-6.72	104.81	112.87
1	B	26	THR	CA-CB-OG1	-6.71	99.53	109.60
1	A	166	ILE	N-CA-C	-6.71	103.69	111.00
1	D	174	ARG	N-CA-C	6.70	121.05	113.01
1	A	231	ALA	N-CA-C	-6.70	103.98	111.28
1	B	78	ASP	CA-C-N	6.70	126.95	119.32
1	B	78	ASP	C-N-CA	6.70	126.95	119.32
1	E	241	GLY	N-CA-C	-6.70	102.36	112.60
1	B	75	SER	N-CA-C	6.69	125.06	110.80
1	C	42	GLY	N-CA-C	-6.69	97.33	113.18
1	E	41	SER	CA-C-O	6.68	130.06	120.51
1	A	328	VAL	CB-CA-C	-6.68	100.75	110.63
1	B	114	VAL	CA-C-N	6.67	127.04	119.83
1	B	114	VAL	C-N-CA	6.67	127.04	119.83
1	F	238	GLN	CG-CD-OE1	-6.67	107.46	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	301	VAL	N-CA-CB	6.67	118.42	110.95
1	A	40	TYR	CA-C-O	6.66	128.97	121.51
1	F	173	LYS	CD-CE-NZ	-6.66	90.59	111.90
1	A	158	GLY	N-CA-C	-6.65	104.66	114.90
1	B	182	THR	O-C-N	6.65	130.85	123.33
1	A	182	THR	CB-CA-C	-6.64	95.46	110.07
1	F	225	VAL	CB-CA-C	-6.64	100.80	110.63
1	F	151	LYS	O-C-N	6.64	131.53	122.37
1	F	207	ASP	CA-C-N	-6.64	108.40	121.41
1	F	207	ASP	C-N-CA	-6.64	108.40	121.41
1	F	166	ILE	CB-CA-C	-6.63	103.07	112.22
1	A	271	ILE	CA-C-N	-6.63	113.77	123.05
1	A	271	ILE	C-N-CA	-6.63	113.77	123.05
1	D	258	VAL	N-CA-CB	-6.62	103.21	112.35
1	E	245	VAL	CA-C-N	-6.62	108.90	121.54
1	E	245	VAL	C-N-CA	-6.62	108.90	121.54
1	F	238	GLN	CG-CD-NE2	6.61	126.32	116.40
1	D	32	ASP	N-CA-C	-6.61	107.09	114.62
1	A	124	GLU	N-CA-CB	6.59	119.81	110.12
1	D	205	VAL	N-CA-C	-6.58	105.33	111.45
1	A	74	VAL	CB-CA-C	-6.57	104.05	111.80
1	C	159	ALA	CA-C-O	-6.57	114.61	122.03
1	A	242	SER	CA-CB-OG	-6.56	97.98	111.10
1	D	270	GLY	CA-C-N	-6.56	114.59	123.12
1	D	270	GLY	C-N-CA	-6.56	114.59	123.12
1	A	159	ALA	CA-C-N	-6.55	109.02	121.54
1	A	159	ALA	C-N-CA	-6.55	109.02	121.54
1	D	263	LEU	N-CA-C	-6.55	105.92	114.04
1	D	26	THR	CB-CA-C	-6.53	100.00	110.84
1	F	95	GLY	N-CA-C	-6.51	106.33	115.32
1	E	106	ALA	N-CA-C	-6.50	98.48	108.76
1	D	226	GLY	N-CA-C	-6.49	102.40	112.85
1	A	327	ILE	CB-CG1-CD1	-6.49	100.17	113.80
1	D	78	ASP	CB-CA-C	6.49	117.25	109.85
1	F	3	THR	CB-CA-C	-6.49	96.84	109.68
1	E	152	GLY	O-C-N	-6.48	117.92	123.43
1	F	209	THR	CA-CB-CG2	6.48	121.51	110.50
1	B	316	ASP	N-CA-C	6.47	118.33	111.28
1	B	113	LEU	CA-C-N	-6.46	117.71	123.33
1	B	113	LEU	C-N-CA	-6.46	117.71	123.33
1	C	258	VAL	N-CA-CB	-6.46	100.58	111.23
1	F	202	ARG	CD-NE-CZ	6.46	133.44	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	THR	N-CA-C	6.44	119.50	109.52
1	C	199	VAL	N-CA-C	6.44	117.12	108.11
1	F	82	ALA	CA-C-N	-6.43	111.73	120.87
1	F	82	ALA	C-N-CA	-6.43	111.73	120.87
1	A	177	ASP	CA-C-N	-6.43	113.71	122.91
1	A	177	ASP	C-N-CA	-6.43	113.71	122.91
1	F	152	GLY	CA-C-O	6.43	127.36	121.76
1	A	41	SER	O-C-N	6.43	131.14	122.59
1	A	182	THR	OG1-CB-CG2	6.42	122.14	109.30
1	D	30	PRO	CA-C-N	-6.42	113.61	123.17
1	D	30	PRO	C-N-CA	-6.42	113.61	123.17
1	F	197	SER	N-CA-C	-6.42	105.49	113.38
1	B	280	VAL	N-CA-C	-6.41	104.01	111.00
1	D	262	ILE	N-CA-C	6.41	120.99	112.98
1	F	105	TYR	N-CA-C	6.41	124.45	110.80
1	D	218	TRP	N-CA-C	6.41	124.45	110.80
1	A	248	LEU	CA-CB-CG	-6.41	93.88	116.30
1	F	141	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	D	218	TRP	O-C-N	-6.39	114.09	122.59
1	B	149	PRO	O-C-N	-6.39	114.01	122.64
1	D	168	VAL	N-CA-C	-6.39	104.10	110.30
1	A	67	ILE	CA-C-O	-6.39	112.80	120.78
1	C	200	ILE	N-CA-C	-6.37	99.50	108.80
1	E	209	THR	CA-C-N	-6.37	112.14	121.76
1	E	209	THR	C-N-CA	-6.37	112.14	121.76
1	B	104	GLU	CA-C-N	-6.36	109.39	121.54
1	B	104	GLU	C-N-CA	-6.36	109.39	121.54
1	C	310	THR	O-C-N	6.36	125.41	120.38
1	F	206	TYR	N-CA-C	6.35	119.92	108.48
1	C	98	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	B	304	GLU	N-CA-C	-6.35	99.56	109.72
1	C	113	LEU	CA-C-N	-6.34	114.34	123.28
1	C	113	LEU	C-N-CA	-6.34	114.34	123.28
1	D	209	THR	CB-CA-C	6.34	123.04	110.42
1	E	238	GLN	CA-CB-CG	6.34	126.78	114.10
1	F	225	VAL	O-C-N	-6.33	116.42	123.26
1	C	207	ASP	CB-CG-OD1	6.33	132.95	118.40
1	A	88	ILE	N-CA-C	-6.32	99.12	108.85
1	D	232	SER	N-CA-C	-6.32	103.69	111.40
1	C	156	VAL	N-CA-C	-6.31	98.54	107.75
1	C	177	ASP	CA-C-N	-6.31	112.48	122.64
1	C	177	ASP	C-N-CA	-6.31	112.48	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ALA	N-CA-C	-6.29	99.44	109.76
1	D	108	VAL	CA-C-N	-6.29	113.03	119.83
1	D	108	VAL	C-N-CA	-6.29	113.03	119.83
1	B	184	ASN	N-CA-C	6.28	119.37	108.76
1	E	307	LEU	CB-CG-CD1	-6.28	91.87	110.70
1	B	218	TRP	CA-C-N	-6.28	109.56	121.54
1	B	218	TRP	C-N-CA	-6.28	109.56	121.54
1	C	182	THR	CB-CA-C	-6.27	95.64	109.56
1	F	299	THR	N-CA-C	6.26	120.01	112.38
1	E	114	VAL	CA-C-N	-6.25	113.53	119.90
1	E	114	VAL	C-N-CA	-6.25	113.53	119.90
1	F	74	VAL	CA-C-N	-6.25	109.60	121.54
1	F	74	VAL	C-N-CA	-6.25	109.60	121.54
1	E	103	SER	N-CA-C	-6.25	99.03	108.52
1	E	328	VAL	CB-CA-C	-6.25	101.90	110.77
1	B	233	LEU	CB-CG-CD1	-6.24	91.98	110.70
1	D	207	ASP	O-C-N	6.24	130.89	122.59
1	D	317	ILE	N-CA-C	-6.24	101.50	109.80
1	B	104	GLU	O-C-N	-6.23	115.46	122.75
1	F	153	SER	CA-CB-OG	-6.23	98.64	111.10
1	C	202	ARG	N-CA-C	-6.22	104.50	111.28
1	A	181	SER	N-CA-CB	-6.21	101.39	110.84
1	D	245	VAL	CB-CA-C	-6.21	101.11	111.29
1	F	299	THR	CA-CB-OG1	-6.19	100.32	109.60
1	A	19	VAL	CB-CA-C	-6.18	101.16	111.29
1	C	238	GLN	N-CA-C	6.18	117.85	110.19
1	E	286	GLU	CG-CD-OE2	-6.18	104.20	118.40
1	D	108	VAL	CB-CA-C	6.17	116.67	110.94
1	E	218	TRP	N-CA-C	6.16	121.37	113.18
1	A	268	LEU	N-CA-C	6.14	118.70	108.20
1	C	276	CYS	CA-C-N	-6.14	113.43	119.76
1	C	276	CYS	C-N-CA	-6.14	113.43	119.76
1	A	274	VAL	N-CA-C	6.14	116.25	110.30
1	F	20	HIS	CB-CA-C	-6.14	97.25	110.45
1	B	106	ALA	CA-C-N	-6.13	113.79	123.24
1	B	106	ALA	C-N-CA	-6.13	113.79	123.24
1	A	33	GLY	N-CA-C	6.13	122.60	112.30
1	A	150	GLU	N-CA-C	6.12	120.30	112.34
1	F	73	VAL	CB-CA-C	-6.12	102.21	111.33
1	A	142	LEU	N-CA-C	-6.11	103.77	111.11
1	C	74	VAL	O-C-N	-6.11	116.19	122.30
1	F	40	TYR	CA-C-O	6.11	129.25	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	LEU	CB-CG-CD2	-6.10	92.39	110.70
1	A	250	GLY	N-CA-C	-6.10	105.16	115.34
1	F	76	SER	CA-C-N	-6.09	112.09	122.56
1	F	76	SER	C-N-CA	-6.09	112.09	122.56
1	F	219	GLN	N-CA-CB	6.07	120.74	110.49
1	A	182	THR	CA-C-O	-6.07	114.55	121.40
1	E	83	GLU	N-CA-CB	6.07	119.23	109.28
1	C	160	THR	CB-CA-C	-6.06	98.36	110.42
1	C	193	GLN	CB-CG-CD	-6.06	102.30	112.60
1	D	119	ASN	N-CA-CB	-6.06	101.23	111.17
1	B	114	VAL	CB-CA-C	6.05	116.00	110.13
1	D	215	LYS	N-CA-C	-6.04	101.47	110.23
1	E	83	GLU	N-CA-C	-6.04	101.24	110.30
1	D	105	TYR	N-CA-C	6.03	123.65	110.80
1	F	61	TYR	N-CA-C	-6.03	101.17	110.58
1	C	243	VAL	CA-C-N	-6.03	114.27	123.07
1	C	243	VAL	C-N-CA	-6.03	114.27	123.07
1	A	78	ASP	N-CA-C	-6.03	97.52	108.85
1	B	150	GLU	N-CA-C	-6.02	105.25	114.16
1	D	252	GLY	CA-C-N	-6.02	113.70	122.19
1	D	252	GLY	C-N-CA	-6.02	113.70	122.19
1	C	105	TYR	N-CA-C	6.02	123.62	110.80
1	F	56	ASN	CB-CA-C	-6.01	103.19	111.73
1	E	131	ALA	N-CA-C	-6.01	104.85	111.82
1	A	131	ALA	CA-C-O	-6.01	109.19	121.03
1	A	32	ASP	CA-C-N	-6.01	112.95	121.54
1	A	32	ASP	C-N-CA	-6.01	112.95	121.54
1	A	201	SER	CA-CB-OG	-6.00	99.09	111.10
1	E	209	THR	CB-CA-C	6.00	122.36	110.42
1	F	34	VAL	CB-CA-C	6.00	119.56	110.62
1	F	41	SER	O-C-N	5.99	130.56	122.59
1	F	245	VAL	N-CA-C	5.99	117.97	108.87
1	F	217	GLN	N-CA-C	5.98	121.63	113.97
1	F	315	LYS	N-CA-C	-5.98	104.70	112.23
1	C	3	THR	CB-CA-C	-5.97	99.83	113.33
1	F	219	GLN	CB-CG-CD	5.97	122.75	112.60
1	F	225	VAL	N-CA-C	-5.97	99.75	108.11
1	F	223	ASP	N-CA-C	5.97	121.69	108.27
1	A	223	ASP	N-CA-C	5.96	122.54	108.40
1	E	298	LEU	CB-CG-CD1	-5.96	92.82	110.70
1	B	238	GLN	CG-CD-OE1	-5.96	108.89	120.80
1	F	330	LEU	CA-CB-CG	-5.96	95.45	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	209	THR	CA-C-O	-5.95	112.00	120.51
1	D	151	LYS	CA-C-O	5.95	126.73	119.11
1	A	219	GLN	CA-CB-CG	-5.95	102.20	114.10
1	D	275	TYR	N-CA-C	5.95	119.84	112.59
1	F	248	LEU	CA-C-O	-5.95	112.01	120.51
1	D	250	GLY	N-CA-C	-5.94	106.89	114.37
1	E	218	TRP	CA-C-N	-5.94	110.19	121.54
1	E	218	TRP	C-N-CA	-5.94	110.19	121.54
1	C	284	VAL	CA-C-N	-5.94	112.32	120.28
1	C	284	VAL	C-N-CA	-5.94	112.32	120.28
1	F	56	ASN	N-CA-C	5.94	119.75	111.74
1	B	71	GLY	N-CA-C	5.92	120.37	111.42
1	D	41	SER	N-CA-C	-5.92	99.95	108.60
1	A	71	GLY	CA-C-N	-5.91	114.43	122.77
1	A	71	GLY	C-N-CA	-5.91	114.43	122.77
1	B	302	ASP	N-CA-C	5.91	117.53	111.14
1	E	316	ASP	CA-C-O	-5.91	114.61	120.70
1	C	114	VAL	CA-C-O	-5.91	114.90	119.98
1	F	182	THR	CB-CA-C	-5.91	97.08	110.07
1	A	176	TYR	CA-C-N	-5.89	114.93	122.77
1	A	176	TYR	C-N-CA	-5.89	114.93	122.77
1	F	286	GLU	N-CA-C	-5.89	104.86	111.28
1	B	308	GLU	CB-CA-C	-5.88	100.84	110.85
1	E	270	GLY	N-CA-C	5.87	120.13	110.97
1	D	306	SER	CA-C-N	-5.87	111.96	120.29
1	D	306	SER	C-N-CA	-5.87	111.96	120.29
1	D	155	LEU	CA-C-N	-5.86	114.05	122.84
1	D	155	LEU	C-N-CA	-5.86	114.05	122.84
1	F	232	SER	N-CA-C	5.86	117.53	111.03
1	E	29	LEU	CA-C-N	5.86	125.88	119.90
1	E	29	LEU	C-N-CA	5.86	125.88	119.90
1	A	78	ASP	CB-CA-C	5.86	117.98	110.13
1	E	164	GLY	N-CA-C	-5.86	105.28	112.77
1	F	277	PRO	CB-CA-C	-5.86	102.52	110.60
1	A	212	ALA	N-CA-C	5.85	118.16	111.02
1	B	156	VAL	CB-CA-C	-5.85	102.53	110.42
1	E	104	GLU	CA-C-O	-5.84	114.01	120.38
1	E	174	ARG	NE-CZ-NH2	5.84	124.45	119.20
1	C	21	VAL	N-CA-C	5.84	121.48	109.34
1	F	179	VAL	CB-CA-C	-5.83	102.00	110.63
1	D	50	ALA	N-CA-C	-5.83	105.43	112.54
1	A	80	ARG	NE-CZ-NH1	-5.82	115.69	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	E	182	THR	CA-C-N	5.82	127.61	120.22
1	E	182	THR	C-N-CA	5.82	127.61	120.22
1	C	256	ALA	N-CA-C	-5.81	101.86	110.46
1	D	158	GLY	N-CA-C	-5.81	104.83	114.48
1	C	151	LYS	O-C-N	5.81	130.31	122.59
1	B	307	LEU	N-CA-C	-5.80	105.10	111.82
1	A	91	SER	N-CA-C	5.79	118.75	109.02
1	A	159	ALA	O-C-N	-5.79	114.89	122.59
1	C	212	ALA	CA-C-N	5.78	130.98	123.00
1	C	212	ALA	C-N-CA	5.78	130.98	123.00
1	D	104	GLU	CA-C-N	-5.77	110.51	121.54
1	D	104	GLU	C-N-CA	-5.77	110.51	121.54
1	B	58	VAL	O-C-N	5.76	129.28	122.83
1	C	271	ILE	CA-CB-CG1	-5.76	100.61	110.40
1	D	288	MSE	CA-C-N	-5.76	113.45	122.49
1	D	288	MSE	C-N-CA	-5.76	113.45	122.49
1	D	298	LEU	N-CA-C	-5.76	106.25	113.28
1	B	319	GLN	CB-CA-C	5.76	121.88	110.42
1	B	219	GLN	CA-C-N	-5.75	113.44	120.92
1	B	219	GLN	C-N-CA	-5.75	113.44	120.92
1	E	38	VAL	CA-C-O	-5.75	114.30	120.85
1	A	304	GLU	N-CA-C	5.74	118.43	107.75
1	A	323	GLN	CB-CA-C	-5.74	101.65	111.41
1	E	260	PRO	CA-C-N	-5.74	112.63	120.44
1	E	260	PRO	C-N-CA	-5.74	112.63	120.44
1	E	210	LEU	CA-C-O	-5.74	112.29	120.15
1	F	160	THR	CB-CA-C	-5.74	99.00	110.42
1	F	74	VAL	N-CA-C	-5.74	99.91	108.46
1	C	248	LEU	CB-CG-CD2	-5.73	93.50	110.70
1	C	144	GLN	N-CA-C	-5.73	106.24	113.18
1	C	164	GLY	N-CA-C	-5.73	105.69	113.37
1	C	207	ASP	CA-C-O	-5.73	112.32	120.51
1	D	245	VAL	N-CA-C	5.72	121.24	109.34
1	A	62	PRO	CA-C-N	5.72	129.92	120.94
1	A	62	PRO	C-N-CA	5.72	129.92	120.94
1	E	153	SER	CA-C-N	-5.72	116.10	123.19
1	E	153	SER	C-N-CA	-5.72	116.10	123.19
1	E	105	TYR	N-CA-CB	5.72	120.15	110.49
1	F	235	SER	CA-C-N	-5.72	114.11	122.86
1	F	235	SER	C-N-CA	-5.72	114.11	122.86
1	D	108	VAL	N-CA-C	5.71	113.55	108.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	327	ILE	CB-CA-C	-5.71	103.38	111.38
1	B	217	GLN	CA-C-N	-5.71	110.63	121.54
1	B	217	GLN	C-N-CA	-5.71	110.63	121.54
1	A	151	LYS	N-CA-C	-5.71	106.48	113.50
1	D	199	VAL	N-CA-C	5.71	116.70	108.48
1	E	58	VAL	N-CA-C	5.70	116.41	108.89
1	E	318	LEU	N-CA-CB	5.70	120.12	110.49
1	F	11	GLU	CB-CG-CD	5.70	122.29	112.60
1	F	167	ALA	N-CA-C	-5.70	105.15	111.36
1	F	76	SER	N-CA-C	5.70	118.77	109.59
1	E	175	GLY	N-CA-C	5.70	122.33	114.92
1	A	170	MSE	N-CA-C	-5.69	105.22	111.82
1	F	160	THR	N-CA-CB	5.69	120.10	110.49
1	F	202	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	C	257	THR	N-CA-C	-5.68	100.63	109.72
1	F	308	GLU	N-CA-CB	-5.68	100.52	109.78
1	D	31	LYS	N-CA-C	5.68	120.56	111.81
1	E	99	ASP	N-CA-C	-5.68	101.44	109.96
1	E	18	SER	CA-C-N	-5.67	111.76	121.97
1	E	18	SER	C-N-CA	-5.67	111.76	121.97
1	F	73	VAL	CA-C-N	5.67	130.82	122.94
1	F	73	VAL	C-N-CA	5.67	130.82	122.94
1	B	230	LEU	N-CA-C	-5.67	104.72	111.69
1	D	273	SER	N-CA-C	-5.67	106.35	113.72
1	B	215	LYS	CB-CG-CD	5.67	124.33	111.30
1	C	193	GLN	CB-CA-C	5.67	118.59	109.07
1	F	169	SER	CB-CA-C	-5.67	99.14	110.42
1	B	21	VAL	N-CA-C	5.67	121.12	109.34
1	C	182	THR	OG1-CB-CG2	5.67	120.63	109.30
1	D	279	ASP	N-CA-C	5.66	122.86	110.80
1	F	105	TYR	N-CA-CB	5.66	120.06	110.49
1	B	253	GLU	CA-C-N	-5.66	117.02	123.25
1	B	253	GLU	C-N-CA	-5.66	117.02	123.25
1	E	11	GLU	N-CA-C	-5.66	100.17	109.40
1	C	303	ARG	N-CA-C	5.66	122.85	110.80
1	F	305	VAL	N-CA-CB	-5.65	105.31	112.60
1	C	199	VAL	CA-C-N	-5.65	114.78	122.92
1	C	199	VAL	C-N-CA	-5.65	114.78	122.92
1	B	327	ILE	N-CA-C	5.65	116.24	107.99
1	D	22	LYS	CA-C-N	-5.64	115.01	122.85
1	D	22	LYS	C-N-CA	-5.64	115.01	122.85
1	D	152	GLY	CA-C-N	-5.64	112.48	122.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	152	GLY	C-N-CA	-5.64	112.48	122.74
1	E	152	GLY	N-CA-C	5.63	117.82	111.85
1	C	271	ILE	N-CA-C	5.63	115.70	107.37
1	B	159	ALA	CA-C-N	-5.62	110.80	121.54
1	B	159	ALA	C-N-CA	-5.62	110.80	121.54
1	A	160	THR	N-CA-C	5.62	122.78	110.80
1	F	22	LYS	CA-CB-CG	5.62	125.34	114.10
1	E	75	SER	CA-C-N	-5.62	115.25	123.00
1	E	75	SER	C-N-CA	-5.62	115.25	123.00
1	B	319	GLN	CA-C-N	5.61	132.26	121.54
1	B	319	GLN	C-N-CA	5.61	132.26	121.54
1	F	88	ILE	N-CA-C	-5.61	100.40	108.48
1	C	149	PRO	O-C-N	-5.61	115.26	122.44
1	D	153	SER	CA-C-O	-5.61	114.82	121.66
1	C	249	THR	CA-C-N	-5.61	111.90	122.05
1	C	249	THR	C-N-CA	-5.61	111.90	122.05
1	C	58	VAL	CA-C-N	-5.61	112.72	122.36
1	C	58	VAL	C-N-CA	-5.61	112.72	122.36
1	C	207	ASP	O-C-N	5.60	130.04	122.59
1	B	58	VAL	CA-C-N	5.60	132.24	121.54
1	B	58	VAL	C-N-CA	5.60	132.24	121.54
1	D	85	ASP	CA-C-N	-5.60	112.15	120.94
1	D	85	ASP	C-N-CA	-5.60	112.15	120.94
1	F	233	LEU	N-CA-CB	-5.60	100.65	109.78
1	D	15	ASP	N-CA-C	5.60	120.99	112.54
1	B	107	SER	CA-C-N	-5.59	111.79	122.13
1	B	107	SER	C-N-CA	-5.59	111.79	122.13
1	D	61	TYR	N-CA-C	5.59	118.48	109.15
1	C	4	LEU	CB-CA-C	5.59	121.06	109.38
1	A	209	THR	CA-C-N	-5.59	112.76	122.37
1	A	209	THR	C-N-CA	-5.59	112.76	122.37
1	B	3	THR	N-CA-C	5.58	122.68	110.80
1	F	291	ASP	N-CA-CB	-5.58	101.07	110.49
1	C	248	LEU	CB-CA-C	-5.57	99.71	109.07
1	D	222	VAL	N-CA-CB	-5.57	104.93	111.39
1	D	206	TYR	N-CA-C	-5.57	100.84	109.14
1	D	212	ALA	CA-C-N	-5.57	115.32	123.00
1	D	212	ALA	C-N-CA	-5.57	115.32	123.00
1	E	90	THR	N-CA-C	-5.56	100.06	108.46
1	A	246	SER	N-CA-C	5.56	120.94	112.54
1	B	207	ASP	N-CA-C	-5.56	98.96	110.80
1	A	131	ALA	N-CA-C	-5.55	96.06	107.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	36	ILE	CA-C-N	-5.55	115.62	122.84
1	F	36	ILE	C-N-CA	-5.55	115.62	122.84
1	B	58	VAL	CB-CA-C	-5.55	104.59	111.08
1	E	120	LEU	CB-CA-C	5.55	118.11	110.34
1	B	249	THR	CA-C-N	-5.54	110.94	120.87
1	B	249	THR	C-N-CA	-5.54	110.94	120.87
1	E	182	THR	OG1-CB-CG2	5.54	120.39	109.30
1	C	6	GLN	CB-CA-C	-5.54	102.37	111.68
1	C	102	LEU	N-CA-C	5.54	118.89	111.24
1	F	229	GLN	N-CA-C	5.54	117.40	111.36
1	F	103	SER	N-CA-C	5.53	116.81	108.46
1	B	58	VAL	N-CA-CB	5.53	117.14	110.95
1	A	147	LEU	CA-CB-CG	5.53	135.64	116.30
1	B	223	ASP	O-C-N	5.53	126.03	121.44
1	D	154	VAL	N-CA-C	5.52	115.84	108.11
1	E	153	SER	N-CA-C	5.52	117.86	110.35
1	C	286	GLU	CB-CA-C	5.52	119.55	110.88
1	F	130	THR	N-CA-C	5.52	116.97	111.07
1	A	305	VAL	N-CA-CB	-5.52	102.13	111.23
1	B	130	THR	CA-CB-OG1	-5.51	101.33	109.60
1	F	199	VAL	CB-CA-C	-5.51	102.47	110.63
1	A	219	GLN	N-CA-CB	5.51	119.80	110.49
1	C	284	VAL	N-CA-C	-5.51	104.59	112.35
1	D	245	VAL	O-C-N	-5.50	115.70	122.57
1	B	327	ILE	N-CA-CB	-5.49	104.78	111.21
1	F	322	ILE	O-C-N	-5.49	118.03	122.97
1	E	67	ILE	CA-CB-CG2	5.48	119.82	110.50
1	F	316	ASP	CB-CA-C	-5.48	100.14	110.67
1	D	104	GLU	N-CA-C	-5.47	100.76	109.96
1	C	34	VAL	N-CA-CB	-5.47	104.56	111.46
1	F	38	VAL	N-CA-C	5.47	116.32	108.93
1	D	3	THR	N-CA-C	5.47	117.59	110.53
1	F	218	TRP	CA-C-N	-5.47	111.09	121.54
1	F	218	TRP	C-N-CA	-5.47	111.09	121.54
1	D	210	LEU	N-CA-C	5.47	117.50	109.24
1	E	80	ARG	N-CA-C	-5.47	106.11	112.89
1	A	29	LEU	N-CA-C	-5.46	103.16	109.93
1	B	101	GLY	CA-C-N	-5.46	114.12	122.21
1	B	101	GLY	C-N-CA	-5.46	114.12	122.21
1	C	103	SER	N-CA-C	-5.46	99.17	110.80
1	E	179	VAL	CB-CA-C	-5.46	103.01	110.77
1	C	279	ASP	CB-CG-OD1	-5.46	105.84	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	TYR	N-CA-C	5.46	117.09	111.03
1	F	329	LYS	CG-CD-CE	5.46	123.86	111.30
1	A	33	GLY	CA-C-N	5.46	127.81	120.50
1	A	33	GLY	C-N-CA	5.46	127.81	120.50
1	A	215	LYS	CA-CB-CG	5.45	125.01	114.10
1	C	76	SER	CA-C-N	-5.45	111.41	122.31
1	C	76	SER	C-N-CA	-5.45	111.41	122.31
1	F	248	LEU	CA-C-N	-5.45	114.50	122.78
1	F	248	LEU	C-N-CA	-5.45	114.50	122.78
1	B	41	SER	CA-C-O	5.45	128.30	120.51
1	A	164	GLY	N-CA-C	-5.44	105.80	112.77
1	A	309	GLU	CB-CA-C	5.44	119.78	111.02
1	D	88	ILE	N-CA-C	-5.44	100.64	108.48
1	B	12	LYS	CA-C-N	-5.44	115.76	122.84
1	B	12	LYS	C-N-CA	-5.44	115.76	122.84
1	D	29	LEU	CA-C-N	5.44	125.75	119.93
1	D	29	LEU	C-N-CA	5.44	125.75	119.93
1	D	149	PRO	N-CA-C	-5.44	102.65	111.19
1	A	12	LYS	CA-C-N	-5.44	114.27	122.81
1	A	12	LYS	C-N-CA	-5.44	114.27	122.81
1	A	197	SER	CB-CA-C	-5.44	98.50	109.55
1	A	155	LEU	CA-CB-CG	5.44	135.33	116.30
1	A	83	GLU	CA-CB-CG	5.44	124.97	114.10
1	E	211	LYS	CG-CD-CE	-5.43	98.81	111.30
1	F	177	ASP	CA-C-N	-5.43	116.10	123.10
1	F	177	ASP	C-N-CA	-5.43	116.10	123.10
1	A	236	LYS	N-CA-C	5.43	119.21	112.59
1	C	151	LYS	N-CA-C	5.42	122.36	110.80
1	E	182	THR	N-CA-CB	5.42	120.41	111.62
1	F	16	ASP	CA-C-N	-5.42	115.16	122.91
1	F	16	ASP	C-N-CA	-5.42	115.16	122.91
1	F	209	THR	N-CA-CB	5.42	119.65	110.49
1	A	298	LEU	CB-CG-CD1	5.42	126.96	110.70
1	B	127	VAL	N-CA-C	-5.42	104.44	110.62
1	D	319	GLN	CB-CA-C	5.41	117.95	110.16
1	A	68	ASP	CB-CA-C	-5.40	98.08	109.38
1	E	274	VAL	CB-CA-C	-5.40	104.84	112.14
1	F	223	ASP	CA-C-N	5.40	125.49	119.87
1	F	223	ASP	C-N-CA	5.40	125.49	119.87
1	D	150	GLU	N-CA-C	5.39	122.28	110.80
1	E	284	VAL	CA-C-N	-5.39	111.72	120.72
1	E	284	VAL	C-N-CA	-5.39	111.72	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	83	GLU	CA-C-O	-5.39	114.98	120.80
1	E	174	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	B	127	VAL	N-CA-CB	5.38	117.20	110.47
1	D	168	VAL	CA-C-N	-5.38	111.99	120.60
1	D	168	VAL	C-N-CA	-5.38	111.99	120.60
1	F	21	VAL	CB-CA-C	-5.38	106.10	111.80
1	C	63	LEU	N-CA-C	5.38	117.85	108.76
1	B	102	LEU	N-CA-C	-5.38	102.37	110.70
1	F	305	VAL	CA-C-N	-5.38	113.37	122.67
1	F	305	VAL	C-N-CA	-5.38	113.37	122.67
1	D	185	ARG	CA-C-N	-5.37	115.00	122.74
1	D	185	ARG	C-N-CA	-5.37	115.00	122.74
1	C	173	LYS	CB-CA-C	-5.37	101.87	110.79
1	A	292	LEU	N-CA-C	-5.36	105.57	113.61
1	A	233	LEU	N-CA-C	5.35	117.80	111.33
1	B	327	ILE	CB-CG1-CD1	-5.34	102.58	113.80
1	F	178	VAL	O-C-N	5.34	128.59	123.14
1	D	32	ASP	CB-CG-OD1	-5.34	106.12	118.40
1	D	91	SER	CA-CB-OG	-5.34	100.43	111.10
1	E	247	GLY	O-C-N	-5.34	118.95	123.59
1	B	151	LYS	O-C-N	5.33	129.01	122.34
1	C	193	GLN	CA-CB-CG	5.33	124.76	114.10
1	E	317	ILE	N-CA-C	-5.33	98.25	109.34
1	B	246	SER	CA-CB-OG	-5.33	100.45	111.10
1	B	249	THR	CA-C-O	5.33	125.89	120.88
1	A	151	LYS	O-C-N	5.32	129.62	122.49
1	E	257	THR	N-CA-C	-5.32	101.33	109.41
1	F	202	ARG	CB-CG-CD	5.32	123.53	111.30
1	F	225	VAL	CA-C-N	-5.32	110.99	121.41
1	F	225	VAL	C-N-CA	-5.32	110.99	121.41
1	A	318	LEU	N-CA-C	5.31	122.11	110.80
1	A	316	ASP	CA-C-O	-5.31	112.92	120.51
1	C	102	LEU	CA-CB-CG	5.30	134.86	116.30
1	A	187	ALA	N-CA-C	-5.30	99.51	110.80
1	D	98	ARG	N-CA-C	-5.30	101.01	109.23
1	C	304	GLU	CA-CB-CG	5.29	124.69	114.10
1	E	113	LEU	N-CA-C	5.29	118.11	110.28
1	F	113	LEU	N-CA-C	5.29	117.90	109.96
1	A	105	TYR	N-CA-C	5.29	122.06	110.80
1	B	180	ALA	CA-C-N	-5.29	114.51	122.81
1	B	180	ALA	C-N-CA	-5.29	114.51	122.81
1	D	36	ILE	CA-C-N	-5.29	113.60	122.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	ILE	C-N-CA	-5.29	113.60	122.17
1	F	57	ILE	N-CA-C	-5.29	98.34	109.34
1	B	90	THR	CA-CB-OG1	-5.28	101.67	109.60
1	F	266	VAL	N-CA-C	5.28	117.06	109.51
1	E	166	ILE	N-CA-C	-5.28	104.36	111.44
1	E	201	SER	N-CA-C	-5.28	102.94	110.59
1	F	38	VAL	N-CA-CB	-5.27	104.42	110.49
1	A	46	LYS	N-CA-C	-5.27	105.70	111.82
1	C	142	LEU	CA-C-N	-5.27	112.30	120.31
1	C	142	LEU	C-N-CA	-5.27	112.30	120.31
1	D	237	ILE	O-C-N	5.26	128.94	122.83
1	D	117	PRO	N-CA-C	5.26	119.49	111.34
1	C	279	ASP	N-CA-C	5.26	116.69	111.07
1	E	19	VAL	N-CA-C	5.26	120.28	109.34
1	B	210	LEU	CA-CB-CG	5.25	134.69	116.30
1	C	199	VAL	O-C-N	-5.25	117.59	123.26
1	A	271	ILE	N-CA-C	5.24	115.13	107.37
1	B	160	THR	N-CA-CB	5.24	119.34	110.49
1	A	3	THR	CB-CA-C	5.24	120.53	109.79
1	A	209	THR	N-CA-C	5.24	117.82	109.81
1	B	182	THR	N-CA-CB	5.24	121.26	111.52
1	C	309	GLU	N-CA-C	5.23	121.94	110.80
1	F	320	ASN	N-CA-C	5.23	121.93	110.80
1	C	74	VAL	CA-C-N	-5.22	111.56	121.54
1	C	74	VAL	C-N-CA	-5.22	111.56	121.54
1	D	65	LEU	CA-C-N	-5.22	111.17	121.41
1	D	65	LEU	C-N-CA	-5.22	111.17	121.41
1	D	131	ALA	N-CA-C	-5.22	98.04	107.75
1	A	13	ASN	N-CA-C	5.22	118.07	109.72
1	B	172	ASN	N-CA-C	5.21	116.96	111.28
1	E	26	THR	CA-C-N	-5.21	112.02	121.14
1	E	26	THR	C-N-CA	-5.21	112.02	121.14
1	F	47	ASP	N-CA-C	-5.21	105.05	111.40
1	C	102	LEU	CB-CG-CD1	-5.21	95.08	110.70
1	E	129	GLY	CA-C-N	5.20	127.25	120.28
1	E	129	GLY	C-N-CA	5.20	127.25	120.28
1	A	85	ASP	CA-C-N	-5.20	113.98	121.42
1	A	85	ASP	C-N-CA	-5.20	113.98	121.42
1	E	312	GLY	N-CA-C	-5.20	100.85	113.18
1	F	59	ARG	CA-CB-CG	-5.20	103.70	114.10
1	F	325	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	28	ASP	N-CA-C	5.20	116.95	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	GLN	CB-CA-C	-5.20	100.07	110.42
1	C	96	VAL	CA-C-N	-5.19	114.51	122.60
1	C	96	VAL	C-N-CA	-5.19	114.51	122.60
1	A	187	ALA	CA-C-N	5.18	131.44	121.54
1	A	187	ALA	C-N-CA	5.18	131.44	121.54
1	B	274	VAL	N-CA-C	5.18	115.80	110.36
1	E	168	VAL	N-CA-CB	5.18	116.61	110.55
1	A	268	LEU	O-C-N	-5.18	116.89	123.05
1	D	281	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	C	184	ASN	N-CA-C	5.17	117.83	109.40
1	A	218	TRP	O-C-N	-5.17	115.72	122.59
1	A	37	LYS	N-CA-C	-5.17	98.90	107.99
1	A	36	ILE	CB-CG1-CD1	-5.16	102.96	113.80
1	A	153	SER	CA-CB-OG	-5.16	100.78	111.10
1	A	309	GLU	CA-C-N	5.16	127.17	120.26
1	A	309	GLU	C-N-CA	5.16	127.17	120.26
1	D	153	SER	CB-CA-C	5.16	118.31	109.80
1	C	110	GLY	N-CA-C	5.15	119.11	112.83
1	E	133	PHE	N-CA-C	-5.14	105.85	111.82
1	A	321	ARG	CD-NE-CZ	5.14	131.60	124.40
1	B	159	ALA	N-CA-C	-5.14	103.70	110.33
1	D	67	ILE	CA-C-O	-5.14	114.35	120.78
1	A	81	PHE	CA-C-O	-5.14	114.44	120.60
1	A	41	SER	CA-C-N	5.14	131.48	121.41
1	A	41	SER	C-N-CA	5.14	131.48	121.41
1	A	214	SER	CA-C-N	5.14	128.40	121.05
1	A	214	SER	C-N-CA	5.14	128.40	121.05
1	D	290	SER	CA-C-N	5.14	131.35	121.54
1	D	290	SER	C-N-CA	5.14	131.35	121.54
1	B	3	THR	N-CA-CB	5.13	119.17	110.49
1	E	174	ARG	N-CA-C	5.13	119.03	112.87
1	F	274	VAL	N-CA-C	-5.13	105.59	110.42
1	B	3	THR	OG1-CB-CG2	5.13	119.56	109.30
1	D	74	VAL	CA-C-N	-5.13	111.75	121.54
1	D	74	VAL	C-N-CA	-5.13	111.75	121.54
1	F	38	VAL	O-C-N	-5.13	117.17	122.66
1	F	286	GLU	N-CA-CB	5.13	117.66	110.12
1	E	190	TYR	N-CA-C	-5.12	105.13	111.33
1	C	277	PRO	N-CA-C	5.12	119.13	111.14
1	F	104	GLU	N-CA-CB	-5.12	101.73	109.92
1	A	279	ASP	CA-CB-CG	-5.12	107.48	112.60
1	C	200	ILE	CA-C-O	-5.12	116.45	121.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	141	ARG	NE-CZ-NH1	-5.12	116.39	121.50
1	E	56	ASN	CB-CA-C	5.11	118.99	111.73
1	A	186	GLU	CA-C-N	5.11	131.30	121.54
1	A	186	GLU	C-N-CA	5.11	131.30	121.54
1	A	229	GLN	CA-CB-CG	-5.11	103.88	114.10
1	D	149	PRO	CA-C-O	-5.11	115.18	121.31
1	B	278	MSE	CG-SE-CE	-5.10	87.70	98.92
1	C	171	LEU	CA-C-O	5.10	125.96	120.55
1	C	166	ILE	CA-C-O	-5.10	115.65	120.95
1	E	237	ILE	N-CA-C	5.09	115.92	108.58
1	F	42	GLY	N-CA-C	5.09	125.25	113.18
1	D	215	LYS	CB-CA-C	5.09	118.17	109.72
1	B	300	ILE	N-CA-C	-5.09	107.79	112.83
1	D	320	ASN	N-CA-C	5.09	121.64	110.80
1	C	229	GLN	CA-CB-CG	-5.08	103.93	114.10
1	C	232	SER	N-CA-C	-5.08	105.66	111.14
1	D	249	THR	CB-CA-C	-5.08	100.66	109.64
1	B	202	ARG	CA-CB-CG	5.07	124.25	114.10
1	B	276	CYS	N-CA-CB	-5.07	102.01	109.98
1	D	20	HIS	CA-C-N	5.07	127.96	120.91
1	D	20	HIS	C-N-CA	5.07	127.96	120.91
1	F	174	ARG	CA-CB-CG	5.07	124.24	114.10
1	D	178	VAL	CA-C-N	-5.07	116.53	123.12
1	D	178	VAL	C-N-CA	-5.07	116.53	123.12
1	E	204	ASP	CA-C-N	-5.07	117.45	122.77
1	E	204	ASP	C-N-CA	-5.07	117.45	122.77
1	F	248	LEU	CB-CG-CD2	-5.06	95.51	110.70
1	F	325	ARG	CA-C-N	-5.05	116.55	123.12
1	F	325	ARG	C-N-CA	-5.05	116.55	123.12
1	A	299	THR	OG1-CB-CG2	5.05	119.40	109.30
1	B	131	ALA	N-CA-C	-5.05	105.69	111.14
1	B	225	VAL	CG1-CB-CG2	-5.04	99.70	110.80
1	E	219	GLN	CB-CA-C	-5.04	100.38	110.42
1	E	245	VAL	O-C-N	-5.04	116.27	122.57
1	A	118	GLN	CB-CA-C	-5.04	102.11	110.68
1	E	103	SER	CA-C-O	-5.04	115.11	120.75
1	E	242	SER	CA-CB-OG	-5.04	101.03	111.10
1	D	182	THR	N-CA-CB	5.03	119.77	111.62
1	E	59	ARG	N-CA-C	-5.03	105.89	112.23
1	B	74	VAL	CA-C-N	-5.02	111.95	121.54
1	B	74	VAL	C-N-CA	-5.02	111.95	121.54
1	B	218	TRP	N-CA-C	5.01	121.48	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	SER	CA-C-O	5.01	127.67	120.51
1	E	151	LYS	CD-CE-NZ	-5.01	95.88	111.90
1	E	279	ASP	N-CA-CB	5.01	117.48	110.12
1	B	80	ARG	NE-CZ-NH1	5.00	126.50	121.50
1	C	258	VAL	N-CA-C	5.00	119.75	109.34
1	F	229	GLN	CB-CA-C	-5.00	102.35	110.85

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	43	ILE	CA
1	D	43	ILE	CA

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASN	Peptide
1	A	131	ALA	Peptide
1	A	150	GLU	Peptide
1	A	184	ASN	Peptide
1	A	186	GLU	Peptide
1	A	208	GLY	Peptide
1	A	41	SER	Mainchain,Peptide
1	A	62	PRO	Peptide
1	B	13	ASN	Peptide
1	B	2	SER	Peptide
1	B	209	THR	Peptide
1	B	250	GLY	Peptide
1	B	290	SER	Peptide
1	B	40	TYR	Peptide
1	B	41	SER	Peptide
1	B	60	GLU	Peptide
1	B	61	TYR	Peptide
1	C	186	GLU	Peptide
1	C	208	GLY	Peptide
1	C	209	THR	Peptide
1	C	316	ASP	Peptide
1	C	319	GLN	Peptide
1	C	42	GLY	Peptide
1	C	52	LYS	Peptide
1	C	61	TYR	Peptide
1	D	131	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	247	GLY	Peptide
1	D	284	VAL	Peptide
1	D	301	VAL	Peptide
1	D	61	TYR	Peptide
1	E	13	ASN	Peptide
1	E	249	THR	Peptide
1	E	40	TYR	Peptide
1	E	41	SER	Peptide
1	E	60	GLU	Peptide
1	F	15	ASP	Peptide
1	F	209	THR	Peptide
1	F	251	GLY	Peptide
1	F	40	TYR	Peptide

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	2429	0	2454	163	0
1	B	2421	0	2425	174	0
1	C	2412	0	2405	214	0
1	D	2431	0	2444	177	0
1	E	2433	0	2458	174	0
1	F	2437	0	2460	191	0
2	A	11	0	4	5	0
2	B	11	0	4	5	0
2	C	11	0	4	4	0
2	D	11	0	4	0	0
2	E	11	0	4	0	0
2	F	11	0	4	5	0
3	A	65	0	0	1	0
3	B	56	0	0	3	0
3	C	57	0	0	5	0
3	D	53	0	0	8	0
3	E	60	0	0	7	0
3	F	62	0	0	8	0
All	All	14982	0	14670	1076	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 37.

All (1076) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:THR:CG2	1:B:3:THR:CB	1.75	1.60
1:A:24:ILE:CD1	1:A:24:ILE:CG1	1.81	1.58
1:E:83:GLU:CD	1:E:83:GLU:CG	1.75	1.58
1:C:207:ASP:CG	1:C:207:ASP:CB	1.77	1.58
1:B:303:ARG:CG	1:B:303:ARG:CB	1.75	1.57
1:D:26:THR:CB	1:D:26:THR:CG2	1.76	1.57
1:B:215:LYS:CB	1:B:215:LYS:CG	1.81	1.57
1:F:67:ILE:CD1	1:F:67:ILE:CG1	1.78	1.56
1:F:322:ILE:CD1	1:F:322:ILE:CG1	1.75	1.56
1:E:59:ARG:CG	1:E:59:ARG:CD	1.80	1.55
1:A:286:GLU:CG	1:A:286:GLU:CD	1.75	1.55
1:F:315:LYS:NZ	1:F:315:LYS:CE	1.67	1.55
1:B:286:GLU:CD	1:B:286:GLU:CG	1.78	1.55
1:D:225:VAL:CB	1:D:225:VAL:CG2	1.82	1.55
1:D:286:GLU:CD	1:D:286:GLU:CG	1.75	1.54
1:F:228:LYS:CE	1:F:228:LYS:NZ	1.70	1.54
1:E:319:GLN:CG	1:E:319:GLN:CD	1.78	1.54
1:D:198:GLU:CD	1:D:198:GLU:CG	1.79	1.53
1:F:105:TYR:N	1:F:105:TYR:CA	1.67	1.52
1:F:329:LYS:CE	1:F:329:LYS:NZ	1.73	1.52
1:A:322:ILE:CD1	1:A:322:ILE:CG1	1.87	1.51
1:E:207:ASP:CG	1:E:208:GLY:H	1.05	1.51
1:A:298:LEU:CG	1:A:298:LEU:CD1	1.90	1.50
1:A:238:GLN:CD	1:A:238:GLN:CG	1.82	1.49
1:B:248:LEU:CD1	1:B:248:LEU:CG	1.90	1.49
1:C:62:PRO:CG	1:C:62:PRO:CB	1.76	1.46
1:F:209:THR:CB	1:F:209:THR:CA	1.92	1.45
1:F:278:MSE:SE	1:F:278:MSE:CE	2.15	1.44
1:E:62:PRO:CG	1:E:62:PRO:CB	1.78	1.43
1:B:207:ASP:O	1:B:209:THR:HG23	1.14	1.26
1:C:8:LEU:CD1	1:C:310:THR:HG21	1.72	1.19
1:A:317:ILE:O	1:A:319:GLN:N	1.74	1.18
1:C:21:VAL:HG12	1:C:21:VAL:O	1.44	1.14
1:E:249:THR:O	1:E:249:THR:CG2	1.96	1.14
1:C:74:VAL:O	1:C:75:SER:HB3	1.37	1.13
1:E:41:SER:OG	1:E:42:GLY:N	1.62	1.13
1:E:207:ASP:CG	1:E:208:GLY:N	1.91	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TRP:O	1:A:219:GLN:HB3	1.34	1.11
1:F:11:GLU:HG3	1:F:12:LYS:H	1.08	1.10
1:A:218:TRP:O	1:A:219:GLN:CB	1.93	1.10
1:C:74:VAL:O	1:C:75:SER:CB	1.98	1.10
1:C:8:LEU:HD13	1:C:310:THR:HG21	1.19	1.09
1:C:21:VAL:O	1:C:21:VAL:CG1	2.00	1.08
1:D:218:TRP:O	1:D:219:GLN:CB	1.97	1.08
1:D:149:PRO:O	1:D:150:GLU:HB3	1.54	1.07
1:B:151:LYS:O	1:B:238:GLN:NE2	1.87	1.07
1:C:159:ALA:O	1:C:160:THR:HB	1.45	1.07
1:D:151:LYS:O	1:D:238:GLN:NE2	1.89	1.06
1:A:80:ARG:HH11	1:A:80:ARG:CG	1.60	1.06
1:B:142:LEU:CD2	1:B:242:SER:HB3	1.86	1.06
1:B:207:ASP:O	1:B:209:THR:CG2	2.03	1.05
1:C:157:THR:CG2	1:C:224:PRO:HD2	1.85	1.05
1:C:244:ALA:HB1	1:C:271:ILE:HD12	1.33	1.04
1:C:157:THR:HG21	1:C:223:ASP:OD1	1.58	1.03
1:C:305:VAL:CG1	1:C:306:SER:H	1.69	1.03
1:E:41:SER:HB2	1:E:328:VAL:H	1.22	1.03
1:C:43:ILE:CG2	1:C:317:ILE:HD11	1.88	1.03
1:E:13:ASN:N	1:E:13:ASN:HD22	1.54	1.02
1:D:218:TRP:O	1:D:219:GLN:HB2	1.60	1.02
1:B:218:TRP:O	1:B:219:GLN:HB3	1.59	1.01
1:C:305:VAL:HG13	1:C:306:SER:H	1.25	1.01
1:F:41:SER:HB2	1:F:328:VAL:H	1.21	1.01
1:C:157:THR:HG22	1:C:224:PRO:HD2	1.03	1.01
1:B:218:TRP:O	1:B:219:GLN:CB	2.08	1.00
1:F:244:ALA:HB1	1:F:271:ILE:HD11	1.43	1.00
1:A:80:ARG:NH1	1:A:80:ARG:HG3	1.51	1.00
1:A:151:LYS:O	1:A:238:GLN:NE2	1.95	0.99
1:D:49:LEU:HB2	1:D:57:ILE:HD12	1.41	0.99
1:A:151:LYS:O	1:A:238:GLN:CD	2.06	0.98
1:C:157:THR:HG22	1:C:224:PRO:CD	1.93	0.98
1:A:103:SER:HB2	1:A:104:GLU:O	1.64	0.98
1:F:185:ARG:O	1:F:186:GLU:HB2	1.62	0.98
1:D:98:ARG:HG3	1:D:98:ARG:HH11	1.26	0.98
1:A:66:GLY:HA3	1:A:101:GLY:H	1.29	0.97
1:C:244:ALA:HB1	1:C:271:ILE:CD1	1.92	0.97
1:E:90:THR:HG22	1:E:91:SER:OG	1.65	0.97
1:C:8:LEU:CD1	1:C:310:THR:CG2	2.42	0.96
1:E:249:THR:O	1:E:249:THR:HG22	1.64	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:GLU:C	1:F:105:TYR:CA	2.38	0.96
1:C:317:ILE:O	1:C:318:LEU:HB2	1.62	0.96
1:A:41:SER:OG	1:A:42:GLY:HA2	1.66	0.95
1:F:8:LEU:HD13	1:F:310:THR:CG2	1.97	0.95
1:F:11:GLU:HG3	1:F:12:LYS:N	1.63	0.94
1:A:41:SER:OG	1:A:42:GLY:N	1.99	0.94
1:D:207:ASP:CG	1:D:208:GLY:H	1.69	0.94
1:F:8:LEU:HD13	1:F:310:THR:HG22	1.48	0.94
1:A:41:SER:OG	1:A:42:GLY:CA	2.15	0.93
1:F:41:SER:HB3	1:F:327:ILE:HG22	1.49	0.93
1:C:313:ALA:C	1:C:315:LYS:H	1.71	0.93
1:D:32:ASP:OD1	1:D:32:ASP:N	1.98	0.92
1:B:304:GLU:HG2	1:B:327:ILE:HG22	1.50	0.92
1:C:172:ASN:C	1:C:172:ASN:HD22	1.77	0.91
1:F:151:LYS:O	1:F:238:GLN:NE2	2.03	0.91
1:D:297:LEU:O	1:D:300:ILE:HG22	1.69	0.91
1:D:24:ILE:HG22	1:D:25:SER:H	1.35	0.91
1:B:41:SER:HB3	1:B:42:GLY:CA	1.66	0.91
1:B:19:VAL:HG12	1:B:19:VAL:O	1.71	0.90
1:F:105:TYR:N	1:F:105:TYR:HA	1.85	0.90
1:E:159:ALA:O	1:E:160:THR:HB	1.69	0.90
1:C:305:VAL:CG1	1:C:306:SER:N	2.31	0.90
1:A:41:SER:HG	1:A:42:GLY:HA2	1.36	0.90
1:C:90:THR:HG22	1:C:91:SER:OG	1.72	0.89
1:E:219:GLN:HA	1:E:238:GLN:HG3	1.53	0.89
1:A:166:ILE:HG13	1:A:300:ILE:HD13	1.54	0.89
1:A:296:GLN:HB2	1:A:299:THR:HG23	1.54	0.89
1:E:151:LYS:O	1:E:238:GLN:NE2	2.05	0.89
1:B:141:ARG:HE	2:B:2255:NAD:H2A	1.36	0.89
1:E:319:GLN:HE21	1:E:321:ARG:HD3	1.36	0.88
1:F:11:GLU:CG	1:F:12:LYS:N	2.35	0.88
1:F:183:GLY:H	1:F:202:ARG:HH11	1.16	0.88
1:C:185:ARG:O	1:C:186:GLU:HB2	1.71	0.88
1:C:43:ILE:HG22	1:C:317:ILE:HD11	1.55	0.88
1:C:304:GLU:OE2	1:C:329:LYS:HE3	1.73	0.87
1:E:80:ARG:HG3	1:E:80:ARG:HH11	1.37	0.87
1:A:182:THR:HG23	1:A:182:THR:O	1.71	0.87
1:A:296:GLN:HB2	1:A:299:THR:CG2	2.03	0.87
1:F:244:ALA:HB1	1:F:271:ILE:CD1	2.04	0.87
1:F:159:ALA:O	1:F:160:THR:HB	1.75	0.87
1:C:126:MSE:O	1:C:325:ARG:NH1	2.06	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ALA:C	1:C:315:LYS:N	2.30	0.87
1:D:55:GLY:O	1:D:56:ASN:HB2	1.74	0.86
1:B:41:SER:OG	1:B:328:VAL:N	2.08	0.86
1:B:141:ARG:NE	2:B:2255:NAD:H2A	1.89	0.86
1:A:151:LYS:O	1:A:238:GLN:OE1	1.93	0.86
1:E:41:SER:OG	1:E:42:GLY:CA	2.24	0.86
1:F:296:GLN:HB3	1:F:299:THR:HB	1.55	0.86
1:A:162:GLY:O	1:A:166:ILE:HD12	1.76	0.85
1:A:245:VAL:CG2	1:A:268:LEU:HD11	2.06	0.85
1:B:142:LEU:HD23	1:B:242:SER:HB3	1.57	0.85
1:B:185:ARG:O	1:B:187:ALA:N	2.08	0.85
1:E:149:PRO:O	1:E:150:GLU:HB3	1.78	0.84
1:F:228:LYS:HG2	3:F:6313:HOH:O	1.78	0.84
1:A:182:THR:O	1:A:182:THR:CG2	2.25	0.84
1:D:8:LEU:HD13	1:D:310:THR:HG22	1.59	0.84
1:E:83:GLU:CD	1:E:83:GLU:H	1.86	0.84
1:E:181:SER:HB2	1:E:200:ILE:HG13	1.60	0.83
1:D:55:GLY:O	1:D:56:ASN:CB	2.24	0.83
1:D:207:ASP:CG	1:D:208:GLY:N	2.30	0.83
1:F:227:GLY:HA3	1:F:251:GLY:HA3	1.58	0.82
1:C:11:GLU:H	1:C:18:SER:HB2	1.44	0.82
1:B:317:ILE:HD13	1:B:322:ILE:HD12	1.61	0.82
1:E:13:ASN:HD22	1:E:13:ASN:H	1.21	0.82
1:B:206:TYR:CE1	1:B:209:THR:HA	2.14	0.81
1:A:80:ARG:HH11	1:A:80:ARG:HG3	0.69	0.81
1:D:149:PRO:O	1:D:150:GLU:CB	2.27	0.81
1:D:248:LEU:O	1:D:248:LEU:HD23	1.81	0.81
1:E:319:GLN:NE2	1:E:321:ARG:HD3	1.95	0.81
1:E:207:ASP:O	1:E:209:THR:HG23	1.79	0.81
1:E:319:GLN:HE21	1:E:321:ARG:CD	1.94	0.81
1:D:108:VAL:HG11	1:D:113:LEU:HD21	1.61	0.80
1:C:8:LEU:HD11	1:C:310:THR:CG2	2.12	0.80
1:F:18:SER:O	1:F:19:VAL:HB	1.81	0.80
1:E:218:TRP:O	1:E:219:GLN:CB	2.26	0.80
1:D:207:ASP:C	1:D:209:THR:H	1.90	0.80
1:F:305:VAL:CG2	1:F:309:GLU:HB2	2.12	0.80
1:B:3:THR:CG2	1:B:3:THR:HB	2.08	0.80
1:A:46:LYS:HG3	1:A:57:ILE:HD13	1.64	0.80
1:E:13:ASN:N	1:E:13:ASN:ND2	2.26	0.80
1:F:104:GLU:O	1:F:105:TYR:CA	2.29	0.79
1:B:7:ALA:HB1	1:B:64:ILE:HD13	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:HG2	1:B:299:THR:HG21	1.64	0.79
1:E:2:SER:N	1:E:27:GLU:OE2	2.15	0.79
1:C:138:SER:HA	1:C:271:ILE:HD13	1.62	0.79
1:D:24:ILE:HG22	1:D:25:SER:N	1.97	0.79
1:D:307:LEU:O	1:D:310:THR:HB	1.82	0.79
1:F:272:ASP:H	2:F:6255:NAD:H62A	1.30	0.79
1:A:141:ARG:HE	2:A:1255:NAD:H2A	1.47	0.79
1:F:209:THR:HG22	1:F:228:LYS:HE3	1.63	0.79
1:F:31:LYS:O	1:F:32:ASP:HB3	1.81	0.78
1:A:245:VAL:HG22	1:A:268:LEU:HD11	1.66	0.78
1:B:41:SER:HB3	1:B:42:GLY:HA2	1.63	0.78
1:A:298:LEU:CD1	1:A:298:LEU:HG	2.10	0.78
1:D:225:VAL:O	1:D:225:VAL:CG1	2.30	0.78
1:A:8:LEU:HD13	1:A:310:THR:HG22	1.66	0.78
1:F:209:THR:CG2	1:F:228:LYS:HE3	2.13	0.78
1:C:329:LYS:C	1:C:330:LEU:HD23	2.08	0.77
1:F:35:LEU:C	1:F:36:ILE:HD12	2.09	0.77
1:C:316:ASP:O	1:C:319:GLN:N	2.17	0.77
1:B:184:ASN:O	1:B:185:ARG:O	2.02	0.77
1:C:313:ALA:O	1:C:315:LYS:N	2.17	0.77
1:D:225:VAL:O	1:D:225:VAL:HG13	1.85	0.77
1:A:185:ARG:O	1:A:186:GLU:O	2.02	0.77
1:A:225:VAL:HG13	1:A:249:THR:HG22	1.67	0.77
1:B:64:ILE:HB	1:B:99:ASP:HB3	1.67	0.76
1:D:223:ASP:OD2	1:D:230:LEU:HD13	1.86	0.76
1:F:41:SER:CB	1:F:327:ILE:HG22	2.15	0.76
1:A:46:LYS:HG3	1:A:57:ILE:CD1	2.16	0.76
1:C:287:ARG:NE	1:C:291:ASP:OD2	2.17	0.76
1:F:66:GLY:HA3	1:F:101:GLY:H	1.51	0.76
1:A:225:VAL:HG12	1:A:225:VAL:O	1.86	0.76
1:B:136:ALA:HB2	1:B:170:MSE:SE	2.34	0.76
1:E:7:ALA:HB1	1:E:64:ILE:HD13	1.68	0.76
1:F:216:GLN:HE21	1:F:238:GLN:HG2	1.49	0.75
1:F:218:TRP:O	1:F:219:GLN:HB3	1.87	0.75
1:D:103:SER:OG	1:D:105:TYR:O	2.04	0.75
1:B:166:ILE:HG13	1:B:300:ILE:HD13	1.69	0.75
1:F:218:TRP:O	1:F:219:GLN:CB	2.30	0.75
1:F:184:ASN:ND2	1:F:185:ARG:O	2.19	0.75
1:E:207:ASP:C	1:E:209:THR:H	1.95	0.74
1:C:305:VAL:HG12	1:C:306:SER:N	2.02	0.74
1:E:13:ASN:O	1:E:15:ASP:N	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:HB3	1:A:267:SER:OG	1.87	0.74
1:D:317:ILE:O	1:D:318:LEU:CB	2.35	0.74
1:E:18:SER:O	1:E:19:VAL:HB	1.85	0.74
1:E:41:SER:HG	1:E:42:GLY:H	1.34	0.74
1:D:18:SER:O	1:D:19:VAL:HB	1.87	0.74
1:F:6:GLN:HE22	1:F:23:THR:HB	1.53	0.74
1:B:271:ILE:N	1:B:271:ILE:HD13	2.00	0.74
1:B:61:TYR:HD2	1:B:61:TYR:O	1.70	0.74
1:E:16:ASP:O	1:E:17:VAL:HB	1.88	0.74
1:A:158:GLY:O	1:A:159:ALA:O	2.06	0.74
1:E:249:THR:O	1:E:249:THR:HG23	1.84	0.74
1:D:207:ASP:OD2	1:D:208:GLY:N	2.20	0.73
1:D:308:GLU:O	1:D:311:PRO:HD2	1.88	0.73
1:E:19:VAL:HG12	1:E:19:VAL:O	1.86	0.73
1:E:90:THR:CG2	1:E:91:SER:OG	2.34	0.73
1:F:315:LYS:HE3	1:F:315:LYS:HA	1.70	0.73
1:B:27:GLU:OE2	1:B:27:GLU:HA	1.88	0.73
1:C:40:TYR:OH	1:C:329:LYS:NZ	2.19	0.73
1:E:16:ASP:O	1:E:17:VAL:CB	2.31	0.73
1:F:300:ILE:O	1:F:300:ILE:HG13	1.86	0.73
1:E:218:TRP:O	1:E:219:GLN:HB2	1.89	0.73
1:F:136:ALA:HA	1:F:170:MSE:HE1	1.70	0.73
1:E:7:ALA:CB	1:E:64:ILE:HD13	2.18	0.72
1:B:7:ALA:CB	1:B:64:ILE:HD13	2.19	0.72
1:C:147:LEU:HD22	1:C:219:GLN:OE1	1.89	0.72
1:C:159:ALA:O	1:C:160:THR:CB	2.25	0.72
1:B:197:SER:O	1:B:198:GLU:HG3	1.89	0.72
1:C:151:LYS:O	1:C:238:GLN:NE2	2.22	0.72
1:A:152:GLY:HA3	1:A:238:GLN:OE1	1.89	0.72
1:B:61:TYR:O	1:B:61:TYR:CD2	2.42	0.72
1:A:219:GLN:H	1:A:238:GLN:H	1.36	0.72
1:B:166:ILE:HG13	1:B:300:ILE:CD1	2.20	0.72
1:B:308:GLU:O	1:B:311:PRO:HD2	1.89	0.72
1:F:41:SER:HB2	1:F:328:VAL:N	2.00	0.72
1:A:246:SER:HA	1:D:262:ILE:HG22	1.72	0.71
1:B:270:GLY:C	1:B:271:ILE:HD13	2.14	0.71
1:D:49:LEU:CB	1:D:57:ILE:HD12	2.17	0.71
1:B:44:ASN:O	1:B:47:ASP:HB2	1.91	0.71
1:E:220:GLY:HA2	1:E:237:ILE:HD12	1.71	0.71
1:F:159:ALA:O	1:F:160:THR:CB	2.35	0.71
1:E:207:ASP:OD1	1:E:208:GLY:N	2.16	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:O	1:C:186:GLU:CB	2.39	0.71
1:C:316:ASP:O	1:C:319:GLN:HG2	1.91	0.71
1:D:86:GLU:HG2	1:D:122:LEU:HD11	1.73	0.71
1:D:8:LEU:HD13	1:D:310:THR:CG2	2.20	0.70
1:D:24:ILE:CG2	1:D:25:SER:H	2.03	0.70
1:B:206:TYR:HE1	1:B:209:THR:HA	1.53	0.70
1:A:206:TYR:CD1	1:A:232:SER:HB2	2.26	0.70
1:C:44:ASN:ND2	1:C:68:ASP:OD2	2.23	0.70
1:E:11:GLU:O	1:E:17:VAL:HA	1.92	0.70
1:B:68:ASP:HB3	1:B:126:MSE:SE	2.41	0.70
1:C:141:ARG:HE	2:C:3255:NAD:H2A	1.55	0.70
1:C:242:SER:HB3	1:C:267:SER:OG	1.91	0.70
1:B:19:VAL:O	1:B:19:VAL:CG1	2.39	0.70
1:B:41:SER:CB	1:B:42:GLY:CA	2.48	0.70
1:C:207:ASP:O	1:C:209:THR:HG23	1.90	0.70
1:E:219:GLN:CA	1:E:238:GLN:HG3	2.20	0.70
1:A:272:ASP:H	2:A:1255:NAD:H62A	1.39	0.70
1:B:152:GLY:O	1:B:219:GLN:NE2	2.25	0.70
1:F:183:GLY:N	1:F:202:ARG:HH11	1.89	0.70
1:F:41:SER:CB	1:F:328:VAL:H	2.03	0.69
1:B:318:LEU:O	1:B:320:ASN:N	2.25	0.69
1:D:67:ILE:O	1:D:90:THR:HA	1.93	0.69
1:D:108:VAL:CG1	1:D:113:LEU:HD21	2.22	0.69
1:C:206:TYR:CZ	1:C:209:THR:HG22	2.27	0.69
1:D:150:GLU:OE1	1:D:151:LYS:HD2	1.92	0.69
1:F:36:ILE:O	1:F:105:TYR:HA	1.93	0.69
1:A:141:ARG:NE	2:A:1255:NAD:H2A	2.08	0.69
1:D:303:ARG:HG2	1:D:304:GLU:H	1.56	0.68
1:B:153:SER:O	1:B:218:TRP:O	2.11	0.68
1:B:181:SER:HB2	1:B:200:ILE:HG13	1.74	0.68
1:E:173:LYS:HD3	1:E:293:LYS:O	1.93	0.68
1:F:208:GLY:O	1:F:209:THR:C	2.35	0.68
1:A:296:GLN:CB	1:A:299:THR:HG23	2.24	0.68
1:F:141:ARG:HE	2:F:6255:NAD:H2A	1.57	0.68
1:A:59:ARG:NE	1:A:59:ARG:HA	2.08	0.68
1:C:120:LEU:HG	1:C:289:SER:HB2	1.76	0.68
1:C:329:LYS:O	1:C:330:LEU:HD23	1.94	0.68
1:D:303:ARG:HG2	1:D:304:GLU:N	2.09	0.68
1:F:209:THR:CB	1:F:209:THR:HA	2.16	0.68
1:C:138:SER:HA	1:C:271:ILE:CD1	2.24	0.68
1:B:83:GLU:CD	1:B:83:GLU:H	2.02	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:LEU:C	1:F:233:LEU:HD23	2.17	0.68
1:F:330:LEU:HD12	1:F:330:LEU:H	1.60	0.67
1:D:201:SER:HB2	1:D:203:GLU:OE1	1.94	0.67
1:F:307:LEU:O	1:F:310:THR:HB	1.95	0.67
1:F:36:ILE:HD12	1:F:36:ILE:N	2.08	0.67
1:B:174:ARG:HB3	1:B:174:ARG:NH1	2.09	0.67
1:A:141:ARG:HE	2:A:1255:NAD:C2A	2.08	0.67
1:C:65:LEU:C	1:C:102:LEU:HD12	2.20	0.67
1:F:233:LEU:C	1:F:233:LEU:CD2	2.67	0.67
1:D:296:GLN:OE1	1:D:296:GLN:N	2.19	0.67
1:A:13:ASN:O	1:A:15:ASP:N	2.27	0.66
1:D:36:ILE:HG12	1:D:108:VAL:HG12	1.77	0.66
1:E:322:ILE:HG13	3:E:5269:HOH:O	1.94	0.66
1:C:37:LYS:HD2	3:C:3307:HOH:O	1.95	0.66
1:D:126:MSE:O	1:D:325:ARG:NH1	2.16	0.66
1:E:207:ASP:OD1	1:E:208:GLY:CA	2.43	0.66
1:A:298:LEU:CD1	1:A:298:LEU:H	2.07	0.66
1:B:230:LEU:HA	1:B:233:LEU:HD23	1.75	0.66
1:D:316:ASP:O	1:D:319:GLN:O	2.13	0.66
1:D:181:SER:HB2	1:D:200:ILE:HG13	1.76	0.66
1:F:120:LEU:HG	1:F:289:SER:CB	2.26	0.66
1:F:209:THR:HB	1:F:210:LEU:HD23	1.78	0.66
1:F:310:THR:HG22	1:F:311:PRO:HD3	1.78	0.66
1:F:6:GLN:N	1:F:104:GLU:OE1	2.26	0.65
1:E:316:ASP:C	1:E:317:ILE:O	2.36	0.65
1:B:181:SER:HB2	1:B:200:ILE:CG1	2.26	0.65
1:D:74:VAL:HG12	1:D:74:VAL:O	1.95	0.65
1:F:321:ARG:HD2	1:F:321:ARG:O	1.96	0.65
1:F:208:GLY:O	1:F:209:THR:O	2.15	0.65
1:F:98:ARG:NH2	1:F:107:SER:O	2.28	0.65
1:A:158:GLY:C	1:A:159:ALA:O	2.36	0.65
1:C:68:ASP:HB3	1:C:126:MSE:SE	2.47	0.65
1:C:230:LEU:HA	1:C:233:LEU:HD13	1.79	0.64
1:B:27:GLU:OE2	1:B:27:GLU:O	2.15	0.64
1:C:43:ILE:HD12	1:C:326:VAL:HG12	1.78	0.64
1:D:142:LEU:HB3	1:D:147:LEU:HG	1.77	0.64
1:C:151:LYS:HB3	1:C:219:GLN:CD	2.22	0.64
1:C:317:ILE:O	1:C:318:LEU:CB	2.35	0.64
1:A:298:LEU:H	1:A:298:LEU:HD12	1.62	0.64
1:B:83:GLU:CD	1:B:83:GLU:N	2.55	0.64
1:D:98:ARG:HG3	1:D:98:ARG:NH1	2.06	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:PRO:O	1:D:266:VAL:HG13	1.97	0.64
1:B:197:SER:C	1:B:198:GLU:HG3	2.23	0.64
1:C:145:ASN:OD1	1:F:141:ARG:NH2	2.27	0.64
1:D:8:LEU:CD1	1:D:310:THR:HG22	2.28	0.64
1:E:9:GLN:O	1:E:19:VAL:HA	1.97	0.64
1:C:26:THR:HB	3:C:3297:HOH:O	1.98	0.64
1:C:65:LEU:O	1:C:102:LEU:HD12	1.97	0.64
1:D:49:LEU:HB2	1:D:57:ILE:CD1	2.23	0.64
1:D:90:THR:CG2	1:D:91:SER:OG	2.46	0.63
1:E:126:MSE:O	1:E:325:ARG:NH1	2.31	0.63
1:E:159:ALA:O	1:E:160:THR:CB	2.40	0.63
1:D:26:THR:CG2	1:D:26:THR:C	2.70	0.63
1:D:302:ASP:OD1	1:D:302:ASP:C	2.40	0.63
1:C:206:TYR:CE1	1:C:209:THR:HG22	2.33	0.63
1:D:74:VAL:O	1:D:75:SER:CB	2.45	0.63
1:E:224:PRO:O	1:E:247:GLY:HA3	1.97	0.63
1:F:209:THR:HG22	3:F:6313:HOH:O	1.97	0.63
1:C:305:VAL:HG12	1:C:306:SER:H	1.58	0.63
1:E:317:ILE:O	1:E:318:LEU:HB2	1.97	0.63
1:B:142:LEU:HD22	1:B:242:SER:HB3	1.77	0.63
1:F:330:LEU:HD12	1:F:330:LEU:N	2.13	0.63
1:E:229:GLN:O	1:E:229:GLN:HG2	1.98	0.63
1:D:98:ARG:HH11	1:D:98:ARG:CG	2.05	0.62
1:B:69:ALA:C	1:B:126:MSE:HE3	2.23	0.62
1:F:316:ASP:C	1:F:317:ILE:O	2.38	0.62
1:A:130:THR:HG22	1:A:130:THR:O	1.99	0.62
1:A:66:GLY:CA	1:A:101:GLY:H	2.08	0.62
1:B:304:GLU:HG2	1:B:327:ILE:CG2	2.27	0.62
1:C:91:SER:O	1:C:92:TYR:C	2.42	0.62
1:C:219:GLN:HA	1:C:238:GLN:HG3	1.82	0.62
1:E:21:VAL:HG12	1:E:21:VAL:O	2.00	0.62
1:A:219:GLN:N	1:A:238:GLN:H	1.97	0.62
1:C:19:VAL:O	1:C:19:VAL:CG1	2.46	0.62
1:C:272:ASP:H	2:C:3255:NAD:H62A	1.48	0.62
1:F:305:VAL:HG22	1:F:309:GLU:HB2	1.82	0.62
1:F:120:LEU:HG	1:F:289:SER:HB3	1.81	0.62
1:B:66:GLY:HA3	1:B:100:GLY:HA3	1.81	0.61
1:D:120:LEU:HG	1:D:289:SER:HB3	1.81	0.61
1:D:207:ASP:O	1:D:209:THR:N	2.23	0.61
1:E:61:TYR:HD2	1:E:61:TYR:O	1.83	0.61
1:A:44:ASN:O	1:A:47:ASP:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ARG:HD3	1:C:275:TYR:HB3	1.81	0.61
1:B:307:LEU:O	1:B:310:THR:OG1	2.09	0.61
1:C:40:TYR:OH	1:C:329:LYS:HE2	2.00	0.61
1:D:43:ILE:O	1:D:43:ILE:HG22	2.01	0.61
1:C:67:ILE:O	1:C:90:THR:HA	2.00	0.61
1:C:207:ASP:C	1:C:209:THR:H	2.09	0.61
1:A:193:GLN:O	1:A:296:GLN:HG3	2.01	0.61
1:A:317:ILE:HA	1:A:322:ILE:HG12	1.82	0.61
1:E:272:ASP:OD1	1:E:274:VAL:HG23	2.01	0.61
1:F:61:TYR:HB3	1:F:62:PRO:HA	1.82	0.61
1:B:24:ILE:HB	1:B:28:ASP:OD1	2.01	0.60
1:C:8:LEU:HD11	1:C:310:THR:HG22	1.81	0.60
1:E:78:ASP:OD1	1:E:80:ARG:HG3	2.02	0.60
1:A:207:ASP:O	1:A:208:GLY:C	2.38	0.60
1:C:207:ASP:O	1:C:209:THR:N	2.26	0.60
1:A:41:SER:CB	1:A:42:GLY:CA	2.79	0.60
1:D:68:ASP:HB3	1:D:126:MSE:SE	2.51	0.60
1:A:18:SER:OG	1:A:20:HIS:NE2	2.35	0.60
1:C:172:ASN:C	1:C:172:ASN:ND2	2.54	0.60
1:E:64:ILE:HG13	1:E:99:ASP:OD1	2.01	0.60
1:C:7:ALA:CB	1:C:64:ILE:HD13	2.32	0.60
1:E:35:LEU:HD13	1:E:74:VAL:CG2	2.32	0.60
1:E:305:VAL:HG13	1:E:309:GLU:HB2	1.84	0.60
1:B:45:TYR:CE1	1:B:318:LEU:HD23	2.37	0.59
1:C:127:VAL:HG12	1:C:127:VAL:O	2.01	0.59
1:D:182:THR:HG22	1:D:183:GLY:H	1.68	0.59
1:E:32:ASP:N	1:E:32:ASP:OD1	2.35	0.59
1:C:141:ARG:NE	2:C:3255:NAD:H2A	2.17	0.59
1:D:37:LYS:HG3	3:D:4273:HOH:O	2.02	0.59
1:B:35:LEU:HD13	1:B:74:VAL:HG13	1.84	0.59
1:F:74:VAL:O	1:F:75:SER:HB2	2.02	0.59
1:A:66:GLY:HA3	1:A:101:GLY:N	2.10	0.59
1:C:216:GLN:HE21	1:C:238:GLN:HB3	1.68	0.59
1:A:327:ILE:HG22	1:A:328:VAL:N	2.15	0.59
1:D:207:ASP:C	1:D:209:THR:N	2.61	0.59
1:F:296:GLN:H	1:F:296:GLN:CD	2.10	0.59
1:C:312:GLY:O	1:C:315:LYS:CB	2.51	0.59
1:E:67:ILE:O	1:E:90:THR:HA	2.02	0.59
1:F:227:GLY:O	1:F:228:LYS:C	2.44	0.59
1:F:305:VAL:HG22	1:F:306:SER:N	2.15	0.59
1:A:147:LEU:HD22	1:A:219:GLN:OE1	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:VAL:H	1:E:105:TYR:H	1.50	0.59
1:E:303:ARG:HG3	1:E:305:VAL:HG23	1.85	0.58
1:F:68:ASP:HB3	1:F:126:MSE:HE1	1.85	0.58
1:B:317:ILE:CD1	1:B:322:ILE:HD12	2.32	0.58
1:F:147:LEU:HD22	1:F:219:GLN:OE1	2.04	0.58
1:C:120:LEU:HG	1:C:289:SER:CB	2.33	0.58
1:B:248:LEU:CD1	1:B:248:LEU:CD2	2.80	0.58
1:C:43:ILE:HD12	1:C:326:VAL:CG1	2.32	0.58
1:C:305:VAL:HG13	1:C:306:SER:N	2.04	0.58
1:D:171:LEU:HD12	1:D:176:TYR:CD1	2.38	0.58
1:B:27:GLU:OE2	1:B:27:GLU:CA	2.51	0.58
1:D:301:VAL:HG13	3:D:4296:HOH:O	2.02	0.58
1:C:138:SER:CA	1:C:271:ILE:HD13	2.34	0.58
1:D:233:LEU:C	1:D:233:LEU:HD23	2.27	0.58
1:E:9:GLN:HG3	1:E:10:ALA:N	2.18	0.58
1:F:66:GLY:HA3	1:F:101:GLY:N	2.19	0.58
1:E:37:LYS:HG3	3:E:5261:HOH:O	2.03	0.58
1:F:224:PRO:O	1:F:247:GLY:HA3	2.03	0.58
1:A:29:LEU:O	1:A:30:PRO:C	2.45	0.58
1:D:170:MSE:HG2	1:D:292:LEU:HB3	1.86	0.58
1:D:305:VAL:HG22	1:D:309:GLU:HB2	1.86	0.58
1:F:116:LEU:HD12	1:F:117:PRO:HD2	1.85	0.58
1:A:159:ALA:O	1:A:160:THR:HB	2.04	0.57
1:B:10:ALA:HA	1:B:19:VAL:HA	1.85	0.57
1:B:25:SER:O	1:B:26:THR:C	2.47	0.57
1:B:166:ILE:CG2	1:B:170:MSE:HE3	2.34	0.57
1:F:136:ALA:CA	1:F:170:MSE:HE1	2.33	0.57
1:F:183:GLY:H	1:F:202:ARG:NH1	1.96	0.57
1:A:25:SER:O	1:A:26:THR:C	2.42	0.57
1:A:296:GLN:H	1:A:296:GLN:CD	2.12	0.57
1:E:303:ARG:HH11	1:E:303:ARG:HB3	1.69	0.57
1:F:148:SER:O	1:F:150:GLU:N	2.37	0.57
1:F:220:GLY:HA2	1:F:242:SER:O	2.04	0.57
1:F:320:ASN:CG	1:F:320:ASN:O	2.47	0.57
1:B:43:ILE:HD12	1:B:313:ALA:HB1	1.86	0.57
1:B:292:LEU:O	1:B:294:PRO:HD3	2.04	0.57
1:C:319:GLN:HG3	1:C:321:ARG:HG2	1.87	0.57
1:E:219:GLN:H	1:E:238:GLN:H	1.52	0.57
1:F:227:GLY:HA2	1:F:253:GLU:O	2.04	0.57
1:B:38:VAL:HG12	1:B:330:LEU:HD13	1.86	0.57
1:D:45:TYR:O	1:D:48:GLY:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:GLN:N	1:E:238:GLN:HG3	2.19	0.57
1:F:296:GLN:O	1:F:298:LEU:N	2.38	0.57
1:B:190:TYR:O	1:B:193:GLN:HB3	2.05	0.57
1:D:182:THR:O	1:D:201:SER:HA	2.05	0.57
1:E:36:ILE:O	1:E:105:TYR:HA	2.03	0.57
1:B:300:ILE:HG12	1:B:300:ILE:O	2.04	0.57
1:F:88:ILE:HB	1:F:114:VAL:HG13	1.87	0.57
1:C:49:LEU:HD23	1:C:318:LEU:HD21	1.86	0.56
1:C:40:TYR:OH	1:C:329:LYS:CE	2.53	0.56
1:C:148:SER:O	1:C:151:LYS:HB2	2.05	0.56
1:E:43:ILE:HG22	1:E:43:ILE:O	2.05	0.56
1:A:147:LEU:HD22	1:A:219:GLN:CD	2.30	0.56
1:B:220:GLY:HA2	1:B:242:SER:O	2.05	0.56
1:D:26:THR:CG2	1:D:26:THR:HB	2.16	0.56
1:E:316:ASP:HB3	3:E:5269:HOH:O	2.05	0.56
1:C:206:TYR:CE1	1:C:209:THR:HA	2.41	0.56
1:C:211:LYS:O	1:C:212:ALA:C	2.47	0.56
1:E:41:SER:OG	1:E:42:GLY:HA2	2.04	0.56
1:B:203:GLU:O	1:B:207:ASP:HB2	2.05	0.56
1:C:119:ASN:O	1:C:120:LEU:HD23	2.04	0.56
1:A:41:SER:HA	1:A:328:VAL:HB	1.87	0.56
1:C:19:VAL:O	1:C:19:VAL:HG12	2.05	0.56
1:C:123:LYS:O	1:C:124:GLU:C	2.46	0.56
1:A:305:VAL:HG22	1:A:309:GLU:HG3	1.87	0.56
1:B:34:VAL:O	1:B:107:SER:HA	2.06	0.56
1:B:111:ASP:OD1	1:B:111:ASP:N	2.35	0.56
1:C:164:GLY:O	1:C:168:VAL:HG23	2.05	0.56
1:E:240:GLY:HA2	1:E:265:GLY:O	2.06	0.56
1:F:90:THR:HG23	1:F:91:SER:OG	2.06	0.56
1:F:302:ASP:HB2	1:F:323:GLN:O	2.04	0.56
1:A:63:LEU:HD23	1:A:63:LEU:C	2.31	0.56
1:C:44:ASN:ND2	1:C:325:ARG:HH21	2.03	0.56
1:D:44:ASN:O	1:D:45:TYR:C	2.49	0.56
1:F:155:LEU:O	1:F:221:ALA:HA	2.05	0.56
1:F:317:ILE:O	1:F:318:LEU:HB2	2.06	0.56
1:B:296:GLN:O	1:B:298:LEU:N	2.37	0.56
1:C:316:ASP:OD2	1:C:316:ASP:N	2.39	0.56
1:A:8:LEU:HD11	1:A:19:VAL:HG12	1.87	0.55
1:B:142:LEU:HD23	1:B:242:SER:CB	2.34	0.55
1:C:245:VAL:CG2	1:C:268:LEU:HD11	2.37	0.55
1:B:90:THR:O	1:B:91:SER:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:HA	1:C:24:ILE:O	2.06	0.55
1:C:53:ALA:O	1:C:54:GLY:C	2.48	0.55
1:D:90:THR:HG23	1:D:91:SER:OG	2.05	0.55
1:B:38:VAL:CG1	1:B:330:LEU:HD13	2.36	0.55
1:D:38:VAL:HG12	1:D:330:LEU:HD13	1.88	0.55
1:F:149:PRO:HA	1:F:176:TYR:CD2	2.41	0.55
1:C:142:LEU:HD23	1:C:242:SER:OG	2.07	0.55
1:A:49:LEU:HB2	1:A:57:ILE:HD12	1.89	0.55
1:A:261:PHE:CZ	1:D:268:LEU:HD23	2.42	0.55
1:D:177:ASP:OD1	1:E:118:GLN:NE2	2.39	0.55
1:D:308:GLU:C	1:D:310:THR:H	2.15	0.55
1:C:136:ALA:HB2	1:C:170:MSE:HE1	1.89	0.55
1:F:31:LYS:O	1:F:32:ASP:CB	2.52	0.55
1:F:138:SER:OG	1:F:271:ILE:HD13	2.06	0.55
1:C:253:GLU:OE1	1:C:253:GLU:HA	2.07	0.54
1:E:6:GLN:NE2	1:E:23:THR:OG1	2.39	0.54
1:C:66:GLY:HA3	1:C:101:GLY:H	1.72	0.54
1:C:245:VAL:HG22	1:C:268:LEU:HD11	1.88	0.54
1:D:34:VAL:HG13	1:D:76:SER:HB2	1.89	0.54
1:E:7:ALA:HA	1:E:103:SER:HA	1.89	0.54
1:B:219:GLN:H	1:B:238:GLN:H	1.53	0.54
1:F:227:GLY:CA	1:F:251:GLY:HA3	2.32	0.54
1:D:202:ARG:O	1:D:206:TYR:O	2.25	0.54
1:E:297:LEU:O	1:E:300:ILE:HG22	2.07	0.54
1:C:173:LYS:HD3	1:C:293:LYS:O	2.07	0.54
1:C:44:ASN:HD21	1:C:325:ARG:NH2	2.05	0.54
1:D:104:GLU:O	1:D:105:TYR:HB2	2.08	0.54
1:D:249:THR:HB	3:D:4290:HOH:O	2.07	0.54
1:F:319:GLN:O	1:F:319:GLN:HG3	2.08	0.54
1:A:117:PRO:HG2	1:A:120:LEU:HD12	1.90	0.54
1:A:262:ILE:HD11	1:D:248:LEU:HD12	1.89	0.54
1:C:25:SER:O	1:C:28:ASP:N	2.29	0.54
1:C:312:GLY:O	1:C:315:LYS:HB2	2.08	0.54
1:F:104:GLU:O	1:F:105:TYR:O	2.24	0.54
1:A:130:THR:O	1:A:130:THR:CG2	2.55	0.54
1:B:141:ARG:HE	2:B:2255:NAD:C2A	2.16	0.54
1:E:46:LYS:HG3	1:E:57:ILE:CD1	2.38	0.54
1:A:3:THR:O	1:A:25:SER:HB2	2.08	0.54
1:E:128:TYR:OH	1:E:293:LYS:HA	2.08	0.54
1:B:166:ILE:CG1	1:B:300:ILE:HD13	2.36	0.53
1:C:101:GLY:O	1:C:102:LEU:C	2.51	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LEU:HD21	1:E:128:TYR:HE1	1.72	0.53
1:F:41:SER:HB2	1:F:328:VAL:HB	1.90	0.53
1:A:32:ASP:OD1	1:A:32:ASP:N	2.39	0.53
1:B:127:VAL:O	1:B:325:ARG:HD2	2.09	0.53
1:E:61:TYR:O	1:E:61:TYR:CD2	2.61	0.53
1:F:16:ASP:HB2	3:F:6272:HOH:O	2.07	0.53
1:A:225:VAL:O	1:A:225:VAL:CG1	2.54	0.53
1:A:248:LEU:HD23	1:D:258:VAL:HG11	1.89	0.53
1:B:18:SER:O	1:B:19:VAL:HB	2.08	0.53
1:D:90:THR:HG22	1:D:91:SER:OG	2.08	0.53
1:D:308:GLU:C	1:D:310:THR:N	2.66	0.53
1:E:78:ASP:OD2	1:E:80:ARG:NH1	2.42	0.53
1:F:281:ARG:HD3	3:F:6285:HOH:O	2.08	0.53
1:B:7:ALA:HA	1:B:103:SER:HB2	1.91	0.53
1:C:7:ALA:HB1	1:C:64:ILE:HD13	1.91	0.53
1:C:153:SER:HB3	1:C:177:ASP:HB2	1.91	0.53
1:D:7:ALA:HB1	1:D:103:SER:HB2	1.89	0.53
1:E:138:SER:OG	1:E:271:ILE:HG13	2.09	0.53
1:C:316:ASP:C	1:C:317:ILE:O	2.52	0.53
1:A:272:ASP:N	2:A:1255:NAD:H62A	2.07	0.53
1:B:98:ARG:CZ	1:B:109:PRO:HD3	2.39	0.53
1:F:11:GLU:HG2	3:F:6310:HOH:O	2.09	0.53
1:E:308:GLU:HA	1:E:308:GLU:OE2	2.09	0.52
1:F:140:HIS:O	1:F:144:GLN:HG3	2.10	0.52
1:F:184:ASN:ND2	1:F:184:ASN:C	2.66	0.52
1:A:316:ASP:O	1:A:317:ILE:O	2.28	0.52
1:C:173:LYS:HG3	1:C:173:LYS:O	2.08	0.52
1:D:8:LEU:HD12	1:D:311:PRO:HD3	1.90	0.52
1:E:83:GLU:CD	1:E:83:GLU:N	2.64	0.52
1:F:209:THR:CA	1:F:210:LEU:HD23	2.39	0.52
1:A:148:SER:HB3	1:A:151:LYS:HD3	1.91	0.52
1:A:153:SER:O	1:A:218:TRP:O	2.28	0.52
1:E:103:SER:O	1:E:330:LEU:HD22	2.09	0.52
1:A:244:ALA:HB1	1:A:271:ILE:CD1	2.39	0.52
1:D:225:VAL:HG22	1:D:249:THR:OG1	2.09	0.52
1:F:216:GLN:NE2	1:F:238:GLN:HG2	2.21	0.52
1:F:325:ARG:HH11	1:F:325:ARG:HB3	1.73	0.52
1:F:308:GLU:HA	1:F:308:GLU:OE1	2.10	0.52
1:A:185:ARG:O	1:A:186:GLU:C	2.49	0.52
1:B:306:SER:O	1:B:310:THR:HG23	2.10	0.52
1:E:12:LYS:HD2	1:E:61:TYR:CD1	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:GLN:OE1	1:F:296:GLN:N	2.33	0.52
1:A:261:PHE:HB3	1:D:270:GLY:HA2	1.90	0.52
1:D:37:LYS:H	1:D:74:VAL:HG23	1.75	0.52
1:E:66:GLY:HA3	1:E:100:GLY:HA3	1.91	0.52
1:F:34:VAL:HG12	1:F:36:ILE:HD11	1.92	0.52
1:F:207:ASP:O	1:F:208:GLY:C	2.44	0.52
1:A:173:LYS:HE2	1:A:293:LYS:O	2.10	0.51
1:B:43:ILE:HD12	1:B:313:ALA:CB	2.39	0.51
1:A:316:ASP:OD2	1:A:321:ARG:HD3	2.10	0.51
1:C:103:SER:O	1:C:104:GLU:C	2.53	0.51
1:E:66:GLY:HA3	1:E:101:GLY:H	1.75	0.51
1:E:219:GLN:O	1:E:241:GLY:HA3	2.10	0.51
1:B:259:TYR:CE1	1:E:248:LEU:HD23	2.46	0.51
1:B:275:TYR:CE2	1:C:79:PRO:HG2	2.45	0.51
1:F:153:SER:O	1:F:218:TRP:O	2.28	0.51
1:A:245:VAL:CG2	1:A:268:LEU:CD1	2.83	0.51
1:A:272:ASP:OD2	1:A:274:VAL:N	2.41	0.51
1:B:63:LEU:C	1:B:63:LEU:HD23	2.36	0.51
1:C:142:LEU:O	1:C:147:LEU:HB2	2.11	0.51
1:E:319:GLN:O	1:E:321:ARG:N	2.43	0.51
1:F:233:LEU:O	1:F:234:LEU:C	2.51	0.51
1:C:40:TYR:CZ	1:C:329:LYS:HE2	2.46	0.51
1:D:129:GLY:O	1:D:130:THR:C	2.53	0.51
1:D:248:LEU:HD23	1:D:248:LEU:C	2.32	0.51
1:A:287:ARG:HB3	1:A:292:LEU:HD12	1.91	0.51
1:F:278:MSE:CE	1:F:278:MSE:HB2	2.41	0.51
1:C:171:LEU:HB3	1:C:178:VAL:HG22	1.92	0.51
1:F:227:GLY:O	1:F:229:GLN:N	2.43	0.51
1:B:216:GLN:HG2	1:B:238:GLN:HA	1.92	0.51
1:D:221:ALA:HB3	1:D:243:VAL:HG13	1.92	0.51
1:E:208:GLY:C	1:E:209:THR:OG1	2.51	0.51
1:F:219:GLN:HA	1:F:238:GLN:HB2	1.92	0.51
1:A:3:THR:HG23	1:A:26:THR:HG21	1.93	0.51
1:A:36:ILE:O	1:A:105:TYR:HA	2.10	0.51
1:A:206:TYR:CD1	1:A:232:SER:CB	2.94	0.51
1:A:225:VAL:O	1:A:226:GLY:O	2.29	0.50
1:B:310:THR:OG1	1:B:311:PRO:HD3	2.10	0.50
1:D:38:VAL:CG1	1:D:330:LEU:HD13	2.41	0.50
1:F:36:ILE:N	1:F:36:ILE:CD1	2.74	0.50
1:A:68:ASP:HB3	1:A:126:MSE:SE	2.61	0.50
1:F:68:ASP:CB	1:F:126:MSE:HE1	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:NE	1:A:291:ASP:OD1	2.42	0.50
1:A:307:LEU:O	1:A:310:THR:HB	2.12	0.50
1:C:49:LEU:HD23	1:C:318:LEU:CD2	2.42	0.50
1:C:313:ALA:O	1:C:314:LEU:C	2.53	0.50
1:E:76:SER:OG	1:E:78:ASP:O	2.29	0.50
1:F:325:ARG:HB3	1:F:325:ARG:NH1	2.27	0.50
1:A:206:TYR:HB2	1:A:232:SER:HB3	1.93	0.50
1:C:11:GLU:N	1:C:18:SER:HB2	2.19	0.50
1:C:88:ILE:HG21	1:C:285:TRP:CZ2	2.47	0.50
1:C:141:ARG:HE	2:C:3255:NAD:C2A	2.21	0.50
1:E:80:ARG:HG3	1:E:80:ARG:NH1	2.14	0.50
1:F:147:LEU:HD13	1:F:176:TYR:CE2	2.47	0.50
1:F:158:GLY:C	1:F:159:ALA:O	2.51	0.50
1:F:220:GLY:CA	1:F:242:SER:O	2.60	0.50
1:A:245:VAL:HG21	1:A:268:LEU:HD11	1.93	0.50
1:A:255:PRO:O	1:A:255:PRO:HG2	2.12	0.50
1:E:202:ARG:HG3	3:E:5303:HOH:O	2.12	0.50
1:E:260:PRO:O	1:E:266:VAL:HG13	2.12	0.50
1:F:209:THR:C	1:F:210:LEU:HD23	2.36	0.50
1:A:49:LEU:HD23	1:A:318:LEU:HD21	1.92	0.50
1:A:157:THR:OG1	1:A:224:PRO:HD2	2.12	0.50
1:C:305:VAL:HG13	1:C:309:GLU:HB3	1.93	0.50
1:F:184:ASN:C	1:F:184:ASN:HD22	2.18	0.50
1:B:59:ARG:HG3	1:B:97:SER:HB3	1.92	0.49
1:D:17:VAL:CG2	1:D:53:ALA:HB2	2.42	0.49
1:E:61:TYR:HB2	3:E:5270:HOH:O	2.11	0.49
1:E:294:PRO:O	1:E:297:LEU:HB2	2.12	0.49
1:F:138:SER:O	1:F:142:LEU:HG	2.12	0.49
1:D:81:PHE:CZ	1:D:113:LEU:HB2	2.47	0.49
1:D:292:LEU:O	1:D:294:PRO:HD3	2.12	0.49
1:F:47:ASP:O	1:F:48:GLY:C	2.55	0.49
1:C:14:ALA:C	1:C:15:ASP:OD1	2.55	0.49
1:D:170:MSE:O	1:D:173:LYS:HB3	2.11	0.49
1:F:104:GLU:O	1:F:105:TYR:C	2.55	0.49
1:B:185:ARG:HA	1:B:185:ARG:NE	2.26	0.49
1:C:147:LEU:HD22	1:C:219:GLN:CD	2.37	0.49
1:D:121:SER:O	1:D:122:LEU:C	2.51	0.49
1:D:287:ARG:NE	1:D:291:ASP:OD2	2.45	0.49
1:E:153:SER:O	1:E:218:TRP:O	2.31	0.49
1:F:209:THR:HB	1:F:210:LEU:CD2	2.42	0.49
1:A:245:VAL:HG22	1:A:268:LEU:CD1	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:SER:OG	1:C:42:GLY:N	2.29	0.49
1:C:284:VAL:O	1:C:288:MSE:HG3	2.12	0.49
1:D:43:ILE:HD12	1:D:43:ILE:N	2.28	0.49
1:D:246:SER:HB3	1:D:271:ILE:HB	1.93	0.49
1:F:209:THR:CA	1:F:209:THR:HB	2.21	0.49
1:F:260:PRO:O	1:F:266:VAL:HG13	2.12	0.49
1:A:329:LYS:O	1:A:330:LEU:HG	2.12	0.49
1:C:138:SER:O	1:C:142:LEU:HD12	2.13	0.49
1:F:278:MSE:HB2	1:F:278:MSE:HE2	1.94	0.49
1:F:19:VAL:HG12	1:F:19:VAL:O	2.12	0.49
1:D:165:GLY:O	1:D:168:VAL:HB	2.12	0.49
1:F:216:GLN:NE2	1:F:238:GLN:HA	2.28	0.49
1:A:296:GLN:CA	1:A:299:THR:HG23	2.43	0.49
1:C:219:GLN:O	1:C:219:GLN:HG2	2.13	0.49
1:E:93:GLU:HB2	1:E:112:TRP:CH2	2.47	0.49
1:F:210:LEU:CD2	3:F:6313:HOH:O	2.61	0.49
1:C:127:VAL:O	1:C:127:VAL:CG1	2.61	0.49
1:D:192:LYS:HD3	1:D:196:ALA:O	2.13	0.49
1:F:272:ASP:O	2:F:6255:NAD:N6A	2.46	0.49
1:B:261:PHE:CZ	1:E:268:LEU:HD23	2.48	0.48
1:C:5:PHE:HB2	1:C:104:GLU:CG	2.43	0.48
1:C:44:ASN:HD21	1:C:325:ARG:HH21	1.60	0.48
1:A:317:ILE:CD1	1:A:318:LEU:H	2.26	0.48
1:B:219:GLN:HA	1:B:238:GLN:HB2	1.94	0.48
1:D:199:VAL:C	1:D:200:ILE:HG23	2.39	0.48
1:B:23:THR:HG22	1:B:23:THR:O	2.13	0.48
1:B:259:TYR:CE1	1:E:248:LEU:CD2	2.96	0.48
1:C:39:ALA:C	1:C:40:TYR:CD1	2.91	0.48
1:E:311:PRO:O	1:E:312:GLY:C	2.55	0.48
1:A:24:ILE:CD1	1:A:24:ILE:CB	2.82	0.48
1:A:306:SER:O	1:A:307:LEU:C	2.55	0.48
1:C:65:LEU:O	1:C:102:LEU:HB2	2.13	0.48
1:C:222:VAL:O	1:C:224:PRO:HD3	2.14	0.48
1:D:5:PHE:CD1	1:D:5:PHE:C	2.92	0.48
1:D:12:LYS:HG2	1:D:12:LYS:O	2.13	0.48
1:C:157:THR:HG23	1:C:158:GLY:N	2.28	0.48
1:D:147:LEU:HD13	1:D:176:TYR:CE2	2.49	0.48
1:D:245:VAL:HG22	1:D:268:LEU:HD11	1.95	0.48
1:F:40:TYR:CZ	1:F:123:LYS:HB2	2.49	0.48
1:F:141:ARG:HE	2:F:6255:NAD:C2A	2.24	0.48
1:A:327:ILE:HG21	1:A:327:ILE:HD13	1.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD23	1:B:49:LEU:HA	1.65	0.48
1:C:157:THR:HG23	1:C:225:VAL:HB	1.96	0.48
1:F:120:LEU:HG	1:F:289:SER:HB2	1.95	0.48
1:B:93:GLU:HB3	1:B:97:SER:OG	2.14	0.48
1:C:43:ILE:HG23	1:C:317:ILE:HD11	1.84	0.48
1:E:246:SER:HB3	1:E:271:ILE:HB	1.96	0.48
1:D:270:GLY:O	1:D:271:ILE:HD13	2.14	0.48
1:A:166:ILE:CG2	1:A:170:MSE:HE3	2.44	0.47
1:D:93:GLU:HB3	1:D:97:SER:HB3	1.96	0.47
1:D:185:ARG:O	1:D:186:GLU:HB2	2.13	0.47
1:E:135:ALA:O	1:E:139:VAL:HG23	2.14	0.47
1:F:69:ALA:HB2	1:F:101:GLY:HA3	1.95	0.47
1:F:114:VAL:HA	1:F:115:PRO:HD3	1.76	0.47
1:F:242:SER:HB3	1:F:267:SER:OG	2.13	0.47
1:F:297:LEU:O	1:F:300:ILE:HG22	2.14	0.47
1:A:317:ILE:HD13	1:A:318:LEU:H	1.79	0.47
1:B:220:GLY:CA	1:B:242:SER:O	2.62	0.47
1:C:43:ILE:CG2	1:C:317:ILE:CD1	2.76	0.47
1:E:64:ILE:HG21	1:E:103:SER:HB2	1.97	0.47
1:A:159:ALA:O	1:A:160:THR:CB	2.57	0.47
1:C:39:ALA:O	1:C:40:TYR:CD1	2.67	0.47
1:D:74:VAL:O	1:D:75:SER:HB2	2.13	0.47
1:D:91:SER:HB3	1:D:274:VAL:HA	1.96	0.47
1:E:170:MSE:HE1	1:E:288:MSE:HE3	1.96	0.47
1:F:209:THR:CB	1:F:210:LEU:HD23	2.45	0.47
1:B:41:SER:CB	1:B:42:GLY:HA2	2.35	0.47
1:B:43:ILE:HD13	1:B:314:LEU:HD23	1.96	0.47
1:B:63:LEU:HD12	1:B:98:ARG:N	2.29	0.47
1:F:237:ILE:HD13	1:F:243:VAL:CG2	2.44	0.47
1:C:225:VAL:HA	1:C:249:THR:HB	1.97	0.47
1:E:308:GLU:O	1:E:311:PRO:HD2	2.14	0.47
1:A:25:SER:O	1:A:28:ASP:N	2.44	0.47
1:A:120:LEU:HA	1:A:124:GLU:OE1	2.15	0.47
1:B:94:LEU:HD21	1:B:108:VAL:HB	1.97	0.47
1:D:69:ALA:C	1:D:126:MSE:HE3	2.39	0.47
1:D:178:VAL:HA	3:D:4261:HOH:O	2.14	0.47
1:D:248:LEU:C	1:D:249:THR:O	2.54	0.47
1:E:159:ALA:HB1	1:E:191:LEU:HD21	1.97	0.47
1:B:174:ARG:HB3	1:B:174:ARG:CZ	2.45	0.47
1:C:225:VAL:HG12	1:C:225:VAL:O	2.15	0.47
1:C:228:LYS:O	1:C:229:GLN:C	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLY:HA3	1:B:101:GLY:H	1.80	0.47
1:B:217:GLN:O	1:B:218:TRP:CG	2.67	0.47
1:C:38:VAL:N	3:C:3307:HOH:O	2.47	0.47
1:A:47:ASP:OD2	1:A:67:ILE:HG23	2.15	0.46
1:C:45:TYR:HA	1:C:317:ILE:CG2	2.45	0.46
1:C:142:LEU:HB3	1:C:147:LEU:HG	1.97	0.46
1:E:5:PHE:HB2	1:E:104:GLU:HG3	1.97	0.46
1:E:303:ARG:HH11	1:E:303:ARG:CB	2.27	0.46
1:B:157:THR:OG1	1:B:224:PRO:HD2	2.15	0.46
1:C:214:SER:HB2	1:C:236:LYS:HG3	1.98	0.46
1:D:182:THR:CG2	1:D:184:ASN:H	2.28	0.46
1:F:6:GLN:NE2	1:F:23:THR:HB	2.26	0.46
1:F:136:ALA:N	1:F:170:MSE:HE1	2.31	0.46
1:A:238:GLN:CD	1:A:238:GLN:CB	2.82	0.46
1:B:34:VAL:HG13	1:B:76:SER:HB2	1.96	0.46
1:B:70:ALA:N	1:B:126:MSE:HE3	2.31	0.46
1:D:13:ASN:O	1:D:14:ALA:HB3	2.15	0.46
1:F:147:LEU:HD22	1:F:219:GLN:CD	2.40	0.46
1:F:317:ILE:H	1:F:317:ILE:HG13	1.52	0.46
1:A:13:ASN:HD22	1:A:13:ASN:N	2.13	0.46
1:C:16:ASP:OD1	1:C:16:ASP:N	2.48	0.46
1:D:245:VAL:O	1:D:246:SER:OG	2.30	0.46
1:E:241:GLY:O	1:E:266:VAL:HA	2.16	0.46
1:F:296:GLN:HB2	1:F:297:LEU:H	1.40	0.46
1:C:55:GLY:O	1:C:56:ASN:HB2	2.14	0.46
1:F:48:GLY:HA3	1:F:317:ILE:HD11	1.98	0.46
1:F:185:ARG:O	1:F:186:GLU:CB	2.36	0.46
1:F:190:TYR:CE2	1:F:194:LEU:HD11	2.51	0.46
1:F:233:LEU:HD23	1:F:233:LEU:O	2.16	0.46
1:A:248:LEU:O	1:A:250:GLY:N	2.46	0.46
1:E:24:ILE:HD13	1:E:24:ILE:HG23	1.51	0.46
1:E:78:ASP:HA	1:E:79:PRO:HD3	1.43	0.46
1:A:184:ASN:O	1:A:187:ALA:HB2	2.16	0.46
1:B:303:ARG:HG2	3:B:2301:HOH:O	2.15	0.46
1:C:267:SER:HB3	3:F:6308:HOH:O	2.16	0.46
1:D:24:ILE:CG2	1:D:25:SER:N	2.64	0.46
1:D:158:GLY:O	1:D:160:THR:N	2.43	0.46
1:D:207:ASP:OD2	1:D:208:GLY:CA	2.64	0.46
1:D:279:ASP:HB3	1:D:280:VAL:H	1.46	0.46
1:F:40:TYR:CE1	1:F:123:LYS:HB2	2.50	0.46
1:F:307:LEU:HA	1:F:307:LEU:HD23	1.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:N	1:A:124:GLU:OE1	2.42	0.46
1:B:101:GLY:C	1:B:103:SER:H	2.24	0.46
1:B:207:ASP:HB3	1:B:208:GLY:H	1.33	0.46
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.76	0.46
1:B:304:GLU:OE2	1:B:329:LYS:HB2	2.15	0.46
1:C:167:ALA:O	1:C:171:LEU:HD22	2.16	0.46
1:C:210:LEU:O	1:C:211:LYS:HB2	2.16	0.46
1:D:26:THR:HG22	1:D:27:GLU:N	2.31	0.46
1:D:132:GLY:O	1:D:133:PHE:C	2.57	0.46
1:D:314:LEU:O	1:D:317:ILE:HD13	2.16	0.46
1:E:13:ASN:C	1:E:15:ASP:N	2.74	0.46
1:C:233:LEU:O	1:C:234:LEU:C	2.56	0.46
1:C:253:GLU:OE1	1:C:253:GLU:CA	2.64	0.46
1:D:11:GLU:OE2	1:D:22:LYS:HE3	2.15	0.46
1:D:125:ALA:O	1:D:128:TYR:HB2	2.15	0.46
1:D:160:THR:HB	3:D:4262:HOH:O	2.16	0.46
1:D:219:GLN:H	1:D:238:GLN:H	1.64	0.46
1:E:46:LYS:HG3	1:E:57:ILE:HD13	1.97	0.46
1:E:121:SER:OG	1:E:124:GLU:HG3	2.14	0.46
1:E:208:GLY:C	1:E:209:THR:HG1	2.23	0.46
1:D:8:LEU:HD21	1:D:19:VAL:HG13	1.97	0.45
1:D:233:LEU:C	1:D:233:LEU:CD2	2.89	0.45
1:D:326:VAL:HA	3:D:4296:HOH:O	2.17	0.45
1:C:8:LEU:HD23	1:C:8:LEU:C	2.41	0.45
1:F:307:LEU:C	1:F:307:LEU:HD22	2.40	0.45
1:A:41:SER:CB	1:A:126:MSE:HB3	2.45	0.45
1:C:206:TYR:HE1	1:C:209:THR:HA	1.82	0.45
1:E:147:LEU:CD2	1:E:219:GLN:OE1	2.64	0.45
1:C:207:ASP:CB	1:C:207:ASP:OD2	2.51	0.45
1:E:187:ALA:O	1:E:188:ALA:C	2.60	0.45
1:A:46:LYS:HG3	1:A:57:ILE:HD11	1.96	0.45
1:B:69:ALA:HB2	1:B:101:GLY:HA3	1.98	0.45
1:E:329:LYS:HE3	3:E:5315:HOH:O	2.16	0.45
1:D:9:GLN:HE21	1:D:62:PRO:C	2.25	0.45
1:E:109:PRO:HD2	1:E:112:TRP:CE3	2.52	0.45
1:F:48:GLY:HA3	1:F:317:ILE:CD1	2.47	0.45
1:B:102:LEU:CD2	1:B:328:VAL:HG21	2.47	0.45
1:C:181:SER:OG	1:C:205:VAL:CG2	2.65	0.45
1:C:187:ALA:O	1:C:188:ALA:C	2.60	0.45
1:D:98:ARG:NH1	1:D:98:ARG:CG	2.71	0.45
1:D:167:ALA:O	1:D:171:LEU:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASP:OD2	1:D:226:GLY:CA	2.65	0.45
1:D:298:LEU:H	1:D:298:LEU:HG	1.39	0.45
1:A:296:GLN:HB2	1:A:299:THR:HG21	1.90	0.45
1:A:296:GLN:CB	1:A:299:THR:CG2	2.84	0.45
1:A:317:ILE:N	1:A:317:ILE:HD12	2.32	0.45
1:B:274:VAL:HG12	1:B:275:TYR:CD2	2.52	0.45
1:C:45:TYR:CE2	1:C:49:LEU:HD21	2.52	0.45
1:C:165:GLY:HA3	1:C:300:ILE:HD11	1.98	0.45
1:D:168:VAL:O	1:D:169:SER:C	2.57	0.45
1:B:63:LEU:HD23	1:B:63:LEU:O	2.17	0.45
1:B:302:ASP:HB2	1:B:323:GLN:O	2.17	0.45
1:B:303:ARG:CB	1:B:303:ARG:CD	2.87	0.45
1:C:22:LYS:HB3	1:C:23:THR:H	1.37	0.45
1:E:8:LEU:HD22	1:E:310:THR:OG1	2.16	0.45
1:F:219:GLN:H	1:F:238:GLN:H	1.65	0.45
2:B:2255:NAD:H8A	1:E:239:TYR:HE2	1.82	0.45
1:E:83:GLU:CD	1:E:83:GLU:CB	2.79	0.45
1:F:109:PRO:HG2	1:F:112:TRP:CE3	2.52	0.45
1:A:261:PHE:HB3	1:D:270:GLY:CA	2.47	0.44
1:B:108:VAL:HG22	1:B:113:LEU:HD21	1.98	0.44
1:D:18:SER:O	1:D:19:VAL:CB	2.60	0.44
1:D:222:VAL:O	1:D:224:PRO:HD3	2.18	0.44
1:F:123:LYS:O	1:F:127:VAL:HG23	2.17	0.44
1:A:91:SER:HB3	1:A:274:VAL:O	2.17	0.44
1:B:101:GLY:C	1:B:103:SER:N	2.73	0.44
1:D:307:LEU:O	1:D:310:THR:CB	2.62	0.44
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.81	0.44
1:E:316:ASP:N	1:E:316:ASP:OD2	2.48	0.44
1:E:319:GLN:NE2	1:E:321:ARG:CD	2.66	0.44
1:B:90:THR:HB	3:B:2257:HOH:O	2.17	0.44
1:C:44:ASN:ND2	1:C:325:ARG:NH2	2.64	0.44
1:C:91:SER:HB3	1:C:274:VAL:HA	1.98	0.44
1:F:66:GLY:CA	1:F:101:GLY:H	2.25	0.44
1:B:93:GLU:O	1:B:94:LEU:C	2.59	0.44
1:C:25:SER:O	1:C:28:ASP:HB2	2.18	0.44
1:C:138:SER:OG	1:C:271:ILE:HD13	2.18	0.44
1:D:182:THR:HG22	1:D:183:GLY:N	2.32	0.44
1:F:66:GLY:HA3	1:F:100:GLY:HA3	1.99	0.44
1:B:128:TYR:CD1	1:B:288:MSE:HE2	2.53	0.44
1:E:16:ASP:C	1:E:17:VAL:HG23	2.43	0.44
1:E:102:LEU:CD2	1:E:328:VAL:HG21	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ILE:HD13	1:F:57:ILE:HA	1.82	0.44
1:C:218:TRP:O	1:C:238:GLN:HG2	2.17	0.44
1:E:266:VAL:HG23	1:E:267:SER:N	2.33	0.44
1:E:319:GLN:HE21	1:E:321:ARG:HD2	1.79	0.44
1:E:16:ASP:O	1:E:17:VAL:HG23	2.17	0.44
1:E:25:SER:O	1:E:26:THR:C	2.59	0.44
1:E:35:LEU:HD13	1:E:74:VAL:HG21	1.99	0.44
1:A:59:ARG:NE	1:A:59:ARG:CA	2.78	0.44
1:C:64:ILE:HG21	1:C:103:SER:HB2	1.99	0.44
1:C:123:LYS:HE3	1:C:304:GLU:OE1	2.17	0.44
1:C:166:ILE:O	1:C:169:SER:HB2	2.18	0.44
1:B:57:ILE:HG22	1:B:96:VAL:HG13	2.00	0.44
2:B:2255:NAD:H8A	1:E:239:TYR:CE2	2.53	0.44
1:C:216:GLN:NE2	1:C:238:GLN:HB3	2.32	0.44
1:C:311:PRO:O	1:C:312:GLY:C	2.60	0.44
1:A:41:SER:HB3	1:A:126:MSE:HB3	2.00	0.43
1:C:225:VAL:HG22	1:C:249:THR:HG21	2.00	0.43
1:E:124:GLU:O	1:E:125:ALA:C	2.60	0.43
1:F:52:LYS:HD3	1:F:315:LYS:HZ1	1.82	0.43
1:F:141:ARG:NE	2:F:6255:NAD:C2A	2.80	0.43
1:A:216:GLN:NE2	1:A:238:GLN:HA	2.34	0.43
1:B:296:GLN:O	1:B:297:LEU:CB	2.64	0.43
1:C:44:ASN:O	1:C:47:ASP:HB2	2.18	0.43
1:C:218:TRP:C	1:C:238:GLN:HG2	2.43	0.43
1:C:244:ALA:HB1	1:C:271:ILE:HD11	1.90	0.43
1:E:103:SER:C	1:E:330:LEU:HD22	2.42	0.43
1:F:166:ILE:HD12	1:F:166:ILE:HG23	1.58	0.43
1:A:40:TYR:CB	1:A:126:MSE:HG3	2.48	0.43
1:A:109:PRO:O	1:A:110:GLY:C	2.62	0.43
1:C:307:LEU:O	1:C:310:THR:HB	2.18	0.43
1:D:53:ALA:C	1:D:55:GLY:H	2.25	0.43
1:D:69:ALA:O	1:D:126:MSE:HE3	2.18	0.43
1:E:35:LEU:HD22	1:E:36:ILE:H	1.83	0.43
1:F:317:ILE:O	1:F:319:GLN:N	2.49	0.43
1:A:169:SER:HB3	1:A:294:PRO:CB	2.49	0.43
1:B:25:SER:O	1:B:28:ASP:HB2	2.18	0.43
1:B:219:GLN:N	1:B:238:GLN:HG3	2.33	0.43
1:B:219:GLN:O	1:B:241:GLY:HA3	2.18	0.43
1:C:223:ASP:HA	1:C:224:PRO:HD2	1.78	0.43
1:C:238:GLN:HG2	1:C:238:GLN:H	1.45	0.43
1:D:203:GLU:HA	1:D:206:TYR:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:TYR:CG	1:D:207:ASP:N	2.85	0.43
1:D:245:VAL:O	1:D:246:SER:CB	2.62	0.43
1:E:43:ILE:HD11	1:E:314:LEU:HG	2.00	0.43
1:E:102:LEU:HD21	1:E:328:VAL:HG21	1.99	0.43
1:F:145:ASN:ND2	1:F:269:LEU:HD11	2.33	0.43
1:A:37:LYS:HD2	1:A:105:TYR:CZ	2.53	0.43
1:B:45:TYR:C	1:B:47:ASP:N	2.76	0.43
1:B:124:GLU:O	1:B:125:ALA:C	2.60	0.43
1:B:303:ARG:CG	1:B:303:ARG:CA	2.82	0.43
1:E:66:GLY:HA3	1:E:101:GLY:N	2.32	0.43
1:C:81:PHE:CD1	1:C:81:PHE:N	2.87	0.43
1:C:93:GLU:O	1:C:94:LEU:C	2.59	0.43
1:C:135:ALA:O	1:C:138:SER:HB2	2.19	0.43
1:D:276:CYS:HA	1:D:277:PRO:HD3	1.87	0.43
1:E:16:ASP:O	1:E:17:VAL:CG2	2.66	0.43
1:F:74:VAL:O	1:F:75:SER:CB	2.55	0.43
1:B:27:GLU:OE2	1:B:27:GLU:C	2.62	0.43
1:B:224:PRO:O	1:B:247:GLY:HA3	2.18	0.43
1:F:126:MSE:O	1:F:127:VAL:C	2.60	0.43
1:A:147:LEU:HD13	1:A:176:TYR:CE2	2.54	0.43
1:A:166:ILE:O	1:A:167:ALA:C	2.62	0.43
1:B:248:LEU:CD1	1:B:248:LEU:H	2.32	0.43
1:C:5:PHE:HB2	1:C:104:GLU:HG3	2.00	0.43
1:C:66:GLY:CA	1:C:101:GLY:H	2.31	0.43
1:E:114:VAL:O	1:E:115:PRO:C	2.60	0.43
1:E:219:GLN:N	1:E:238:GLN:CG	2.81	0.43
1:A:166:ILE:CG1	1:A:300:ILE:HD13	2.38	0.43
1:A:261:PHE:CE1	1:D:268:LEU:HD23	2.53	0.43
1:B:78:ASP:HA	1:B:79:PRO:HD2	1.84	0.43
1:B:217:GLN:O	1:B:218:TRP:CD1	2.72	0.43
1:E:155:LEU:O	1:E:221:ALA:HA	2.18	0.43
1:E:258:VAL:HG13	1:E:262:ILE:HG12	2.00	0.43
1:B:36:ILE:O	1:B:36:ILE:HG22	2.18	0.43
1:B:45:TYR:CE1	1:B:318:LEU:CD2	3.01	0.43
1:F:78:ASP:OD1	1:F:78:ASP:C	2.61	0.43
1:B:164:GLY:O	1:B:165:GLY:C	2.62	0.42
1:B:225:VAL:HG12	1:B:249:THR:O	2.18	0.42
1:C:78:ASP:O	1:C:80:ARG:N	2.52	0.42
1:C:124:GLU:O	1:C:125:ALA:C	2.60	0.42
1:C:157:THR:CG2	1:C:225:VAL:HB	2.49	0.42
1:D:66:GLY:HA3	1:D:100:GLY:HA3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:VAL:HG22	1:D:309:GLU:CB	2.49	0.42
1:E:147:LEU:HD22	1:E:219:GLN:OE1	2.19	0.42
1:F:6:GLN:O	1:F:104:GLU:HG3	2.18	0.42
1:A:319:GLN:O	1:A:320:ASN:C	2.61	0.42
1:B:245:VAL:HG22	1:B:268:LEU:HD11	2.01	0.42
1:E:120:LEU:HD21	1:E:128:TYR:CE1	2.53	0.42
1:A:220:GLY:HA2	1:A:242:SER:O	2.19	0.42
1:A:287:ARG:NH2	1:A:291:ASP:OD1	2.52	0.42
1:B:167:ALA:O	1:B:171:LEU:HB2	2.20	0.42
1:C:124:GLU:HG2	1:C:297:LEU:HD13	2.01	0.42
1:C:172:ASN:OD1	1:C:195:GLY:HA2	2.20	0.42
1:B:37:LYS:HG3	3:B:2268:HOH:O	2.19	0.42
1:B:155:LEU:HD23	1:B:179:VAL:HG12	2.02	0.42
1:E:206:TYR:CE1	1:E:209:THR:HA	2.54	0.42
1:B:129:GLY:HA3	1:B:325:ARG:HH21	1.84	0.42
1:C:127:VAL:HG11	1:C:297:LEU:HD22	2.01	0.42
1:D:83:GLU:CD	1:D:83:GLU:H	2.27	0.42
1:E:93:GLU:HB2	1:E:112:TRP:HH2	1.84	0.42
1:F:183:GLY:HA2	3:F:6283:HOH:O	2.18	0.42
1:F:297:LEU:O	1:F:298:LEU:C	2.62	0.42
1:A:260:PRO:HA	1:A:264:ARG:HB2	2.00	0.42
1:B:147:LEU:HD13	1:B:176:TYR:CE2	2.53	0.42
1:C:103:SER:C	1:C:104:GLU:O	2.57	0.42
1:C:312:GLY:O	1:C:315:LYS:HB3	2.20	0.42
1:D:7:ALA:CB	1:D:103:SER:HB2	2.49	0.42
1:E:141:ARG:HH11	1:E:141:ARG:HD2	1.56	0.42
1:F:229:GLN:O	1:F:229:GLN:HG2	2.19	0.42
1:A:120:LEU:HA	1:A:120:LEU:HD23	1.91	0.42
1:B:262:ILE:O	1:E:272:ASP:HB2	2.19	0.42
1:C:13:ASN:HD22	1:C:13:ASN:C	2.26	0.42
1:C:36:ILE:HD12	1:C:108:VAL:HG13	2.02	0.42
1:C:317:ILE:HD13	1:C:317:ILE:HG21	1.60	0.42
1:D:153:SER:HB2	1:D:177:ASP:HB2	2.02	0.42
1:D:248:LEU:O	1:D:249:THR:C	2.60	0.42
1:B:126:MSE:O	1:B:127:VAL:C	2.60	0.42
1:B:208:GLY:O	1:B:209:THR:O	2.37	0.42
1:D:148:SER:HB3	1:D:151:LYS:CD	2.50	0.42
1:D:329:LYS:O	1:D:330:LEU:HG	2.19	0.42
1:E:221:ALA:HB3	1:E:243:VAL:HG13	2.02	0.42
1:F:314:LEU:HD23	1:F:314:LEU:HA	1.92	0.42
1:B:44:ASN:ND2	1:B:67:ILE:HD11	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:TYR:O	1:D:46:LYS:C	2.63	0.42
1:E:306:SER:OG	1:E:308:GLU:HB2	2.20	0.42
1:A:124:GLU:O	1:A:125:ALA:C	2.59	0.42
1:A:170:MSE:HG2	1:A:292:LEU:O	2.20	0.42
1:A:234:LEU:HA	1:A:237:ILE:HD12	2.02	0.42
1:B:114:VAL:HA	1:B:115:PRO:HD3	1.81	0.42
1:D:154:VAL:HB	3:D:4261:HOH:O	2.20	0.42
1:E:258:VAL:HG13	1:E:258:VAL:O	2.20	0.42
1:E:315:LYS:HD2	1:E:319:GLN:OE1	2.20	0.42
1:D:303:ARG:CG	1:D:304:GLU:N	2.80	0.41
1:F:7:ALA:HB1	1:F:64:ILE:HD13	2.02	0.41
1:C:36:ILE:CD1	1:C:108:VAL:HG13	2.50	0.41
1:C:319:GLN:O	1:C:321:ARG:N	2.53	0.41
1:A:257:THR:HB	1:A:259:TYR:CD2	2.54	0.41
1:B:258:VAL:HG11	1:E:248:LEU:HB3	2.02	0.41
1:D:26:THR:CG2	1:D:26:THR:CA	2.83	0.41
1:D:290:SER:OG	1:D:291:ASP:N	2.53	0.41
1:E:42:GLY:HA2	1:E:325:ARG:HH22	1.84	0.41
1:F:233:LEU:HD21	1:F:237:ILE:HD11	2.02	0.41
1:F:248:LEU:O	1:F:249:THR:C	2.58	0.41
1:F:287:ARG:NE	1:F:291:ASP:OD2	2.53	0.41
1:F:298:LEU:HD23	1:F:298:LEU:HA	1.92	0.41
1:A:59:ARG:HA	1:A:59:ARG:HE	1.81	0.41
1:B:41:SER:CB	1:B:328:VAL:H	2.29	0.41
1:C:14:ALA:HB1	3:C:3282:HOH:O	2.19	0.41
1:C:21:VAL:O	1:C:21:VAL:HG13	2.08	0.41
1:C:59:ARG:HB2	3:C:3292:HOH:O	2.19	0.41
1:C:78:ASP:O	1:C:79:PRO:C	2.63	0.41
1:C:109:PRO:HD2	1:C:112:TRP:CE3	2.56	0.41
1:D:281:ARG:HD3	3:D:4268:HOH:O	2.20	0.41
1:E:262:ILE:HD13	1:E:262:ILE:HG21	1.88	0.41
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.81	0.41
1:E:29:LEU:HD23	1:E:29:LEU:HA	1.75	0.41
1:E:286:GLU:O	1:E:287:ARG:C	2.62	0.41
1:F:126:MSE:C	1:F:128:TYR:N	2.73	0.41
1:F:258:VAL:O	1:F:261:PHE:HB2	2.20	0.41
1:F:305:VAL:HG23	1:F:309:GLU:CD	2.45	0.41
1:A:212:ALA:HB1	1:A:259:TYR:CD2	2.56	0.41
1:B:3:THR:CG2	1:B:3:THR:CA	2.87	0.41
1:C:262:ILE:HD13	1:C:262:ILE:HG21	1.80	0.41
1:D:26:THR:C	1:D:26:THR:HG22	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:THR:HB	1:D:184:ASN:H	1.86	0.41
1:C:114:VAL:HG21	1:C:285:TRP:CD1	2.56	0.41
1:C:193:GLN:HE21	1:C:193:GLN:C	2.29	0.41
1:E:322:ILE:HD13	1:E:322:ILE:HG21	1.89	0.41
1:F:233:LEU:C	1:F:233:LEU:HD22	2.46	0.41
1:A:287:ARG:HB3	1:A:292:LEU:CD1	2.50	0.41
1:B:187:ALA:O	1:B:188:ALA:C	2.59	0.41
1:C:98:ARG:HG3	1:C:99:ASP:N	2.35	0.41
1:C:116:LEU:O	1:C:117:PRO:C	2.62	0.41
1:D:109:PRO:HG2	1:D:112:TRP:CD2	2.56	0.41
1:A:152:GLY:CA	1:A:238:GLN:OE1	2.66	0.41
1:B:206:TYR:CD1	1:B:209:THR:HA	2.52	0.41
1:B:228:LYS:HA	1:B:255:PRO:HD2	2.02	0.41
1:C:8:LEU:O	1:C:64:ILE:HA	2.21	0.41
1:C:13:ASN:O	1:C:14:ALA:C	2.61	0.41
1:D:53:ALA:C	1:D:55:GLY:N	2.78	0.41
1:E:78:ASP:OD1	1:E:78:ASP:C	2.64	0.41
1:F:78:ASP:HA	1:F:79:PRO:HD3	1.94	0.41
1:F:78:ASP:OD2	1:F:80:ARG:NH2	2.50	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.76	0.41
1:B:34:VAL:O	1:B:36:ILE:HD12	2.21	0.41
1:B:151:LYS:HB2	1:B:219:GLN:OE1	2.20	0.41
1:C:70:ALA:HB1	1:C:122:LEU:HD23	2.02	0.41
1:C:111:ASP:OD1	1:C:111:ASP:N	2.53	0.41
1:A:63:LEU:HD23	1:A:63:LEU:O	2.21	0.40
1:B:168:VAL:HG13	1:B:178:VAL:HG11	2.02	0.40
1:C:66:GLY:HA3	1:C:101:GLY:N	2.34	0.40
1:C:181:SER:OG	1:C:205:VAL:HG21	2.21	0.40
1:D:171:LEU:HB3	1:D:178:VAL:CG2	2.51	0.40
1:E:149:PRO:HA	1:E:176:TYR:CD2	2.55	0.40
1:E:308:GLU:H	1:E:308:GLU:HG2	1.67	0.40
1:B:166:ILE:CG1	1:B:300:ILE:CD1	2.95	0.40
1:B:327:ILE:HD13	1:B:327:ILE:HG21	1.45	0.40
1:C:219:GLN:HA	1:C:238:GLN:CG	2.50	0.40
1:D:18:SER:HB2	1:D:20:HIS:NE2	2.35	0.40
1:E:148:SER:HA	1:E:149:PRO:HD3	1.71	0.40
1:E:310:THR:O	1:E:311:PRO:C	2.63	0.40
1:F:81:PHE:CZ	1:F:113:LEU:HB2	2.56	0.40
1:A:174:ARG:HD2	3:A:1263:HOH:O	2.21	0.40
1:B:12:LYS:HD3	1:B:14:ALA:O	2.22	0.40
1:B:29:LEU:O	1:B:30:PRO:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ARG:NE	1:B:291:ASP:OD2	2.45	0.40
1:E:25:SER:C	1:E:27:GLU:N	2.77	0.40
1:F:41:SER:HB2	1:F:328:VAL:O	2.22	0.40
1:A:8:LEU:HD11	1:A:19:VAL:CG1	2.51	0.40
1:A:69:ALA:HB2	1:A:101:GLY:HA3	2.03	0.40
1:A:102:LEU:CD2	1:A:328:VAL:HG21	2.51	0.40
1:A:262:ILE:O	1:D:272:ASP:HB2	2.21	0.40
1:B:67:ILE:HG22	1:B:94:LEU:O	2.21	0.40
1:E:136:ALA:HB2	1:E:170:MSE:HE1	2.04	0.40
1:F:7:ALA:HA	1:F:103:SER:HB2	2.04	0.40
1:A:90:THR:CG2	1:A:281:ARG:NH1	2.85	0.40
1:D:199:VAL:C	1:D:200:ILE:CG2	2.95	0.40
1:E:319:GLN:HG2	3:E:5309:HOH:O	2.21	0.40
1:F:108:VAL:HG23	1:F:109:PRO:HD2	2.03	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	327/330 (99%)	268 (82%)	38 (12%)	21 (6%)	1	3
1	B	327/330 (99%)	264 (81%)	37 (11%)	26 (8%)	1	1
1	C	327/330 (99%)	251 (77%)	43 (13%)	33 (10%)	0	1
1	D	327/330 (99%)	257 (79%)	43 (13%)	27 (8%)	0	1
1	E	327/330 (99%)	274 (84%)	37 (11%)	16 (5%)	1	6
1	F	327/330 (99%)	269 (82%)	41 (12%)	17 (5%)	1	5
All	All	1962/1980 (99%)	1583 (81%)	239 (12%)	140 (7%)	1	2

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	A	41	SER
1	A	62	PRO
1	A	105	TYR
1	A	159	ALA
1	A	185	ARG
1	A	186	GLU
1	A	219	GLN
1	A	258	VAL
1	A	317	ILE
1	A	318	LEU
1	B	3	THR
1	B	14	ALA
1	B	22	LYS
1	B	41	SER
1	B	59	ARG
1	B	67	ILE
1	B	75	SER
1	B	105	TYR
1	B	185	ARG
1	B	186	GLU
1	B	227	GLY
1	B	279	ASP
1	B	291	ASP
1	B	296	GLN
1	B	318	LEU
1	B	319	GLN
1	C	21	VAL
1	C	22	LYS
1	C	103	SER
1	C	186	GLU
1	C	208	GLY
1	C	209	THR
1	C	291	ASP
1	C	297	LEU
1	C	303	ARG
1	C	309	GLU
1	C	317	ILE
1	C	320	ASN
1	D	62	PRO
1	D	129	GLY
1	D	207	ASP
1	D	208	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	219	GLN
1	D	279	ASP
1	D	291	ASP
1	D	297	LEU
1	D	302	ASP
1	D	318	LEU
1	D	320	ASN
1	E	14	ALA
1	E	150	GLU
1	E	208	GLY
1	E	219	GLN
1	E	296	GLN
1	F	32	ASP
1	F	105	TYR
1	F	209	THR
1	F	219	GLN
1	F	291	ASP
1	F	296	GLN
1	F	320	ASN
1	A	17	VAL
1	A	187	ALA
1	A	188	ALA
1	A	226	GLY
1	B	17	VAL
1	B	208	GLY
1	B	219	GLN
1	B	320	ASN
1	C	53	ALA
1	C	54	GLY
1	C	312	GLY
1	C	314	LEU
1	D	150	GLU
1	D	159	ALA
1	D	245	VAL
1	E	41	SER
1	F	19	VAL
1	F	250	GLY
1	A	27	GLU
1	A	53	ALA
1	A	279	ASP
1	A	291	ASP
1	B	321	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	26	THR
1	C	75	SER
1	C	91	SER
1	C	105	TYR
1	C	160	THR
1	C	226	GLY
1	C	290	SER
1	D	13	ASN
1	D	19	VAL
1	D	56	ASN
1	D	185	ARG
1	D	285	TRP
1	E	111	ASP
1	E	160	THR
1	F	228	LYS
1	F	297	LEU
1	C	17	VAL
1	C	18	SER
1	C	101	GLY
1	C	188	ALA
1	D	14	ALA
1	D	290	SER
1	E	91	SER
1	E	297	LEU
1	F	204	ASP
1	A	19	VAL
1	B	19	VAL
1	B	61	TYR
1	C	62	PRO
1	C	187	ALA
1	D	17	VAL
1	D	75	SER
1	D	105	TYR
1	D	324	GLY
1	E	17	VAL
1	E	207	ASP
1	E	209	THR
1	F	75	SER
1	C	61	TYR
1	E	105	TYR
1	F	149	PRO
1	F	227	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	21	VAL
1	D	43	ILE
1	D	67	ILE
1	E	19	VAL
1	F	317	ILE
1	A	67	ILE
1	B	54	GLY
1	B	149	PRO
1	C	19	VAL
1	C	305	VAL
1	C	67	ILE
1	E	317	ILE
1	F	30	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	259/258 (100%)	201 (78%)	58 (22%)	1	3
1	B	257/258 (100%)	199 (77%)	58 (23%)	1	3
1	C	255/258 (99%)	200 (78%)	55 (22%)	1	3
1	D	259/258 (100%)	200 (77%)	59 (23%)	1	3
1	E	260/258 (101%)	196 (75%)	64 (25%)	1	2
1	F	261/258 (101%)	209 (80%)	52 (20%)	1	5
All	All	1551/1548 (100%)	1205 (78%)	346 (22%)	1	3

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	8	LEU
1	A	12	LYS
1	A	13	ASN
1	A	25	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	LEU
1	A	41	SER
1	A	43	ILE
1	A	59	ARG
1	A	63	LEU
1	A	65	LEU
1	A	67	ILE
1	A	78	ASP
1	A	80	ARG
1	A	90	THR
1	A	103	SER
1	A	108	VAL
1	A	114	VAL
1	A	124	GLU
1	A	147	LEU
1	A	150	GLU
1	A	151	LYS
1	A	155	LEU
1	A	160	THR
1	A	171	LEU
1	A	178	VAL
1	A	185	ARG
1	A	198	GLU
1	A	215	LYS
1	A	217	GLN
1	A	228	LYS
1	A	230	LEU
1	A	233	LEU
1	A	237	ILE
1	A	245	VAL
1	A	248	LEU
1	A	249	THR
1	A	253	GLU
1	A	258	VAL
1	A	266	VAL
1	A	271	ILE
1	A	272	ASP
1	A	276	CYS
1	A	280	VAL
1	A	286	GLU
1	A	296	GLN
1	A	297	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	298	LEU
1	A	299	THR
1	A	303	ARG
1	A	305	VAL
1	A	307	LEU
1	A	310	THR
1	A	315	LYS
1	A	317	ILE
1	A	322	ILE
1	A	323	GLN
1	A	325	ARG
1	B	3	THR
1	B	4	LEU
1	B	8	LEU
1	B	18	SER
1	B	19	VAL
1	B	21	VAL
1	B	24	ILE
1	B	27	GLU
1	B	35	LEU
1	B	36	ILE
1	B	43	ILE
1	B	46	LYS
1	B	60	GLU
1	B	61	TYR
1	B	63	LEU
1	B	64	ILE
1	B	65	LEU
1	B	67	ILE
1	B	74	VAL
1	B	75	SER
1	B	83	GLU
1	B	90	THR
1	B	103	SER
1	B	108	VAL
1	B	111	ASP
1	B	114	VAL
1	B	147	LEU
1	B	155	LEU
1	B	160	THR
1	B	171	LEU
1	B	181	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	THR
1	B	185	ARG
1	B	186	GLU
1	B	193	GLN
1	B	211	LYS
1	B	215	LYS
1	B	225	VAL
1	B	230	LEU
1	B	233	LEU
1	B	242	SER
1	B	245	VAL
1	B	248	LEU
1	B	266	VAL
1	B	269	LEU
1	B	271	ILE
1	B	276	CYS
1	B	279	ASP
1	B	286	GLU
1	B	297	LEU
1	B	304	GLU
1	B	305	VAL
1	B	306	SER
1	B	307	LEU
1	B	308	GLU
1	B	319	GLN
1	B	325	ARG
1	B	327	ILE
1	C	2	SER
1	C	3	THR
1	C	13	ASN
1	C	16	ASP
1	C	17	VAL
1	C	18	SER
1	C	19	VAL
1	C	21	VAL
1	C	27	GLU
1	C	35	LEU
1	C	43	ILE
1	C	57	ILE
1	C	59	ARG
1	C	60	GLU
1	C	67	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	76	SER
1	C	83	GLU
1	C	93	GLU
1	C	96	VAL
1	C	97	SER
1	C	98	ARG
1	C	108	VAL
1	C	114	VAL
1	C	118	GLN
1	C	147	LEU
1	C	150	GLU
1	C	151	LYS
1	C	157	THR
1	C	160	THR
1	C	171	LEU
1	C	172	ASN
1	C	182	THR
1	C	193	GLN
1	C	199	VAL
1	C	211	LYS
1	C	233	LEU
1	C	236	LYS
1	C	238	GLN
1	C	245	VAL
1	C	246	SER
1	C	258	VAL
1	C	266	VAL
1	C	272	ASP
1	C	297	LEU
1	C	298	LEU
1	C	305	VAL
1	C	306	SER
1	C	307	LEU
1	C	309	GLU
1	C	310	THR
1	C	314	LEU
1	C	319	GLN
1	C	323	GLN
1	C	325	ARG
1	C	330	LEU
1	D	4	LEU
1	D	11	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	13	ASN
1	D	15	ASP
1	D	20	HIS
1	D	22	LYS
1	D	24	ILE
1	D	26	THR
1	D	31	LYS
1	D	36	ILE
1	D	41	SER
1	D	45	TYR
1	D	60	GLU
1	D	64	ILE
1	D	67	ILE
1	D	75	SER
1	D	76	SER
1	D	83	GLU
1	D	90	THR
1	D	98	ARG
1	D	103	SER
1	D	114	VAL
1	D	116	LEU
1	D	123	LYS
1	D	147	LEU
1	D	150	GLU
1	D	151	LYS
1	D	155	LEU
1	D	160	THR
1	D	171	LEU
1	D	181	SER
1	D	182	THR
1	D	185	ARG
1	D	186	GLU
1	D	197	SER
1	D	207	ASP
1	D	211	LYS
1	D	219	GLN
1	D	225	VAL
1	D	228	LYS
1	D	229	GLN
1	D	234	LEU
1	D	245	VAL
1	D	249	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	266	VAL
1	D	272	ASP
1	D	293	LYS
1	D	295	ASP
1	D	296	GLN
1	D	297	LEU
1	D	298	LEU
1	D	300	ILE
1	D	305	VAL
1	D	307	LEU
1	D	308	GLU
1	D	315	LYS
1	D	317	ILE
1	D	327	ILE
1	D	330	LEU
1	E	3	THR
1	E	4	LEU
1	E	9	GLN
1	E	13	ASN
1	E	16	ASP
1	E	17	VAL
1	E	18	SER
1	E	20	HIS
1	E	22	LYS
1	E	24	ILE
1	E	28	ASP
1	E	35	LEU
1	E	37	LYS
1	E	41	SER
1	E	43	ILE
1	E	52	LYS
1	E	59	ARG
1	E	63	LEU
1	E	65	LEU
1	E	67	ILE
1	E	72	THR
1	E	74	VAL
1	E	78	ASP
1	E	80	ARG
1	E	83	GLU
1	E	90	THR
1	E	91	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	108	VAL
1	E	114	VAL
1	E	120	LEU
1	E	147	LEU
1	E	150	GLU
1	E	155	LEU
1	E	166	ILE
1	E	171	LEU
1	E	181	SER
1	E	182	THR
1	E	185	ARG
1	E	193	GLN
1	E	211	LYS
1	E	215	LYS
1	E	219	GLN
1	E	233	LEU
1	E	238	GLN
1	E	242	SER
1	E	245	VAL
1	E	248	LEU
1	E	249	THR
1	E	258	VAL
1	E	266	VAL
1	E	286	GLU
1	E	291	ASP
1	E	292	LEU
1	E	297	LEU
1	E	299	THR
1	E	303	ARG
1	E	305	VAL
1	E	307	LEU
1	E	315	LYS
1	E	317	ILE
1	E	318	LEU
1	E	320	ASN
1	E	325	ARG
1	E	330	LEU
1	F	2	SER
1	F	8	LEU
1	F	12	LYS
1	F	13	ASN
1	F	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	22	LYS
1	F	23	THR
1	F	24	ILE
1	F	25	SER
1	F	31	LYS
1	F	41	SER
1	F	60	GLU
1	F	67	ILE
1	F	74	VAL
1	F	90	THR
1	F	108	VAL
1	F	114	VAL
1	F	118	GLN
1	F	123	LYS
1	F	147	LEU
1	F	155	LEU
1	F	156	VAL
1	F	160	THR
1	F	171	LEU
1	F	181	SER
1	F	182	THR
1	F	185	ARG
1	F	210	LEU
1	F	211	LYS
1	F	217	GLN
1	F	233	LEU
1	F	236	LYS
1	F	237	ILE
1	F	245	VAL
1	F	246	SER
1	F	248	LEU
1	F	255	PRO
1	F	266	VAL
1	F	272	ASP
1	F	297	LEU
1	F	300	ILE
1	F	307	LEU
1	F	310	THR
1	F	315	LYS
1	F	317	ILE
1	F	318	LEU
1	F	319	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	321	ARG
1	F	322	ILE
1	F	323	GLN
1	F	325	ARG
1	F	327	ILE

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	13	ASN
1	A	216	GLN
1	A	229	GLN
1	A	323	GLN
1	B	13	ASN
1	B	44	ASN
1	B	193	GLN
1	B	216	GLN
1	B	229	GLN
1	B	238	GLN
1	B	320	ASN
1	C	44	ASN
1	C	56	ASN
1	C	193	GLN
1	C	216	GLN
1	C	238	GLN
1	C	323	GLN
1	D	6	GLN
1	D	9	GLN
1	D	119	ASN
1	D	172	ASN
1	E	6	GLN
1	E	13	ASN
1	E	216	GLN
1	E	229	GLN
1	E	238	GLN
1	E	296	GLN
1	E	319	GLN
1	F	6	GLN
1	F	119	ASN
1	F	184	ASN
1	F	216	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	229	GLN
1	F	238	GLN
1	F	323	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
2	NAD	C	3255	-	12,12,48	3.13	7 (58%)	17,17,73	3.08	10 (58%)
2	NAD	B	2255	-	12,12,48	2.43	4 (33%)	17,17,73	3.28	9 (52%)
2	NAD	A	1255	-	12,12,48	2.06	5 (41%)	17,17,73	4.09	13 (76%)
2	NAD	D	4255	-	12,12,48	2.53	5 (41%)	17,17,73	3.28	8 (47%)
2	NAD	E	5255	-	12,12,48	5.56	7 (58%)	17,17,73	5.91	13 (76%)
2	NAD	F	6255	-	12,12,48	3.09	7 (58%)	17,17,73	2.82	7 (41%)

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
2	NAD	C	3255	-	-	-	0/2/2/5
2	NAD	B	2255	-	-	-	0/2/2/5
2	NAD	A	1255	-	-	-	0/2/2/5
2	NAD	D	4255	-	-	-	0/2/2/5
2	NAD	E	5255	-	-	-	0/2/2/5
2	NAD	F	6255	-	-	-	0/2/2/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5255	NAD	C4A-N9A	12.95	1.58	1.37
2	E	5255	NAD	C2A-N3A	8.69	1.49	1.33
2	E	5255	NAD	C8A-N9A	6.52	1.50	1.36
2	B	2255	NAD	C4A-N9A	5.75	1.46	1.37
2	E	5255	NAD	C8A-N7A	5.56	1.42	1.31
2	F	6255	NAD	C8A-N7A	5.45	1.42	1.31
2	D	4255	NAD	C8A-N9A	5.26	1.47	1.36
2	C	3255	NAD	C2A-N3A	5.22	1.43	1.33
2	C	3255	NAD	C8A-N9A	4.88	1.47	1.36
2	F	6255	NAD	C2A-N1A	4.84	1.42	1.33
2	E	5255	NAD	C6A-N1A	4.82	1.49	1.35
2	C	3255	NAD	C2A-N1A	4.46	1.41	1.33
2	F	6255	NAD	C8A-N9A	4.29	1.45	1.36
2	D	4255	NAD	C8A-N7A	4.25	1.39	1.31
2	F	6255	NAD	C2A-N3A	4.13	1.41	1.33
2	C	3255	NAD	C8A-N7A	4.01	1.39	1.31
2	E	5255	NAD	C2A-N1A	3.80	1.40	1.33
2	B	2255	NAD	C8A-N7A	3.58	1.38	1.31
2	D	4255	NAD	C2A-N1A	3.43	1.40	1.33
2	C	3255	NAD	C5A-C4A	3.31	1.45	1.39
2	F	6255	NAD	C4A-N3A	3.21	1.40	1.34
2	A	1255	NAD	C6A-N1A	3.11	1.44	1.35
2	A	1255	NAD	C2A-N3A	3.10	1.39	1.33
2	E	5255	NAD	C4A-N3A	3.09	1.40	1.34
2	D	4255	NAD	C6A-N6A	-3.00	1.26	1.34
2	A	1255	NAD	C5A-N7A	-2.90	1.33	1.39
2	B	2255	NAD	C8A-N9A	2.79	1.42	1.36
2	F	6255	NAD	C6A-N1A	2.74	1.43	1.35
2	C	3255	NAD	C4A-N9A	2.68	1.41	1.37
2	A	1255	NAD	C2A-N1A	2.65	1.38	1.33
2	B	2255	NAD	C6A-N6A	-2.61	1.27	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3255	NAD	C5A-N7A	-2.61	1.34	1.39
2	D	4255	NAD	C2A-N3A	2.49	1.38	1.33
2	A	1255	NAD	C8A-N9A	2.49	1.41	1.36
2	F	6255	NAD	C5A-C4A	2.38	1.43	1.39

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5255	NAD	C5A-C4A-N3A	-12.64	109.32	126.72
2	E	5255	NAD	C5A-N7A-C8A	8.56	116.90	103.45
2	E	5255	NAD	N9A-C8A-N7A	-8.34	102.56	114.27
2	B	2255	NAD	C5A-C4A-N3A	-8.24	115.37	126.72
2	D	4255	NAD	N3A-C2A-N1A	-8.10	116.31	128.58
2	E	5255	NAD	C2A-N3A-C4A	7.88	131.08	111.83
2	D	4255	NAD	N9A-C8A-N7A	-7.26	104.08	114.27
2	E	5255	NAD	C5A-C6A-N6A	-7.21	105.43	123.29
2	F	6255	NAD	N3A-C2A-N1A	-6.94	118.08	128.58
2	C	3255	NAD	C5A-C4A-N3A	-6.85	117.29	126.72
2	E	5255	NAD	C2A-N1A-C6A	-6.56	107.95	118.73
2	A	1255	NAD	C5A-C4A-N3A	-6.29	118.05	126.72
2	E	5255	NAD	N3A-C4A-N9A	6.18	142.58	127.01
2	A	1255	NAD	C5A-C6A-N6A	-6.04	108.33	123.29
2	E	5255	NAD	N3A-C2A-N1A	-5.47	120.31	128.58
2	A	1255	NAD	N9A-C8A-N7A	5.45	121.93	114.27
2	A	1255	NAD	C6A-C5A-N7A	-5.09	122.28	132.09
2	A	1255	NAD	C4A-C5A-N7A	5.05	116.35	110.58
2	A	1255	NAD	N6A-C6A-N1A	4.99	129.49	118.38
2	F	6255	NAD	N9A-C8A-N7A	-4.97	107.28	114.27
2	C	3255	NAD	C1B-N9A-C8A	4.90	135.21	126.89
2	A	1255	NAD	C1B-N9A-C8A	4.57	134.65	126.89
2	B	2255	NAD	C5A-C6A-N6A	-4.50	112.15	123.29
2	E	5255	NAD	C5A-C6A-N1A	4.49	128.91	117.51
2	F	6255	NAD	C5A-C6A-N6A	-4.33	112.57	123.29
2	A	1255	NAD	C5A-N7A-C8A	-4.31	96.67	103.45
2	B	2255	NAD	C1B-N9A-C8A	4.27	134.14	126.89
2	D	4255	NAD	C2A-N3A-C4A	4.05	121.73	111.83
2	C	3255	NAD	C2A-N1A-C6A	-4.03	112.12	118.73
2	F	6255	NAD	N6A-C6A-N1A	4.00	127.29	118.38
2	B	2255	NAD	C2A-N1A-C6A	-4.00	112.17	118.73
2	A	1255	NAD	C2A-N3A-C4A	3.89	121.33	111.83
2	E	5255	NAD	C6A-C5A-C4A	3.81	122.38	117.18
2	B	2255	NAD	C2A-N3A-C4A	3.77	121.03	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3255	NAD	C6A-C5A-C4A	3.71	122.25	117.18
2	B	2255	NAD	N3A-C4A-N9A	3.68	136.26	127.01
2	A	1255	NAD	N3A-C2A-N1A	-3.65	123.06	128.58
2	D	4255	NAD	C5A-N7A-C8A	3.61	109.13	103.45
2	C	3255	NAD	C4A-N9A-C8A	-3.59	96.74	105.95
2	E	5255	NAD	C4A-C5A-N7A	-3.41	106.68	110.58
2	E	5255	NAD	N6A-C6A-N1A	3.24	125.59	118.38
2	A	1255	NAD	N3A-C4A-N9A	3.22	135.11	127.01
2	A	1255	NAD	C6A-C5A-C4A	3.07	121.36	117.18
2	B	2255	NAD	C5A-C6A-N1A	3.04	125.22	117.51
2	C	3255	NAD	C6A-C5A-N7A	-3.04	126.23	132.09
2	C	3255	NAD	N9A-C8A-N7A	3.04	118.53	114.27
2	A	1255	NAD	C4A-N9A-C8A	-3.03	98.18	105.95
2	D	4255	NAD	C5A-C6A-N6A	-2.82	116.32	123.29
2	C	3255	NAD	C5A-C6A-N6A	-2.74	116.51	123.29
2	C	3255	NAD	C2A-N3A-C4A	2.55	118.06	111.83
2	D	4255	NAD	C5A-C4A-N3A	-2.46	123.32	126.72
2	E	5255	NAD	C1B-N9A-C8A	2.43	131.01	126.89
2	D	4255	NAD	C5A-C6A-N1A	2.38	123.56	117.51
2	F	6255	NAD	C2A-N3A-C4A	2.38	117.64	111.83
2	F	6255	NAD	C2A-N1A-C6A	2.36	122.61	118.73
2	B	2255	NAD	C4A-N9A-C8A	-2.27	100.12	105.95
2	F	6255	NAD	C1B-N9A-C4A	-2.26	122.45	126.28
2	C	3255	NAD	C5A-C6A-N1A	2.24	123.19	117.51
2	D	4255	NAD	C1B-N9A-C4A	-2.15	122.64	126.28
2	B	2255	NAD	C6A-C5A-C4A	2.07	120.00	117.18

There are no chirality outliers.

There are no torsion outliers.

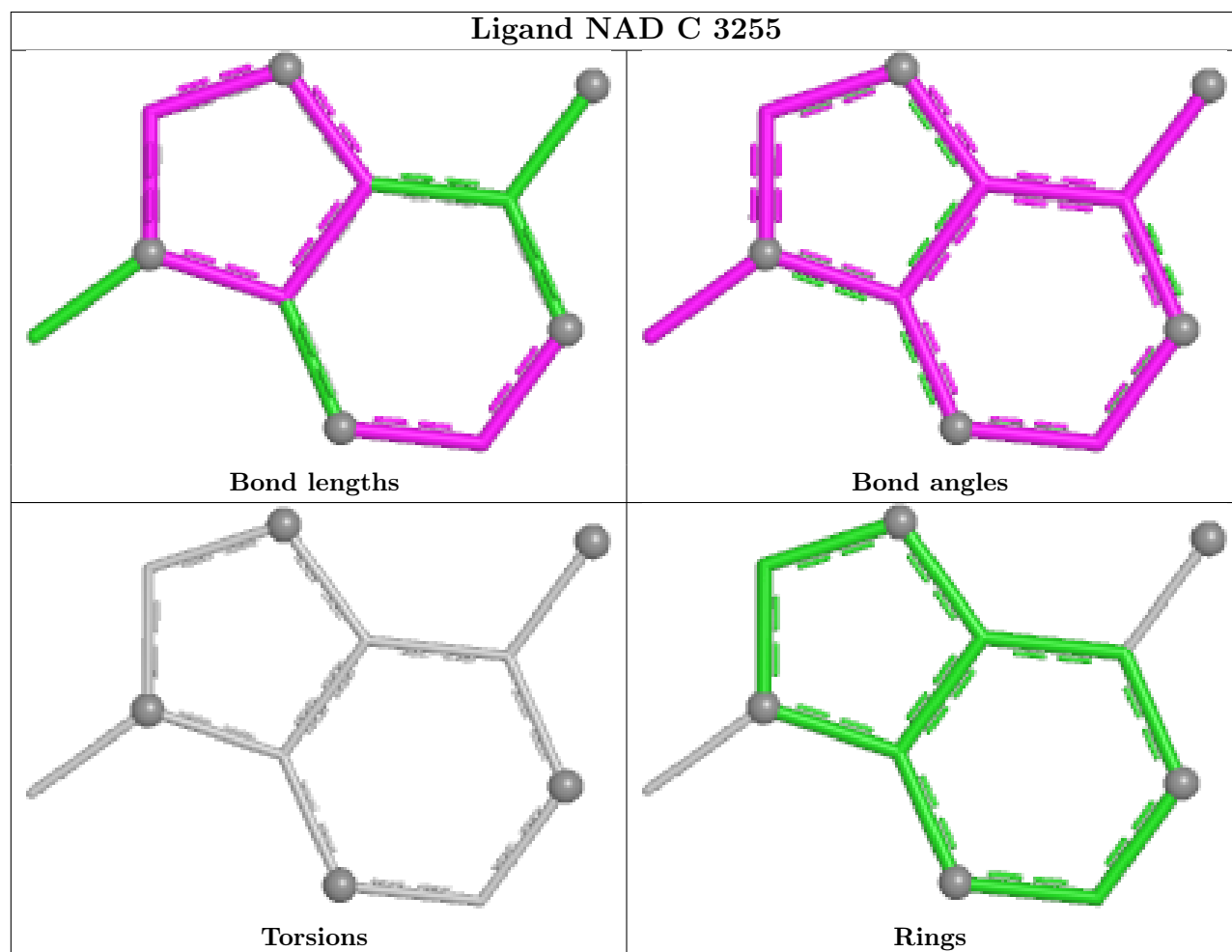
There are no ring outliers.

4 monomers are involved in 19 short contacts:

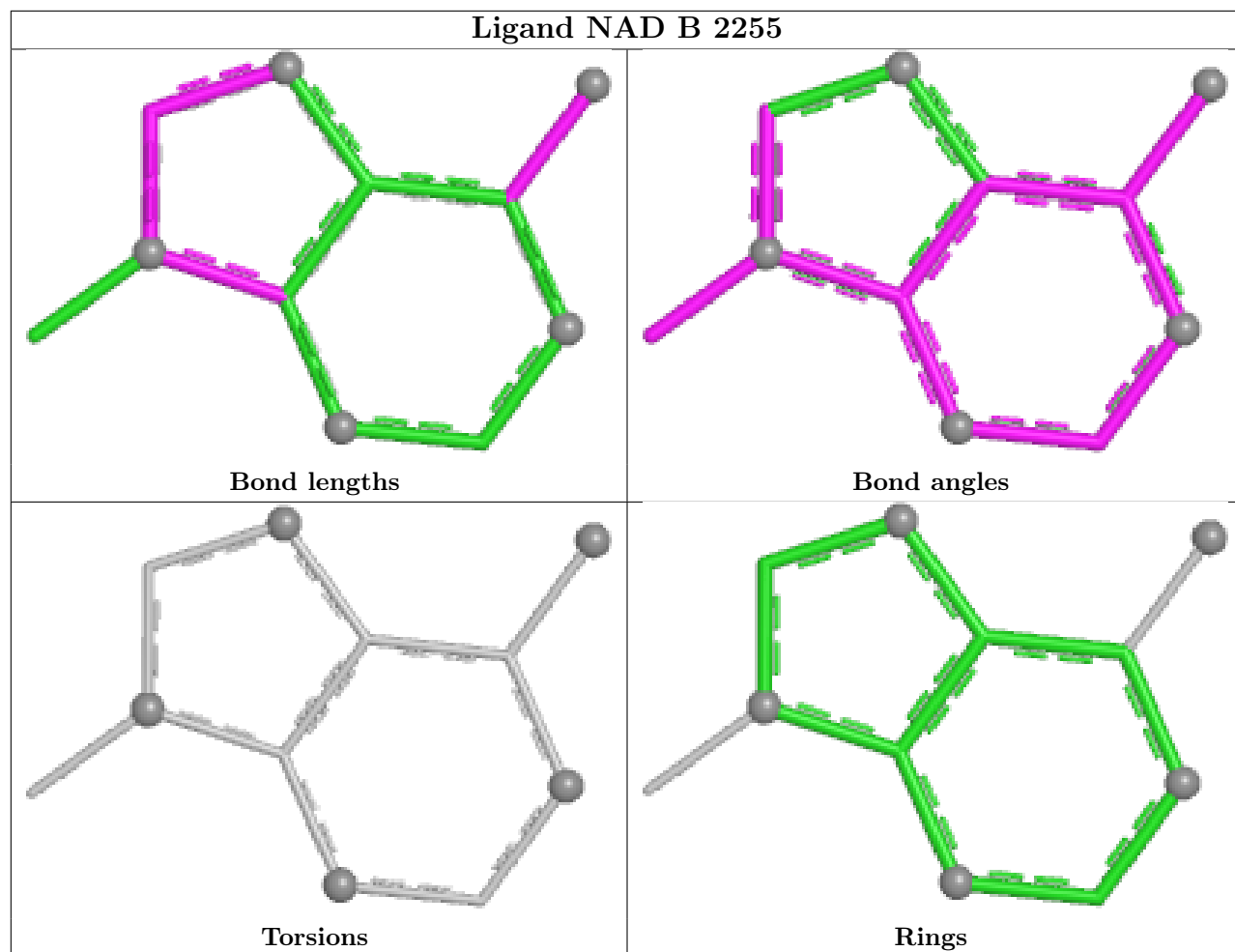
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3255	NAD	4	0
2	B	2255	NAD	5	0
2	A	1255	NAD	5	0
2	F	6255	NAD	5	0

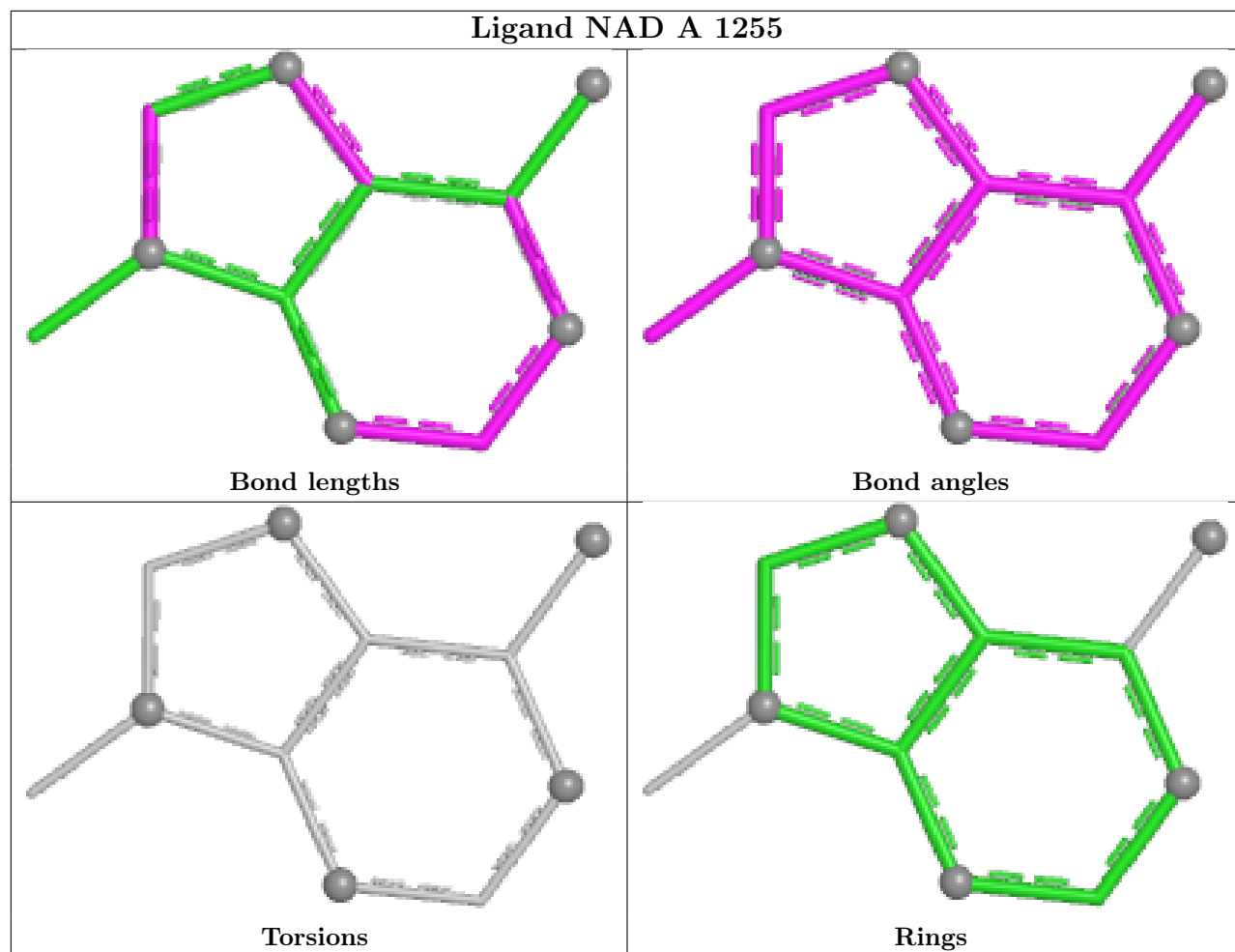
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

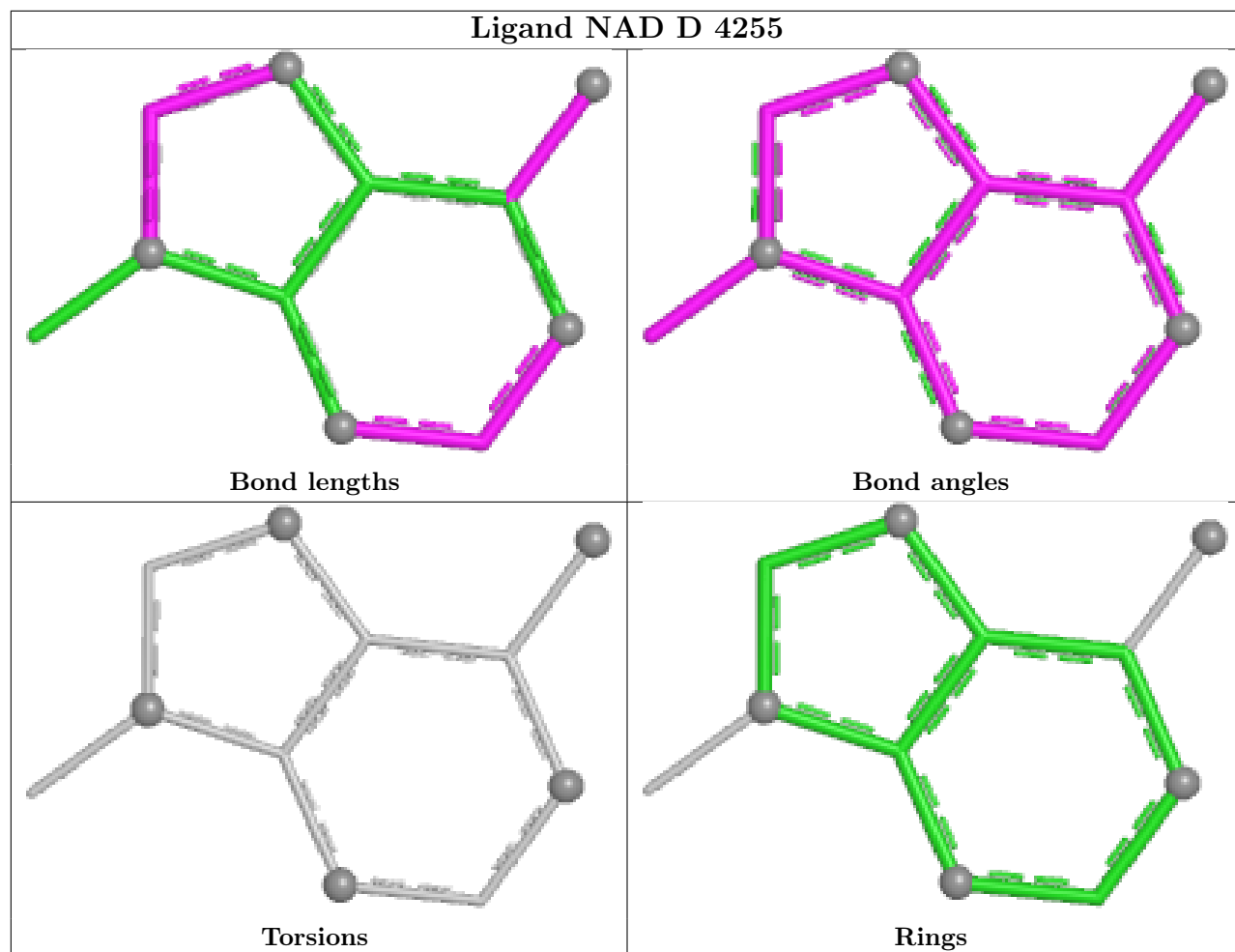


Ligand NAD B 2255

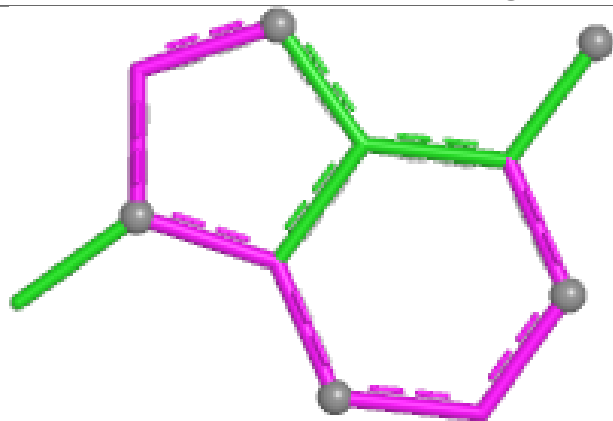




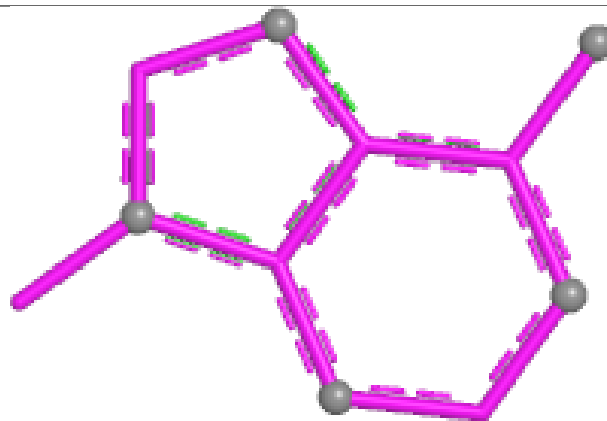
Ligand NAD D 4255



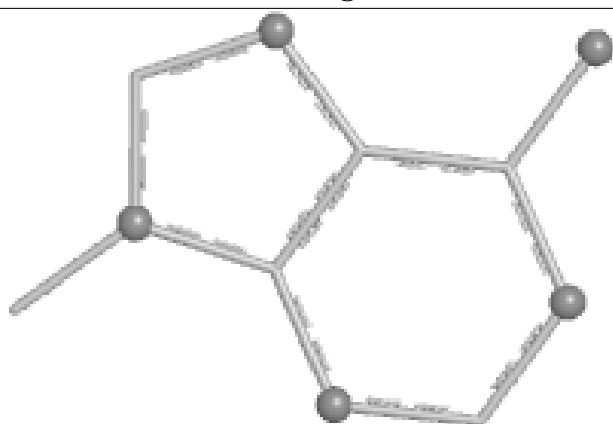
Ligand NAD E 5255



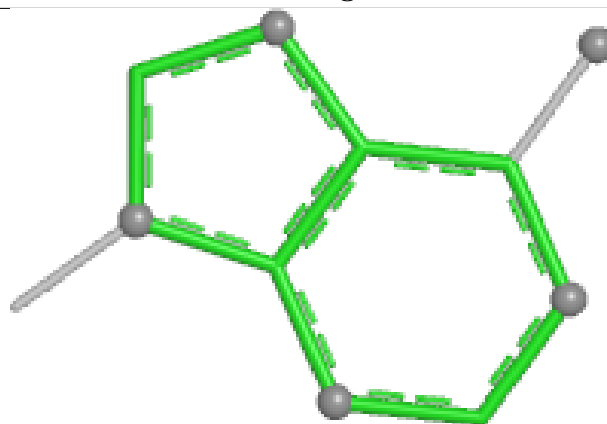
Bond lengths



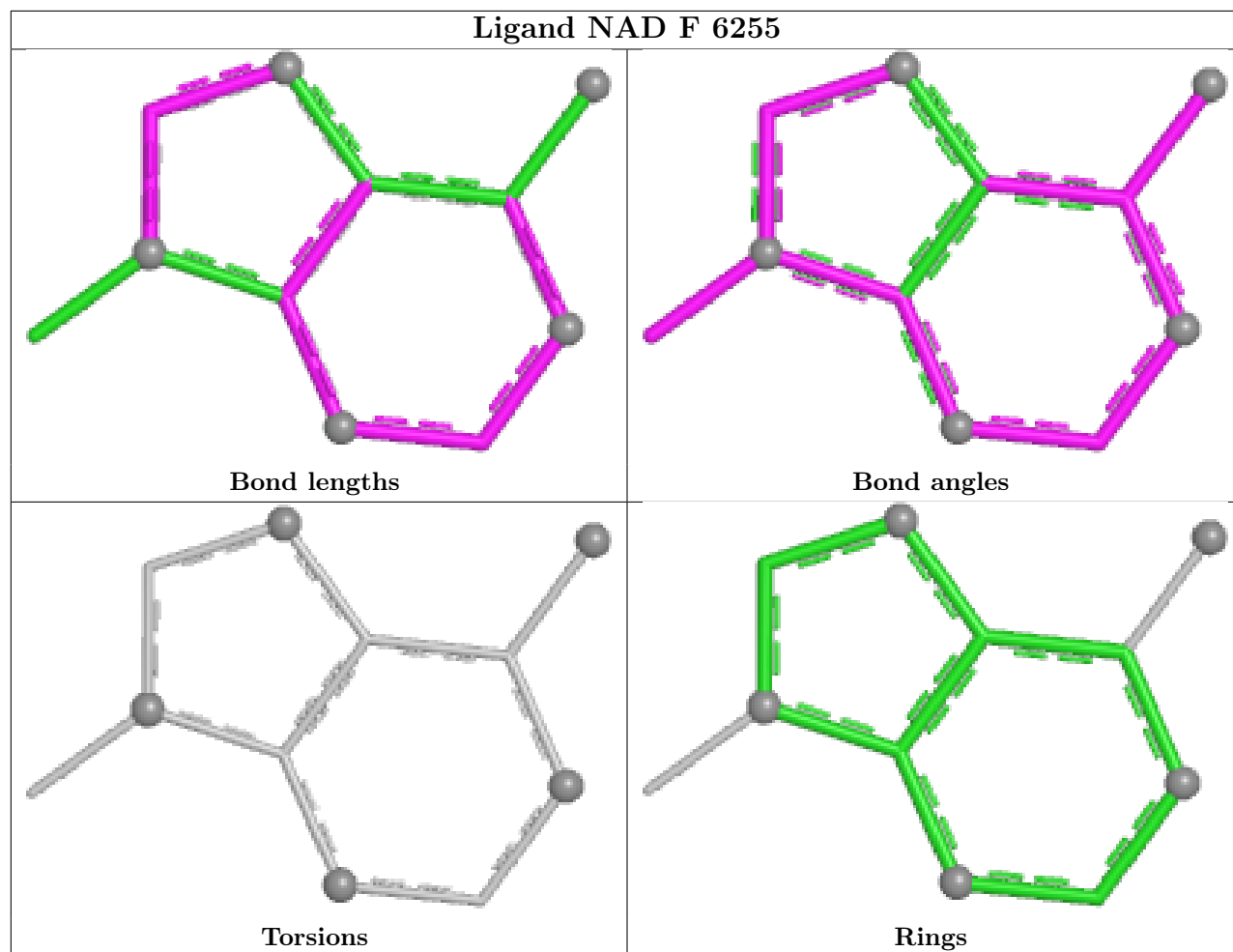
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	325/330 (98%)	-0.00	10 (3%)	51	41	18, 18, 18, 18	0
1	B	325/330 (98%)	0.08	11 (3%)	48	39	18, 18, 18, 18	0
1	C	325/330 (98%)	0.23	17 (5%)	33	25	18, 18, 18, 18	0
1	D	325/330 (98%)	0.09	13 (4%)	42	33	18, 18, 18, 18	0
1	E	325/330 (98%)	-0.05	6 (1%)	67	58	18, 18, 18, 18	0
1	F	325/330 (98%)	0.04	10 (3%)	51	41	18, 18, 18, 18	0
All	All	1950/1980 (98%)	0.06	67 (3%)	48	39	18, 18, 18, 18	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	13	ASN	5.2
1	E	16	ASP	4.7
1	F	209	THR	4.3
1	C	16	ASP	3.8
1	E	13	ASN	3.8
1	D	16	ASP	3.7
1	B	207	ASP	3.6
1	C	14	ALA	3.6
1	B	16	ASP	3.5
1	D	324	GLY	3.3
1	B	13	ASN	3.2
1	D	13	ASN	3.2
1	C	18	SER	3.2
1	F	13	ASN	3.1
1	A	15	ASP	3.1
1	C	2	SER	3.0
1	C	53	ALA	3.0
1	C	60	GLU	2.9
1	B	186	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	2.8
1	F	11	GLU	2.8
1	E	15	ASP	2.8
1	C	15	ASP	2.7
1	B	320	ASN	2.7
1	D	320	ASN	2.7
1	E	209	THR	2.7
1	D	321	ARG	2.7
1	E	185	ARG	2.7
1	B	3	THR	2.7
1	A	16	ASP	2.6
1	A	308	GLU	2.6
1	B	60	GLU	2.6
1	B	59	ARG	2.5
1	A	184	ASN	2.5
1	A	62	PRO	2.5
1	C	11	GLU	2.5
1	F	186	GLU	2.5
1	F	28	ASP	2.4
1	F	319	GLN	2.4
1	A	13	ASN	2.4
1	F	321	ARG	2.4
1	D	44	ASN	2.3
1	F	208	GLY	2.3
1	D	185	ARG	2.3
1	F	185	ARG	2.3
1	E	42	GLY	2.3
1	C	321	ARG	2.3
1	C	320	ASN	2.3
1	C	27	GLU	2.3
1	D	319	GLN	2.3
1	A	59	ARG	2.2
1	B	20	HIS	2.2
1	D	75	SER	2.2
1	C	208	GLY	2.2
1	A	14	ALA	2.2
1	F	30	PRO	2.2
1	B	319	GLN	2.1
1	D	42	GLY	2.1
1	B	14	ALA	2.1
1	C	189	ASP	2.1
1	C	12	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	62	PRO	2.1
1	C	42	GLY	2.1
1	D	14	ALA	2.1
1	C	207	ASP	2.0
1	D	207	ASP	2.0
1	A	20	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

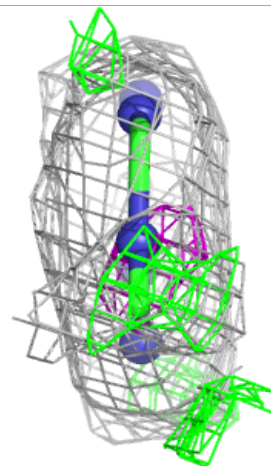
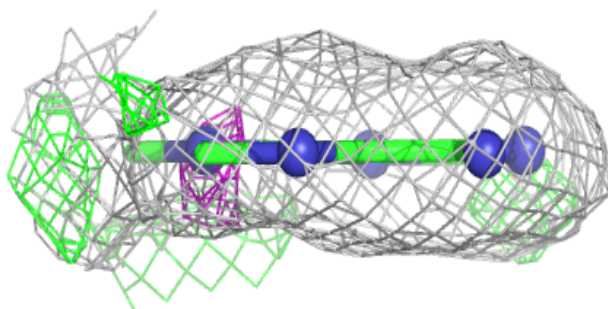
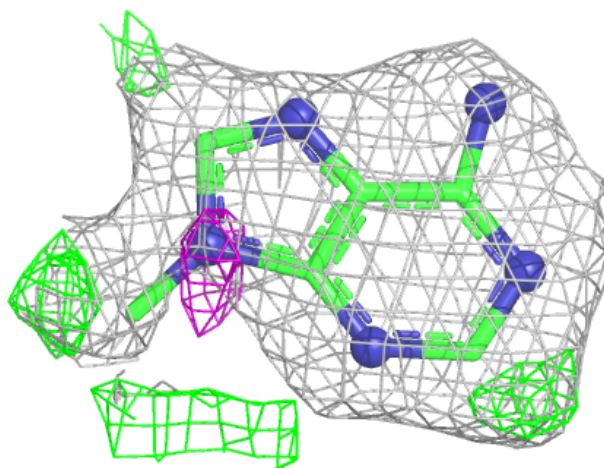
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	E	5255	11/44	0.76	0.16	17,17,17,17	0
2	NAD	A	1255	11/44	0.82	0.14	17,17,17,17	0
2	NAD	C	3255	11/44	0.88	0.12	17,17,17,17	0
2	NAD	F	6255	11/44	0.89	0.11	17,17,17,17	0
2	NAD	B	2255	11/44	0.90	0.11	17,17,17,17	0
2	NAD	D	4255	11/44	0.91	0.11	17,17,17,17	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.

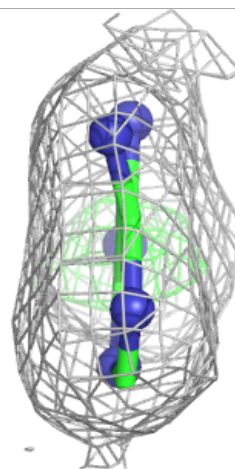
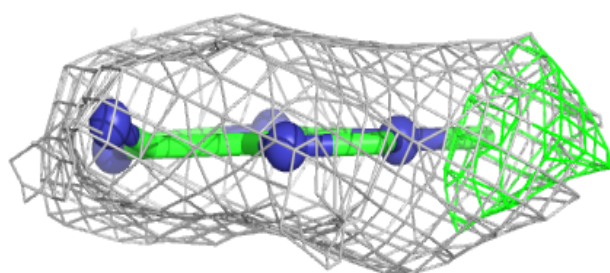
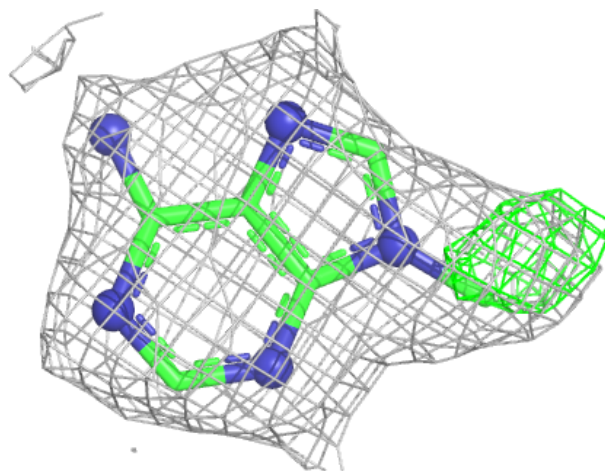
Electron density around NAD E 5255:

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



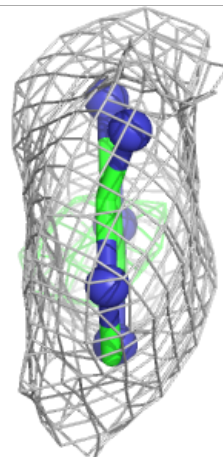
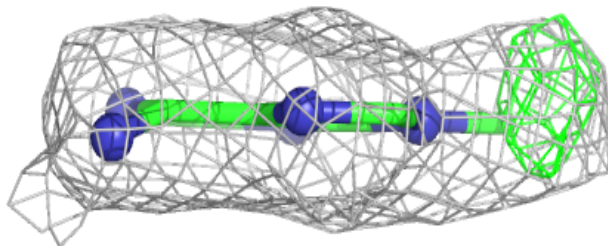
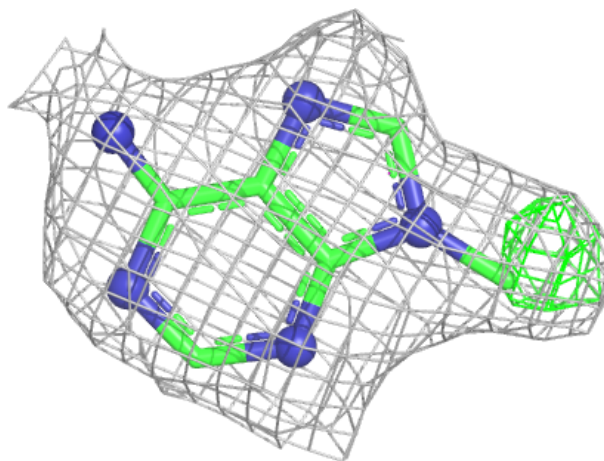
Electron density around NAD A 1255:

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



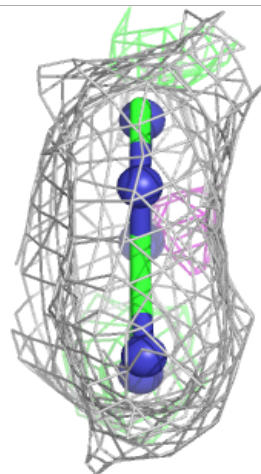
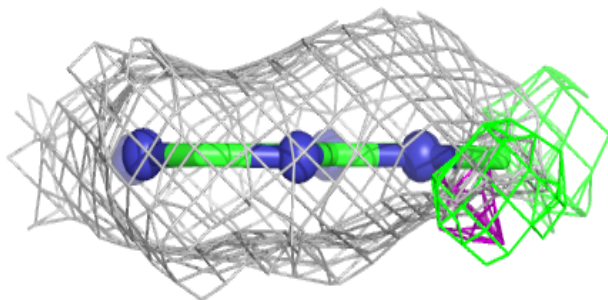
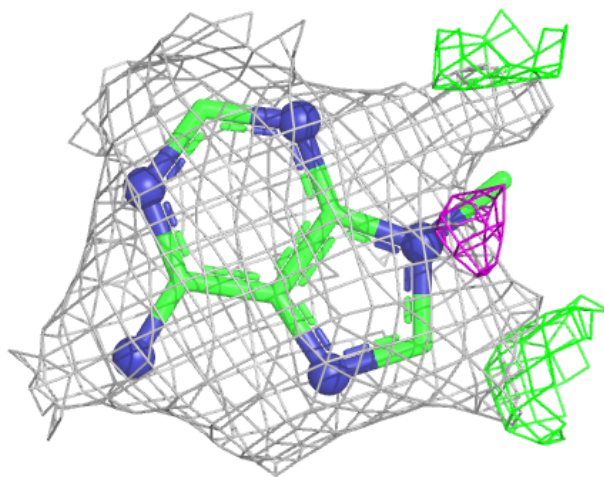
Electron density around NAD C 3255:

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



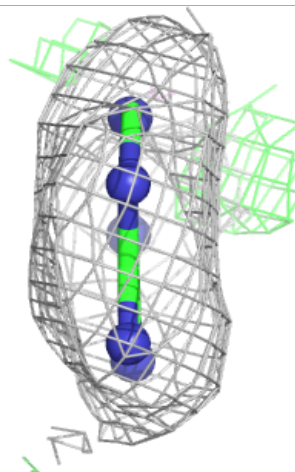
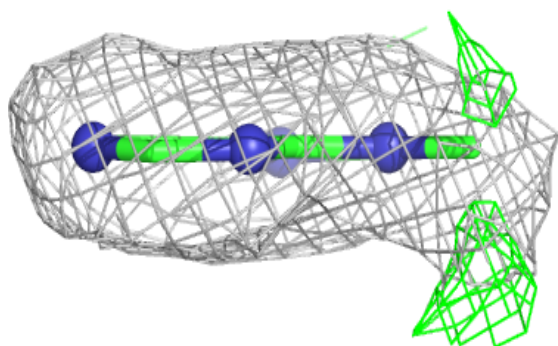
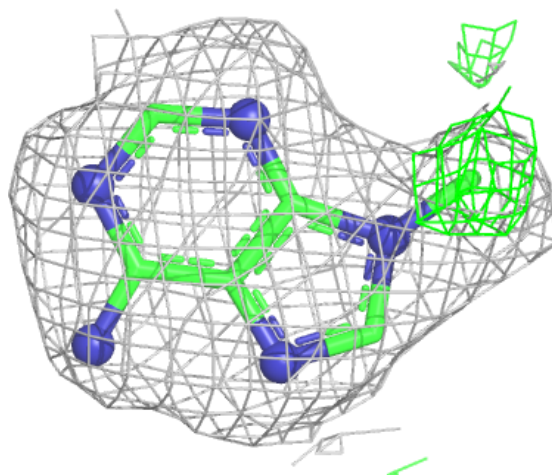
Electron density around NAD F 6255:

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



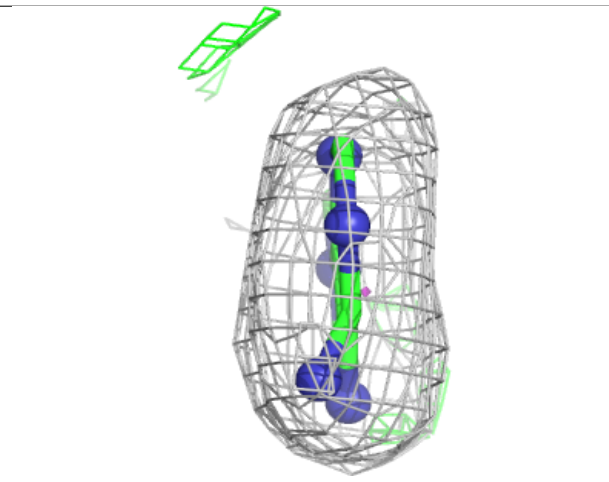
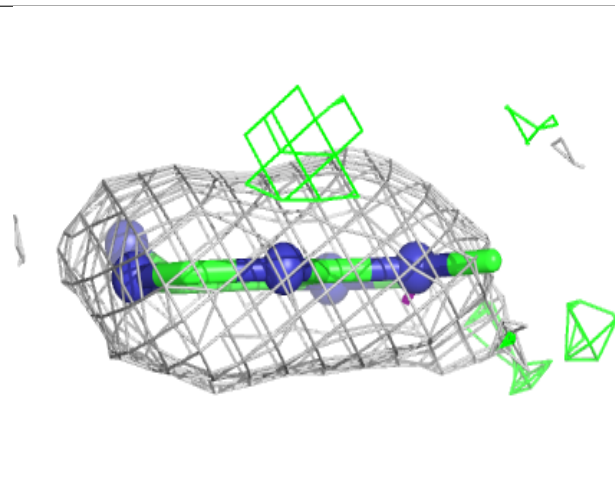
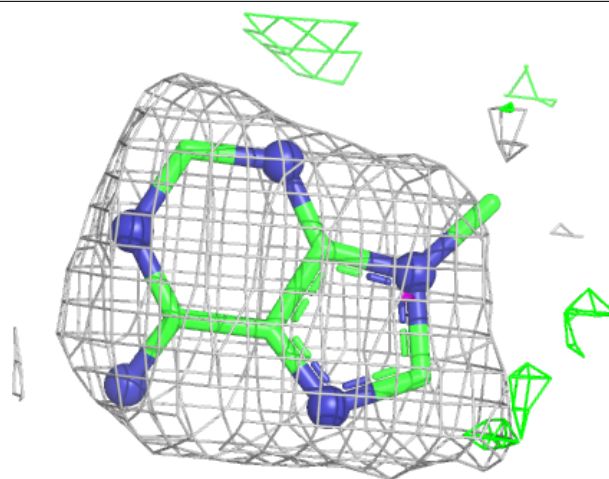
Electron density around NAD B 2255:

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



Electron density around NAD D 4255:

$2mF_o-DF_c$ (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.