



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:01 PM UTC

PDB ID : 2G83 / pdb_00002g83
Title : Structure of activated G-alpha-i1 bound to a nucleotide-state-selective peptide: Minimal determinants for recognizing the active form of a G protein alpha subunit
Authors : Johnston, C.A.; Ramer, J.K.; Blaesius, R.; Kuhlman, B.; Arshavsky, V.Y.; Siderovski, D.P.
Deposited on : 2006-03-01
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](#) ①) 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

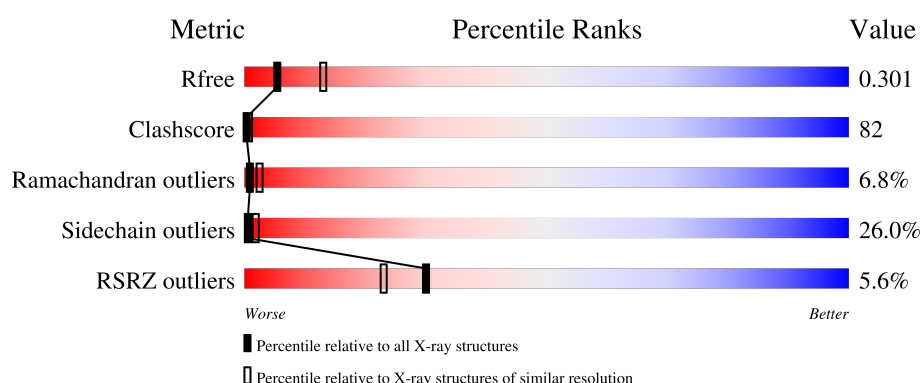
1 Overall quality at a glance

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	313	4% 32% 45% 19%
1	B	313	6% 28% 40% 26%
2	C	11	18% 27% 18% 45% 9%
2	D	11	18% 9% 36% 36% 18%

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
5	GDP	A	355	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5190 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.

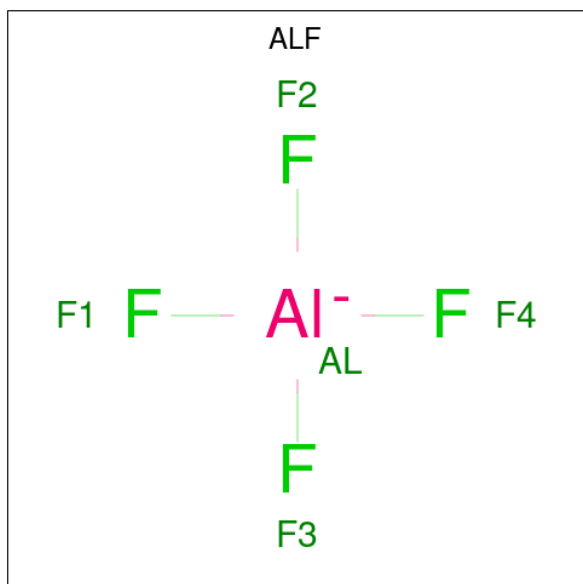
- Molecule 1 is a protein called Guanine nucleotide-binding protein G(i), alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2450	1561	411	464	14			
1	B	303	Total	C	N	O	S	0	0	0
			2450	1561	411	464	14			

- Molecule 2 is a protein called KB-1753 phage display peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	0	0	0
			96	63	17	16			
2	D	11	Total	C	N	O	0	0	0
			96	63	17	16			

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4^-).

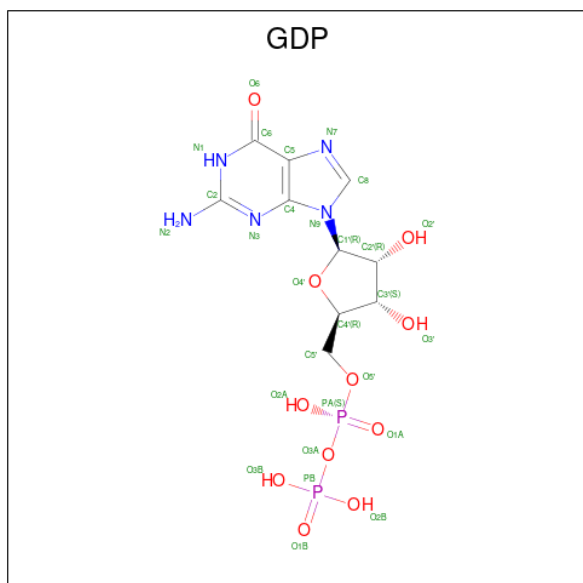


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		
3	B	1	Total	Al	F	0	0
			5	1	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



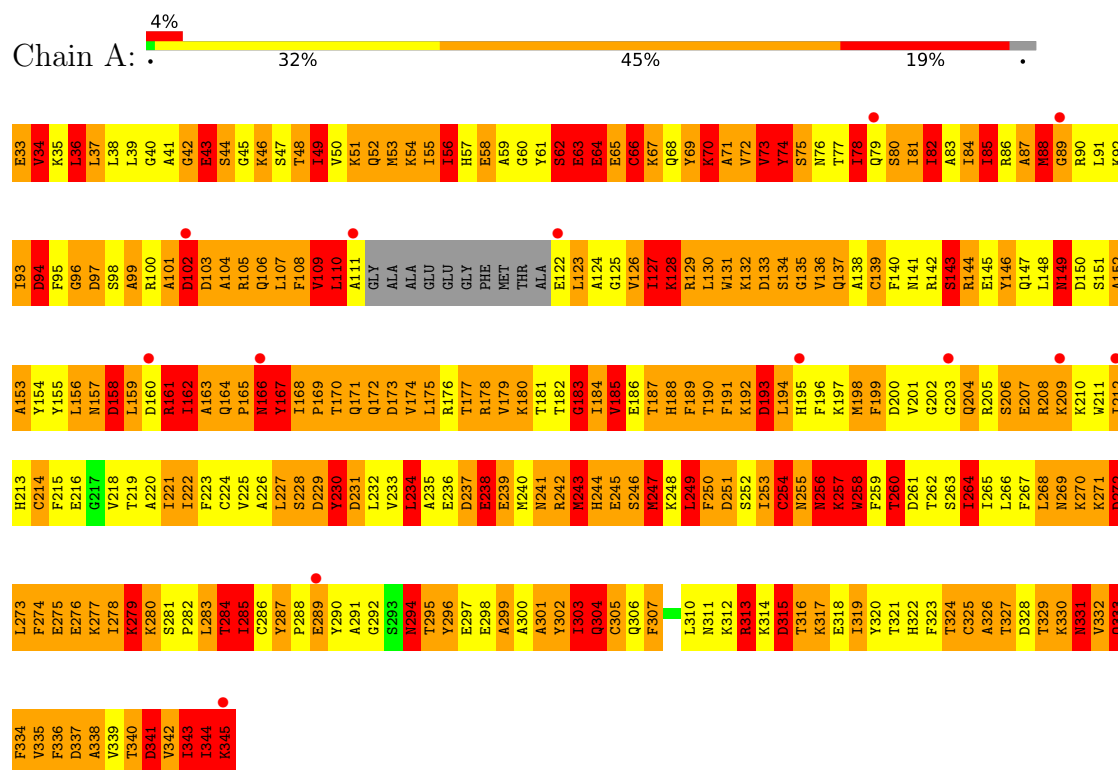
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	12	Total	O	0	0
			12	12		
6	C	1	Total	O	0	0
			1	1		

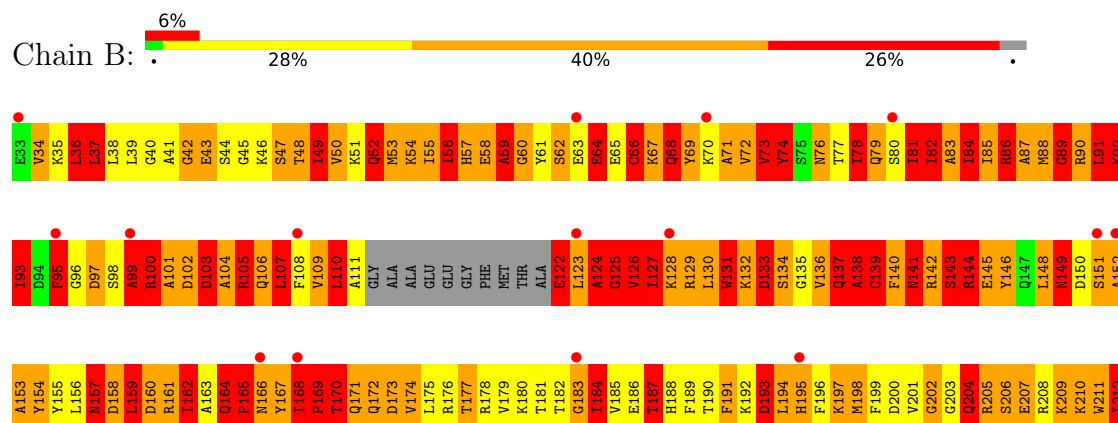
3 Residue-property plots

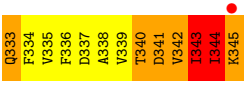
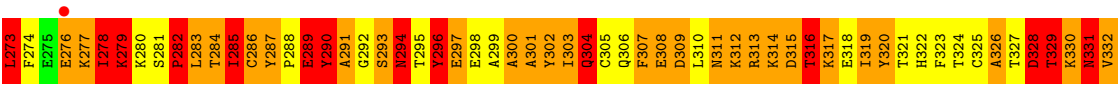
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit

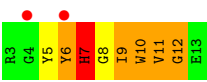


- Molecule 1: Guanine nucleotide-binding protein G(i), alpha-1 subunit

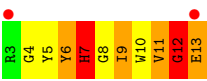




● Molecule 2: KB-1753 phage display peptide



● Molecule 2: KB-1753 phage display peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.13Å 103.13Å 206.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 87.9 (50.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.300 0.271 , 0.301	Depositor DCC
R_{free} test set	3043 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: ALF, GDP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	4.77	707/2494 (28.3%)	2.91	121/3359 (3.6%)
1	B	4.23	531/2494 (21.3%)	2.45	162/3359 (4.8%)
2	C	3.78	17/100 (17.0%)	2.05	5/133 (3.8%)
2	D	4.23	22/100 (22.0%)	1.97	6/133 (4.5%)
All	All	4.49	1277/5188 (24.6%)	2.66	294/6984 (4.2%)

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	18
1	B	0	29
2	D	0	1
All	All	0	48

All (1277) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	VAL	C-N	-59.30	0.73	1.33
1	A	110	LEU	C-N	-33.71	0.86	1.33
1	B	104	ALA	N-CA	22.19	1.86	1.47
1	B	55	ILE	CA-CB	-19.89	1.32	1.54
1	B	226	ALA	CA-CB	-19.56	1.27	1.53
1	B	99	ALA	C-N	17.65	1.58	1.33
1	B	60	GLY	N-CA	-17.47	1.20	1.45
1	B	82	ILE	N-CA	16.22	1.66	1.46
1	A	226	ALA	CA-CB	-15.98	1.31	1.53
1	A	83	ALA	CA-CB	-15.60	1.29	1.53
1	A	291	ALA	CA-CB	-15.24	1.32	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ILE	CA-CB	-15.10	1.39	1.55
1	B	220	ALA	CA-CB	-15.04	1.28	1.53
1	A	84	ILE	CA-CB	-15.04	1.37	1.54
1	B	56	ILE	CA-CB	-14.97	1.36	1.54
1	A	301	ALA	CA-CB	-14.83	1.31	1.53
1	B	285	ILE	CA-CB	-14.83	1.35	1.54
1	B	139	CYS	N-CA	14.68	1.64	1.46
1	B	301	ALA	CA-CB	-14.62	1.30	1.53
1	A	303	ILE	CA-CB	-14.23	1.36	1.54
1	A	98	SER	C-O	-14.05	1.03	1.24
1	A	276	GLU	CA-C	-13.77	1.38	1.52
1	A	299	ALA	CA-CB	-13.77	1.32	1.53
1	B	103	ASP	C-N	-13.71	1.18	1.33
1	B	59	ALA	CA-C	-13.69	1.40	1.53
1	B	338	ALA	CA-CB	-13.62	1.31	1.53
1	A	168	ILE	CA-CB	-13.33	1.36	1.54
1	A	82	ILE	CA-CB	-13.09	1.37	1.54
1	B	344	ILE	CA-CB	-13.02	1.36	1.54
1	B	83	ALA	CA-CB	-13.00	1.32	1.53
1	A	59	ALA	CA-CB	-12.93	1.32	1.53
1	A	264	ILE	CA-CB	-12.72	1.39	1.54
1	A	344	ILE	C-N	-12.70	1.15	1.33
1	A	104	ALA	CA-CB	-12.50	1.33	1.53
1	A	124	ALA	CA-CB	-12.48	1.33	1.53
2	D	6	TYR	CA-C	-12.44	1.45	1.52
1	B	41	ALA	CA-CB	-12.36	1.34	1.53
1	B	174	VAL	CA-CB	-12.35	1.39	1.54
1	A	332	VAL	CA-CB	-12.32	1.38	1.54
1	B	253	ILE	CA-CB	-12.10	1.42	1.55
2	C	11	VAL	CA-CB	-12.09	1.39	1.54
1	B	49	ILE	CA-CB	-12.07	1.39	1.54
1	B	82	ILE	CA-CB	-11.99	1.38	1.54
1	A	101	ALA	CA-CB	-11.98	1.32	1.53
1	A	338	ALA	CA-CB	-11.65	1.33	1.53
1	A	71	ALA	CA-CB	-11.52	1.35	1.53
1	A	221	ILE	CA-CB	-11.44	1.38	1.54
1	B	85	ILE	CA-CB	-11.37	1.40	1.54
1	A	220	ALA	CA-CB	-11.30	1.33	1.53
1	A	319	ILE	CA-CB	-11.18	1.41	1.54
1	A	126	VAL	CA-CB	-11.14	1.38	1.54
1	A	138	ALA	CA-CB	-11.09	1.33	1.53
1	A	218	VAL	CA-CB	-11.06	1.40	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	11	VAL	CA-CB	-11.05	1.39	1.54
1	B	127	ILE	CA-CB	-11.01	1.39	1.54
1	A	41	ALA	CA-CB	-11.01	1.35	1.53
1	A	87	ALA	CA-CB	-11.01	1.33	1.53
1	B	326	ALA	CA-CB	-10.86	1.34	1.53
1	B	73	VAL	CA-CB	-10.71	1.36	1.54
1	A	73	VAL	CA-CB	-10.69	1.40	1.54
1	A	260	THR	CA-CB	-10.53	1.39	1.54
1	A	269	ASN	CA-C	-10.53	1.39	1.52
1	B	222	ILE	CA-CB	-10.52	1.40	1.53
1	A	72	VAL	CA-CB	-10.51	1.41	1.54
2	C	9	ILE	CA-CB	-10.46	1.40	1.54
1	B	319	ILE	CA-CB	-10.46	1.41	1.54
1	B	278	ILE	CA-CB	-10.43	1.40	1.54
1	B	168	ILE	CA-CB	-10.41	1.46	1.55
1	B	165	PRO	N-CA	-10.40	1.34	1.47
1	B	222	ILE	C-O	-10.39	1.12	1.24
1	A	34	VAL	CA-CB	-10.36	1.40	1.54
1	B	299	ALA	CA-CB	-10.36	1.35	1.53
1	B	153	ALA	CA-CB	-10.35	1.37	1.53
1	A	201	VAL	CA-CB	-10.32	1.40	1.54
1	A	212	ILE	CA-CB	-10.18	1.42	1.54
1	A	56	ILE	CA-CB	-10.14	1.41	1.54
1	B	72	VAL	CA-CB	-10.10	1.42	1.54
1	A	182	THR	CA-CB	-10.05	1.38	1.53
2	D	11	VAL	CA-C	-9.99	1.40	1.52
1	A	222	ILE	CA-CB	-9.99	1.41	1.53
1	A	50	VAL	CA-C	-9.94	1.42	1.52
1	A	185	VAL	CA-CB	-9.93	1.42	1.54
1	A	184	ILE	CA-CB	-9.89	1.42	1.54
1	A	300	ALA	CA-C	-9.88	1.38	1.52
1	A	55	ILE	CA-CB	-9.81	1.40	1.54
1	A	344	ILE	CA-CB	-9.79	1.41	1.54
1	B	41	ALA	CA-C	-9.78	1.40	1.53
1	B	225	VAL	CA-CB	-9.77	1.41	1.54
1	A	294	ASN	CA-C	-9.76	1.40	1.53
1	A	269	ASN	C-O	-9.74	1.11	1.23
1	A	199	PHE	C-O	-9.73	1.11	1.24
1	B	179	VAL	CA-CB	-9.68	1.41	1.54
1	B	126	VAL	CA-CB	-9.64	1.41	1.54
1	B	331	ASN	CA-C	-9.62	1.39	1.52
1	B	218	VAL	CA-CB	-9.61	1.43	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	ASN	CA-C	-9.61	1.40	1.53
2	C	7	HIS	CA-C	-9.60	1.40	1.52
1	B	225	VAL	C-O	-9.59	1.14	1.24
1	B	87	ALA	CA-CB	-9.58	1.37	1.53
1	A	82	ILE	C-O	-9.58	1.13	1.24
1	B	343	ILE	CA-CB	-9.58	1.41	1.54
1	B	288	PRO	CA-C	-9.56	1.42	1.52
1	A	256	ASN	CA-C	-9.55	1.41	1.52
1	A	274	PHE	CA-C	-9.55	1.40	1.52
1	B	207	GLU	CA-C	-9.53	1.40	1.52
1	A	99	ALA	CA-CB	-9.49	1.36	1.53
1	B	71	ALA	CA-CB	-9.36	1.38	1.53
1	A	332	VAL	CA-C	-9.35	1.39	1.52
1	A	225	VAL	C-O	-9.33	1.14	1.24
1	B	84	ILE	CA-CB	-9.32	1.41	1.54
1	B	221	ILE	C-O	-9.29	1.14	1.24
1	B	56	ILE	CA-C	-9.28	1.41	1.52
1	B	335	VAL	CA-CB	-9.25	1.41	1.54
1	A	153	ALA	CA-CB	-9.21	1.38	1.53
1	B	201	VAL	CA-CB	-9.20	1.41	1.54
1	B	183	GLY	C-O	-9.19	1.11	1.23
1	B	320	TYR	C-O	-9.13	1.13	1.23
1	B	212	ILE	CA-C	-9.11	1.41	1.52
1	A	170	THR	CA-CB	-9.08	1.39	1.53
1	A	300	ALA	CA-CB	-9.06	1.37	1.53
1	A	335	VAL	CA-CB	-9.05	1.42	1.54
1	A	109	VAL	CA-CB	-8.97	1.42	1.54
1	B	59	ALA	C-O	-8.94	1.15	1.24
1	A	85	ILE	CA-CB	-8.93	1.42	1.54
1	A	278	ILE	CA-CB	-8.90	1.42	1.54
1	B	199	PHE	C-O	-8.90	1.13	1.23
1	A	152	ALA	CA-CB	-8.86	1.38	1.53
1	B	49	ILE	C-O	-8.86	1.14	1.24
1	B	267	PHE	C-O	-8.84	1.14	1.24
1	A	49	ILE	CA-C	-8.82	1.41	1.53
1	A	162	ILE	CA-CB	-8.82	1.45	1.54
1	A	295	THR	N-CA	-8.80	1.34	1.45
1	A	187	THR	CA-CB	-8.79	1.38	1.53
1	B	185	VAL	C-O	-8.78	1.14	1.24
1	A	83	ALA	CA-C	-8.77	1.41	1.52
1	A	165	PRO	CA-C	-8.74	1.42	1.52
2	D	9	ILE	C-O	-8.72	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	GLN	CA-C	-8.72	1.41	1.52
1	A	249	LEU	CA-C	-8.72	1.41	1.52
1	A	138	ALA	C-O	-8.71	1.12	1.24
1	B	332	VAL	CA-CB	-8.71	1.42	1.54
1	A	176	ARG	N-CA	-8.69	1.36	1.46
1	A	241	ASN	CA-C	-8.68	1.41	1.52
1	A	140	PHE	CA-C	-8.68	1.41	1.52
1	A	255	ASN	C-O	-8.64	1.14	1.24
1	A	152	ALA	C-O	-8.63	1.13	1.24
1	B	220	ALA	C-O	-8.63	1.13	1.23
1	A	200	ASP	CA-C	-8.62	1.42	1.52
1	B	124	ALA	CA-CB	-8.61	1.39	1.53
1	B	49	ILE	CA-C	-8.61	1.41	1.52
1	B	171	GLN	CA-C	-8.59	1.41	1.52
1	B	185	VAL	CA-CB	-8.59	1.43	1.54
1	A	245	GLU	CA-C	-8.58	1.40	1.52
1	B	45	GLY	C-O	-8.57	1.12	1.23
1	A	271	LYS	CA-C	-8.56	1.40	1.52
1	A	295	THR	CA-C	-8.56	1.42	1.52
1	B	252	SER	CA-C	-8.55	1.41	1.52
1	B	342	VAL	CA-CB	-8.56	1.45	1.54
1	A	303	ILE	C-O	-8.51	1.14	1.24
1	A	46	LYS	C-O	-8.50	1.14	1.24
1	B	55	ILE	N-CA	-8.48	1.36	1.46
1	A	266	LEU	C-O	-8.46	1.14	1.24
1	B	226	ALA	CA-C	-8.45	1.42	1.52
1	B	300	ALA	CA-CB	-8.45	1.40	1.53
1	A	41	ALA	CA-C	-8.44	1.40	1.53
1	A	177	THR	CA-C	-8.43	1.42	1.52
1	A	212	ILE	CA-C	-8.41	1.42	1.52
1	A	278	ILE	C-O	-8.40	1.14	1.24
1	A	70	LYS	CA-C	-8.39	1.41	1.52
1	B	342	VAL	C-O	-8.38	1.14	1.24
1	A	179	VAL	C-O	-8.37	1.14	1.24
2	D	7	HIS	CA-C	-8.35	1.42	1.53
1	B	109	VAL	CA-CB	-8.31	1.44	1.54
1	B	39	LEU	C-O	-8.29	1.13	1.23
1	A	126	VAL	C-O	-8.28	1.14	1.24
1	A	139	CYS	CA-C	-8.27	1.41	1.52
1	B	220	ALA	CA-C	-8.27	1.42	1.52
1	B	287	TYR	C-O	-8.27	1.15	1.24
1	A	185	VAL	C-O	-8.25	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ARG	C-O	-8.25	1.12	1.24
1	A	207	GLU	CA-C	-8.23	1.41	1.52
1	A	36	LEU	C-O	-8.22	1.13	1.23
1	A	222	ILE	C-O	-8.21	1.15	1.24
1	B	78	ILE	CA-CB	-8.21	1.43	1.54
2	D	10	TRP	CA-C	-8.19	1.42	1.52
1	B	200	ASP	C-O	-8.19	1.14	1.24
1	B	339	VAL	CA-CB	-8.18	1.44	1.54
1	B	283	LEU	CA-C	-8.17	1.41	1.52
1	A	37	LEU	C-O	-8.15	1.13	1.23
1	A	208	ARG	NE-CZ	-8.13	1.24	1.33
2	C	10	TRP	CA-C	-8.12	1.42	1.52
1	A	274	PHE	C-O	-8.11	1.14	1.24
1	B	207	GLU	C-O	-8.09	1.13	1.24
1	A	287	TYR	C-O	-8.09	1.14	1.24
1	B	221	ILE	CA-CB	-8.08	1.43	1.54
1	B	206	SER	CA-C	-8.07	1.41	1.52
1	A	136	VAL	CA-CB	-8.05	1.41	1.54
1	A	179	VAL	CA-CB	-8.05	1.43	1.54
1	A	48	THR	C-O	-8.04	1.13	1.24
1	A	204	GLN	CA-C	-8.04	1.42	1.52
1	A	258	TRP	CA-C	-8.03	1.42	1.52
1	A	78	ILE	CA-CB	-8.03	1.43	1.54
1	A	278	ILE	CA-C	-8.02	1.42	1.52
1	B	184	ILE	CA-CB	-8.02	1.43	1.54
1	A	268	LEU	C-O	-8.01	1.14	1.24
1	B	307	PHE	C-O	-8.01	1.14	1.24
1	A	45	GLY	C-O	-8.01	1.13	1.23
1	B	141	ASN	CA-C	-8.00	1.42	1.52
1	B	179	VAL	C-O	-7.99	1.15	1.24
1	B	272	ASP	C-O	-7.99	1.14	1.24
1	B	37	LEU	C-O	-7.95	1.14	1.24
2	D	13	GLU	C-OXT	7.95	1.39	1.23
1	B	272	ASP	CA-C	-7.94	1.43	1.52
1	A	208	ARG	CA-C	-7.92	1.41	1.52
1	A	285	ILE	CA-CB	-7.92	1.43	1.54
1	A	81	ILE	C-O	-7.91	1.13	1.24
1	A	249	LEU	C-O	-7.91	1.15	1.24
1	A	276	GLU	C-O	-7.90	1.12	1.23
1	A	264	ILE	C-O	-7.90	1.15	1.24
1	A	168	ILE	CA-C	-7.88	1.44	1.52
1	A	265	ILE	C-O	-7.87	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	TYR	CA-C	-7.85	1.42	1.52
1	B	183	GLY	C-N	-7.84	1.23	1.33
1	A	108	PHE	CA-C	-7.84	1.42	1.52
1	B	257	LYS	CA-C	-7.83	1.40	1.52
1	A	224	CYS	C-O	-7.83	1.14	1.23
1	B	301	ALA	C-O	-7.80	1.13	1.24
1	A	231	ASP	CA-C	-7.79	1.43	1.53
1	A	205	ARG	CA-C	-7.79	1.41	1.52
1	A	310	LEU	CG-CD2	-7.78	1.26	1.52
1	B	43	GLU	CA-C	-7.77	1.43	1.53
1	A	97	ASP	C-O	-7.77	1.14	1.23
1	A	200	ASP	C-O	-7.75	1.15	1.23
1	B	324	THR	C-O	-7.75	1.14	1.23
1	A	181	THR	C-O	-7.73	1.14	1.24
1	B	205	ARG	N-CA	-7.72	1.36	1.46
1	B	338	ALA	C-O	-7.72	1.15	1.24
1	A	216	GLU	CA-C	-7.72	1.43	1.52
1	A	80	SER	C-O	-7.71	1.14	1.24
1	B	241	ASN	C-O	-7.69	1.14	1.23
1	A	50	VAL	C-O	-7.68	1.16	1.23
1	A	321	THR	CA-CB	-7.68	1.41	1.53
1	B	198	MET	C-O	-7.68	1.14	1.24
1	B	205	ARG	C-O	-7.67	1.15	1.24
1	B	187	THR	CA-CB	-7.67	1.39	1.53
1	A	337	ASP	C-O	-7.67	1.15	1.24
1	A	305	CYS	C-O	-7.67	1.14	1.24
1	B	266	LEU	C-O	-7.65	1.15	1.23
1	A	227	LEU	C-O	-7.65	1.15	1.24
1	B	241	ASN	CA-C	-7.64	1.42	1.52
1	B	264	ILE	CA-CB	-7.63	1.43	1.53
1	B	300	ALA	CA-C	-7.62	1.42	1.52
1	B	216	GLU	CA-C	-7.62	1.43	1.52
1	B	298	GLU	CA-C	-7.62	1.42	1.52
1	A	284	THR	CB-CG2	-7.61	1.27	1.52
1	A	125	GLY	C-O	-7.59	1.14	1.23
2	C	9	ILE	CA-C	-7.59	1.43	1.52
1	A	72	VAL	C-O	-7.59	1.15	1.24
1	A	128	LYS	CA-C	-7.58	1.42	1.52
1	B	303	ILE	CA-CB	-7.56	1.43	1.54
1	B	224	CYS	C-O	-7.54	1.14	1.24
1	B	211	TRP	C-O	-7.53	1.14	1.24
1	B	271	LYS	CA-C	-7.52	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLN	C-O	-7.51	1.14	1.24
1	B	334	PHE	CA-C	-7.50	1.42	1.52
2	D	5	TYR	C-O	-7.48	1.14	1.24
1	B	245	GLU	C-O	-7.46	1.15	1.24
1	A	332	VAL	N-CA	-7.46	1.36	1.46
1	B	149	ASN	C-O	-7.46	1.15	1.23
1	B	152	ALA	CA-CB	-7.45	1.41	1.53
1	A	201	VAL	C-O	-7.45	1.15	1.24
1	A	270	LYS	C-O	-7.43	1.14	1.24
1	A	83	ALA	N-CA	-7.42	1.36	1.46
1	A	207	GLU	C-O	-7.41	1.14	1.24
1	A	54	LYS	C-O	-7.41	1.14	1.24
1	A	100	ARG	CA-C	-7.41	1.42	1.52
1	A	70	LYS	C-O	-7.39	1.14	1.24
2	D	10	TRP	C-O	-7.39	1.15	1.24
1	B	227	LEU	C-O	-7.38	1.14	1.24
1	A	343	ILE	CA-CB	-7.37	1.44	1.54
1	A	233	VAL	CA-CB	-7.37	1.43	1.54
1	A	38	LEU	CA-C	-7.36	1.43	1.52
1	A	129	ARG	C-O	-7.36	1.14	1.24
1	A	42	GLY	C-O	-7.35	1.15	1.23
1	A	128	LYS	C-O	-7.35	1.14	1.24
1	A	132	LYS	CA-C	-7.34	1.43	1.52
1	A	274	PHE	CE2-CZ	-7.34	1.16	1.38
1	A	181	THR	CB-CG2	-7.33	1.28	1.52
1	A	331	ASN	C-O	-7.32	1.15	1.24
1	B	201	VAL	C-O	-7.32	1.15	1.23
1	A	93	ILE	CA-CB	-7.32	1.43	1.54
1	A	153	ALA	C-O	-7.31	1.14	1.24
1	B	179	VAL	CA-C	-7.31	1.44	1.52
1	A	235	ALA	CA-CB	-7.30	1.40	1.53
1	A	94	ASP	CA-C	-7.29	1.43	1.52
1	A	306	GLN	N-CA	-7.29	1.36	1.46
1	B	248	LYS	CA-C	-7.29	1.42	1.52
1	B	328	ASP	C-O	-7.28	1.15	1.24
1	B	305	CYS	C-O	-7.28	1.14	1.24
1	A	311	ASN	CA-C	-7.27	1.43	1.52
1	A	329	THR	C-O	-7.25	1.14	1.24
1	B	253	ILE	C-O	-7.25	1.15	1.23
1	A	179	VAL	CA-C	-7.25	1.43	1.52
1	B	55	ILE	CA-C	-7.25	1.44	1.52
1	B	104	ALA	CA-C	-7.25	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	ILE	CA-C	-7.24	1.43	1.52
1	B	127	ILE	CA-C	-7.24	1.43	1.52
1	B	269	ASN	CA-C	-7.24	1.44	1.52
1	A	245	GLU	C-O	-7.24	1.14	1.24
1	B	72	VAL	C-O	-7.23	1.15	1.24
1	B	329	THR	CA-C	-7.23	1.42	1.52
1	A	73	VAL	N-CA	-7.22	1.37	1.46
1	A	268	LEU	CA-C	-7.22	1.44	1.52
1	A	84	ILE	C-O	-7.21	1.16	1.24
1	A	172	GLN	C-O	-7.21	1.14	1.24
1	B	79	GLN	CA-C	-7.20	1.43	1.52
1	B	325	CYS	C-O	-7.20	1.15	1.24
1	A	83	ALA	C-O	-7.20	1.14	1.24
1	B	218	VAL	C-O	-7.18	1.16	1.24
1	A	257	LYS	CA-C	-7.18	1.41	1.52
1	B	51	LYS	C-O	-7.17	1.15	1.24
1	B	153	ALA	C-O	-7.17	1.15	1.24
1	B	288	PRO	N-CA	-7.17	1.41	1.47
1	A	156	LEU	CA-C	-7.17	1.42	1.52
2	D	11	VAL	C-O	-7.17	1.15	1.24
1	A	310	LEU	CA-C	-7.17	1.43	1.52
2	D	5	TYR	CA-C	-7.17	1.43	1.52
1	A	340	THR	CA-CB	-7.15	1.42	1.53
1	A	231	ASP	CB-CG	-7.14	1.34	1.52
1	B	282	PRO	CB-CG	-7.14	1.14	1.49
1	B	263	SER	C-O	-7.13	1.14	1.23
1	B	93	ILE	CA-CB	-7.13	1.44	1.54
1	B	303	ILE	C-O	-7.13	1.15	1.24
1	A	50	VAL	CA-CB	-7.11	1.46	1.54
1	A	148	LEU	CA-C	-7.11	1.43	1.52
1	B	310	LEU	CG-CD2	-7.11	1.29	1.52
1	A	148	LEU	C-O	-7.10	1.15	1.23
1	B	343	ILE	CA-C	-7.10	1.42	1.52
1	A	198	MET	SD-CE	-7.08	1.61	1.79
1	B	322	HIS	C-O	-7.08	1.15	1.23
1	A	252	SER	CA-C	-7.08	1.43	1.52
2	C	10	TRP	N-CA	-7.07	1.37	1.46
1	B	78	ILE	CA-C	-7.06	1.43	1.52
1	B	311	ASN	CA-C	-7.06	1.43	1.52
1	B	35	LYS	C-O	-7.05	1.15	1.24
1	A	103	ASP	N-CA	-7.05	1.36	1.46
1	A	289	GLU	C-O	-7.05	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ASP	CA-C	-7.04	1.43	1.52
1	A	171	GLN	CA-C	-7.04	1.43	1.52
1	A	151	SER	C-O	-7.03	1.14	1.24
1	A	175	LEU	CA-C	-7.02	1.43	1.52
1	A	197	LYS	C-O	-7.01	1.16	1.24
1	B	304	GLN	C-O	-7.01	1.16	1.24
1	A	155	TYR	C-O	-7.00	1.15	1.24
1	B	39	LEU	CG-CD1	-7.00	1.29	1.52
1	B	41	ALA	C-O	-7.00	1.15	1.23
1	A	110	LEU	CA-C	-6.99	1.45	1.53
1	B	54	LYS	CA-C	-6.99	1.45	1.52
1	A	149	ASN	C-O	-6.99	1.14	1.23
1	A	127	ILE	CA-C	-6.98	1.43	1.52
1	A	170	THR	C-O	-6.98	1.15	1.23
1	A	282	PRO	C-O	-6.97	1.14	1.24
1	A	47	SER	C-O	-6.97	1.14	1.24
1	A	74	TYR	CA-C	-6.97	1.43	1.52
1	A	149	ASN	CA-C	-6.97	1.43	1.53
1	B	186	GLU	C-O	-6.96	1.15	1.23
1	A	36	LEU	CG-CD2	-6.96	1.29	1.52
1	B	249	LEU	CG-CD1	-6.96	1.29	1.52
1	B	237	ASP	C-O	-6.95	1.15	1.23
1	A	186	GLU	C-O	-6.95	1.15	1.23
1	A	328	ASP	C-O	-6.95	1.16	1.24
1	A	296	TYR	C-O	-6.95	1.16	1.24
1	B	339	VAL	C-O	-6.94	1.16	1.24
1	B	255	ASN	C-O	-6.93	1.15	1.24
1	A	195	HIS	C-O	-6.93	1.15	1.24
1	B	332	VAL	C-O	-6.93	1.15	1.24
1	A	271	LYS	N-CA	-6.92	1.36	1.46
1	A	338	ALA	CA-C	-6.92	1.43	1.52
1	A	38	LEU	N-CA	-6.91	1.37	1.46
2	C	10	TRP	C-O	-6.90	1.15	1.24
1	A	172	GLN	N-CA	-6.90	1.37	1.46
1	A	154	TYR	C-O	-6.89	1.15	1.24
1	A	284	THR	CA-CB	-6.89	1.41	1.53
1	A	302	TYR	CA-C	-6.89	1.43	1.52
1	A	64	GLU	CA-C	-6.89	1.43	1.52
1	A	126	VAL	CB-CG1	-6.89	1.29	1.52
1	A	214	CYS	C-O	-6.89	1.14	1.23
1	B	228	SER	N-CA	-6.89	1.38	1.46
1	A	295	THR	C-O	-6.88	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	ILE	CA-C	-6.88	1.44	1.52
1	A	195	HIS	CA-C	-6.88	1.44	1.52
1	B	301	ALA	CA-C	-6.88	1.43	1.52
1	A	133	ASP	C-O	-6.87	1.15	1.23
1	A	292	GLY	C-O	-6.86	1.17	1.23
1	A	77	THR	C-O	-6.86	1.15	1.24
1	A	97	ASP	CA-C	-6.85	1.44	1.52
1	A	322	HIS	C-O	-6.85	1.15	1.23
1	A	185	VAL	CB-CG1	-6.85	1.29	1.52
1	B	188	HIS	C-O	-6.85	1.15	1.23
1	A	73	VAL	C-O	-6.85	1.16	1.24
1	B	328	ASP	CA-C	-6.84	1.44	1.52
1	A	236	GLU	C-O	-6.84	1.14	1.24
1	B	185	VAL	CB-CG1	-6.84	1.29	1.52
1	B	330	LYS	CA-CB	-6.84	1.44	1.54
1	B	239	GLU	N-CA	-6.83	1.37	1.46
2	C	8	GLY	C-O	-6.83	1.14	1.24
1	A	226	ALA	C-O	-6.83	1.15	1.24
1	B	187	THR	C-O	-6.82	1.15	1.23
1	B	239	GLU	CA-C	-6.82	1.43	1.52
1	A	306	GLN	CA-C	-6.82	1.43	1.52
1	A	267	PHE	C-O	-6.82	1.15	1.24
1	A	124	ALA	CA-C	-6.81	1.43	1.52
1	A	295	THR	CB-CG2	-6.81	1.30	1.52
1	A	147	GLN	C-O	-6.81	1.15	1.24
1	A	177	THR	CA-CB	-6.80	1.43	1.53
1	A	164	GLN	C-O	-6.80	1.15	1.24
1	B	322	HIS	CA-C	-6.80	1.44	1.52
1	B	278	ILE	N-CA	-6.79	1.37	1.46
1	A	265	ILE	CA-C	-6.77	1.44	1.52
1	B	228	SER	CA-CB	-6.77	1.43	1.53
1	B	234	LEU	CA-C	-6.77	1.43	1.53
1	B	76	ASN	CA-C	-6.77	1.43	1.52
1	A	259	PHE	C-O	-6.76	1.15	1.24
1	B	332	VAL	CA-C	-6.76	1.44	1.52
1	A	94	ASP	N-CA	-6.76	1.37	1.46
1	B	344	ILE	CA-C	-6.76	1.44	1.52
1	A	175	LEU	C-O	-6.75	1.15	1.24
1	A	56	ILE	CA-C	-6.75	1.44	1.52
1	A	75	SER	C-O	-6.74	1.16	1.24
1	A	41	ALA	N-CA	-6.74	1.36	1.45
1	A	227	LEU	CG-CD2	-6.74	1.30	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ARG	CA-C	-6.74	1.43	1.52
1	A	180	LYS	C-O	-6.73	1.15	1.23
1	A	314	LYS	CA-C	-6.72	1.43	1.52
1	B	238	GLU	C-O	-6.72	1.15	1.24
1	A	223	PHE	C-O	-6.71	1.15	1.24
1	A	53	MET	CG-SD	-6.71	1.64	1.80
1	A	198	MET	C-O	-6.71	1.16	1.24
1	A	82	ILE	CA-C	-6.71	1.44	1.52
1	A	178	ARG	C-O	-6.71	1.16	1.24
1	A	221	ILE	C-O	-6.71	1.17	1.24
1	A	172	GLN	CA-C	-6.71	1.43	1.52
1	B	217	GLY	C-O	-6.70	1.15	1.24
1	A	39	LEU	C-O	-6.70	1.15	1.23
1	A	80	SER	CA-C	-6.69	1.44	1.52
1	B	204	GLN	N-CA	-6.69	1.37	1.46
1	B	73	VAL	CA-C	-6.68	1.42	1.52
1	A	78	ILE	C-O	-6.68	1.15	1.24
2	C	6	TYR	CA-C	-6.68	1.43	1.52
1	A	54	LYS	CA-C	-6.67	1.43	1.52
1	A	51	LYS	N-CA	-6.67	1.38	1.46
1	A	136	VAL	C-O	-6.67	1.15	1.24
1	A	300	ALA	N-CA	-6.67	1.37	1.46
1	A	76	ASN	CA-C	-6.67	1.43	1.52
1	A	338	ALA	C-O	-6.67	1.15	1.24
1	B	43	GLU	C-O	-6.66	1.14	1.23
1	A	221	ILE	CA-C	-6.66	1.44	1.52
1	A	325	CYS	C-O	-6.65	1.14	1.23
1	B	84	ILE	CA-C	-6.65	1.43	1.52
1	A	81	ILE	CA-C	-6.65	1.43	1.52
1	A	71	ALA	CA-C	-6.65	1.43	1.52
1	A	333	GLN	CA-C	-6.63	1.44	1.52
1	A	41	ALA	C-O	-6.63	1.14	1.24
1	A	108	PHE	CA-CB	-6.62	1.42	1.53
1	A	49	ILE	C-O	-6.61	1.14	1.23
1	A	200	ASP	N-CA	-6.61	1.38	1.46
1	A	273	LEU	CG-CD2	-6.61	1.30	1.52
1	A	340	THR	CA-C	-6.61	1.44	1.52
1	A	35	LYS	C-O	-6.60	1.16	1.24
1	A	108	PHE	N-CA	-6.59	1.38	1.46
1	A	40	GLY	N-CA	-6.59	1.39	1.45
1	A	260	THR	CA-C	-6.59	1.43	1.52
1	B	202	GLY	C-O	-6.59	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	THR	CB-CG2	-6.59	1.30	1.52
1	A	101	ALA	N-CA	-6.58	1.37	1.46
1	A	199	PHE	CE1-CZ	-6.58	1.19	1.38
1	A	265	ILE	CA-CB	-6.57	1.46	1.54
1	B	181	THR	C-O	-6.57	1.15	1.24
1	B	337	ASP	C-O	-6.57	1.16	1.24
1	A	100	ARG	C-O	-6.57	1.14	1.23
1	A	327	THR	C-O	-6.57	1.15	1.24
1	A	263	SER	C-O	-6.56	1.16	1.24
1	A	125	GLY	CA-C	-6.56	1.44	1.52
1	A	310	LEU	CG-CD1	-6.56	1.30	1.52
1	B	338	ALA	CA-C	-6.56	1.44	1.52
1	B	38	LEU	CG-CD2	-6.56	1.30	1.52
1	B	204	GLN	CA-C	-6.56	1.44	1.52
1	A	163	ALA	CA-CB	-6.54	1.42	1.53
1	A	220	ALA	C-O	-6.54	1.15	1.23
1	A	218	VAL	C-O	-6.54	1.15	1.24
1	A	223	PHE	CD1-CE1	-6.54	1.19	1.38
1	A	178	ARG	CA-C	-6.53	1.44	1.52
1	B	46	LYS	CA-C	-6.53	1.44	1.52
1	A	204	GLN	N-CA	-6.53	1.37	1.46
1	A	52	GLN	CA-C	-6.53	1.43	1.52
1	B	176	ARG	NE-CZ	-6.52	1.25	1.33
1	B	201	VAL	CB-CG2	-6.52	1.31	1.52
1	A	110	LEU	CG-CD1	-6.52	1.31	1.52
1	A	235	ALA	CA-C	-6.52	1.43	1.52
1	A	319	ILE	CA-C	-6.52	1.45	1.52
1	B	291	ALA	CA-CB	-6.52	1.42	1.53
1	B	264	ILE	C-O	-6.52	1.16	1.24
1	A	176	ARG	CZ-NH2	-6.51	1.25	1.33
1	A	148	LEU	CG-CD1	-6.51	1.31	1.52
1	B	331	ASN	C-O	-6.51	1.15	1.24
1	B	210	LYS	C-O	-6.50	1.15	1.24
1	A	182	THR	C-O	-6.50	1.15	1.24
1	A	205	ARG	C-O	-6.50	1.15	1.24
1	B	323	PHE	C-O	-6.50	1.16	1.24
1	A	36	LEU	CA-C	-6.50	1.45	1.52
1	B	51	LYS	N-CA	-6.50	1.38	1.46
1	A	44	SER	CA-C	-6.50	1.43	1.52
1	A	144	ARG	N-CA	-6.50	1.38	1.46
1	A	264	ILE	CG1-CD1	-6.49	1.26	1.51
1	A	79	GLN	C-O	-6.49	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	LEU	CA-C	-6.49	1.43	1.52
1	B	198	MET	SD-CE	-6.49	1.63	1.79
1	A	158	ASP	C-O	-6.48	1.17	1.23
1	B	56	ILE	C-O	-6.48	1.16	1.24
1	A	305	CYS	CA-C	-6.48	1.44	1.52
1	A	297	GLU	C-O	-6.47	1.16	1.24
1	B	249	LEU	C-O	-6.47	1.16	1.24
1	B	49	ILE	N-CA	-6.46	1.40	1.46
1	A	202	GLY	C-O	-6.46	1.13	1.23
1	A	284	THR	CA-C	-6.46	1.44	1.52
1	A	146	TYR	CA-C	-6.46	1.44	1.52
1	A	123	LEU	C-O	-6.46	1.15	1.24
1	B	145	GLU	CA-C	-6.46	1.44	1.52
1	B	242	ARG	C-O	-6.46	1.15	1.24
1	B	55	ILE	CB-CG2	-6.45	1.31	1.52
1	B	236	GLU	CA-C	-6.45	1.44	1.52
1	A	55	ILE	N-CA	-6.45	1.38	1.46
1	B	161	ARG	CA-C	-6.44	1.44	1.52
1	A	241	ASN	C-O	-6.44	1.15	1.23
1	B	290	TYR	CE2-CZ	-6.44	1.22	1.38
1	B	187	THR	CB-CG2	-6.43	1.31	1.52
1	A	51	LYS	C-O	-6.43	1.16	1.24
1	A	95	PHE	C-O	-6.43	1.14	1.23
1	A	144	ARG	NE-CZ	-6.42	1.25	1.33
1	A	280	LYS	C-O	-6.42	1.16	1.24
1	A	197	LYS	N-CA	-6.42	1.38	1.46
1	A	103	ASP	C-O	-6.42	1.15	1.24
1	A	181	THR	N-CA	-6.41	1.38	1.46
1	A	243	MET	SD-CE	-6.41	1.63	1.79
1	B	48	THR	CA-C	-6.41	1.44	1.52
1	A	300	ALA	C-O	-6.40	1.15	1.24
1	B	320	TYR	N-CA	-6.40	1.39	1.46
1	A	40	GLY	C-O	-6.39	1.14	1.23
1	B	214	CYS	C-O	-6.39	1.15	1.24
1	A	247	MET	CA-C	-6.39	1.44	1.52
1	B	173	ASP	CA-C	-6.39	1.43	1.52
1	B	344	ILE	C-O	-6.39	1.16	1.24
1	B	235	ALA	CA-CB	-6.38	1.42	1.53
1	A	58	GLU	CA-C	-6.37	1.44	1.52
1	A	248	LYS	C-O	-6.37	1.16	1.24
1	B	324	THR	CB-CG2	-6.37	1.31	1.52
1	B	267	PHE	CA-C	-6.37	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	LYS	C-O	-6.36	1.16	1.24
1	A	333	GLN	C-O	-6.36	1.16	1.24
1	B	40	GLY	C-O	-6.36	1.14	1.23
1	B	218	VAL	CA-C	-6.36	1.44	1.52
1	B	194	LEU	CA-C	-6.35	1.45	1.52
1	A	191	PHE	C-O	-6.35	1.16	1.23
1	A	278	ILE	CB-CG2	-6.35	1.31	1.52
1	A	134	SER	CA-C	-6.34	1.44	1.52
1	A	282	PRO	CB-CG	-6.34	1.18	1.49
1	A	124	ALA	N-CA	-6.34	1.38	1.46
1	B	272	ASP	CB-CG	-6.33	1.36	1.52
1	B	168	ILE	CA-C	-6.32	1.47	1.52
1	B	225	VAL	CB-CG1	-6.32	1.31	1.52
1	A	187	THR	CB-CG2	-6.32	1.31	1.52
1	A	132	LYS	C-O	-6.32	1.15	1.24
1	B	246	SER	C-O	-6.32	1.14	1.24
1	A	341	ASP	C-O	-6.32	1.16	1.24
1	B	226	ALA	C-O	-6.32	1.16	1.24
1	A	193	ASP	CA-C	-6.32	1.44	1.52
1	B	43	GLU	CA-CB	-6.31	1.44	1.53
1	A	320	TYR	C-O	-6.31	1.16	1.23
2	D	8	GLY	C-O	-6.31	1.15	1.24
1	B	87	ALA	CA-C	-6.31	1.44	1.52
1	A	52	GLN	CA-CB	-6.30	1.43	1.53
1	B	48	THR	CA-CB	-6.29	1.42	1.53
1	A	336	PHE	CA-C	-6.29	1.44	1.52
1	B	306	GLN	CA-C	-6.29	1.44	1.52
1	A	324	THR	CB-CG2	-6.29	1.31	1.52
1	B	38	LEU	CG-CD1	-6.29	1.31	1.52
1	B	191	PHE	CE2-CZ	-6.28	1.19	1.38
1	B	208	ARG	CA-C	-6.28	1.43	1.52
1	A	95	PHE	CA-C	-6.27	1.44	1.53
1	A	188	HIS	C-O	-6.27	1.16	1.23
1	A	262	THR	C-O	-6.27	1.16	1.23
1	A	276	GLU	CA-CB	-6.26	1.43	1.54
1	A	226	ALA	CA-C	-6.26	1.45	1.52
1	A	258	TRP	CE2-CZ2	-6.26	1.26	1.39
1	A	126	VAL	CA-C	-6.26	1.44	1.52
1	A	222	ILE	CA-C	-6.26	1.44	1.52
1	A	297	GLU	N-CA	-6.26	1.38	1.46
1	A	137	GLN	CA-C	-6.26	1.44	1.52
1	B	293	SER	CA-C	-6.26	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	VAL	CA-C	-6.25	1.45	1.52
1	A	59	ALA	CA-C	-6.25	1.44	1.52
1	B	244	HIS	C-O	-6.25	1.16	1.24
1	B	151	SER	N-CA	-6.25	1.39	1.46
1	B	329	THR	C-O	-6.25	1.15	1.24
1	A	286	CYS	CA-C	-6.24	1.44	1.52
1	B	317	LYS	CA-C	-6.24	1.45	1.52
1	B	250	PHE	C-O	-6.24	1.17	1.24
1	A	344	ILE	N-CA	-6.23	1.38	1.46
1	A	176	ARG	CA-CB	-6.23	1.45	1.53
1	A	206	SER	CA-C	-6.23	1.44	1.52
1	A	269	ASN	N-CA	-6.23	1.37	1.45
1	A	303	ILE	CA-C	-6.23	1.44	1.52
1	A	99	ALA	CA-C	-6.22	1.44	1.52
1	A	242	ARG	N-CA	-6.22	1.37	1.46
1	B	318	GLU	C-O	-6.22	1.16	1.23
1	B	59	ALA	CA-CB	-6.21	1.41	1.52
1	B	240	MET	CG-SD	-6.21	1.65	1.80
1	B	201	VAL	CA-C	-6.21	1.45	1.52
1	A	156	LEU	CG-CD1	-6.21	1.32	1.52
1	A	152	ALA	CA-C	-6.21	1.44	1.52
1	A	292	GLY	CA-C	-6.20	1.45	1.52
1	A	40	GLY	CA-C	-6.20	1.45	1.51
1	B	286	CYS	C-O	-6.20	1.16	1.24
1	B	174	VAL	N-CA	-6.19	1.38	1.46
1	B	245	GLU	CA-C	-6.19	1.44	1.52
1	A	130	LEU	CA-C	-6.19	1.45	1.52
1	B	284	THR	CA-CB	-6.19	1.42	1.53
1	A	107	LEU	CG-CD1	-6.19	1.32	1.52
1	A	271	LYS	C-O	-6.18	1.16	1.24
1	B	41	ALA	N-CA	-6.18	1.38	1.45
1	A	283	LEU	C-O	-6.18	1.16	1.24
1	B	252	SER	CA-CB	-6.17	1.44	1.54
1	B	281	SER	CA-C	-6.17	1.47	1.52
1	A	109	VAL	C-O	-6.17	1.16	1.24
1	A	230	TYR	CA-C	-6.17	1.44	1.52
1	B	50	VAL	CA-CB	-6.17	1.46	1.54
1	B	290	TYR	C-O	-6.17	1.16	1.24
1	A	177	THR	C-O	-6.17	1.15	1.23
1	A	183	GLY	C-O	-6.17	1.15	1.23
1	A	299	ALA	C-O	-6.17	1.16	1.24
1	B	38	LEU	C-O	-6.17	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	LEU	CG-CD1	-6.16	1.32	1.52
1	A	327	THR	CA-CB	-6.16	1.43	1.53
1	A	234	LEU	CA-C	-6.16	1.44	1.52
1	B	140	PHE	N-CA	-6.16	1.38	1.46
2	D	4	GLY	C-O	-6.15	1.16	1.24
1	A	52	GLN	CB-CG	-6.15	1.33	1.52
1	B	195	HIS	C-O	-6.15	1.16	1.23
1	B	310	LEU	N-CA	-6.15	1.38	1.46
1	A	252	SER	C-O	-6.15	1.16	1.24
1	B	50	VAL	CB-CG2	-6.14	1.32	1.52
1	B	86	ARG	CA-C	-6.14	1.44	1.52
1	B	265	ILE	C-O	-6.14	1.15	1.24
1	A	108	PHE	C-O	-6.14	1.16	1.24
1	A	275	GLU	N-CA	-6.13	1.37	1.46
1	B	300	ALA	C-O	-6.13	1.16	1.24
1	A	214	CYS	CA-C	-6.13	1.45	1.53
1	B	202	GLY	CA-C	-6.13	1.46	1.52
1	A	48	THR	C-N	-6.13	1.27	1.33
1	A	133	ASP	N-CA	-6.13	1.38	1.46
2	D	11	VAL	CB-CG2	-6.13	1.32	1.52
1	A	337	ASP	CA-C	-6.12	1.45	1.52
1	A	331	ASN	C-N	-6.12	1.26	1.33
1	B	256	ASN	C-O	-6.12	1.15	1.23
1	A	298	GLU	C-O	-6.12	1.16	1.24
1	B	270	LYS	CA-C	-6.12	1.45	1.53
1	B	335	VAL	C-O	-6.11	1.16	1.24
1	B	283	LEU	N-CA	-6.10	1.38	1.46
1	B	284	THR	C-O	-6.10	1.16	1.24
1	A	234	LEU	CG-CD2	-6.10	1.32	1.52
1	A	248	LYS	CA-C	-6.10	1.44	1.52
1	A	274	PHE	CG-CD1	-6.09	1.26	1.38
1	A	307	PHE	CE1-CZ	-6.09	1.20	1.38
1	B	53	MET	SD-CE	-6.09	1.64	1.79
1	A	269	ASN	CA-CB	-6.08	1.42	1.54
1	B	171	GLN	C-O	-6.08	1.16	1.24
1	B	221	ILE	CB-CG2	-6.08	1.32	1.52
1	A	248	LYS	N-CA	-6.08	1.39	1.46
1	B	174	VAL	CB-CG2	-6.08	1.32	1.52
1	A	268	LEU	CG-CD2	-6.08	1.32	1.52
1	A	238	GLU	C-O	-6.07	1.16	1.24
1	B	42	GLY	C-O	-6.07	1.17	1.24
1	B	212	ILE	C-O	-6.07	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CA-C	-6.06	1.44	1.52
1	A	55	ILE	CA-C	-6.06	1.44	1.52
1	B	278	ILE	C-O	-6.05	1.16	1.24
1	A	136	VAL	CA-C	-6.05	1.43	1.52
1	A	94	ASP	C-O	-6.05	1.17	1.23
1	A	291	ALA	CA-C	-6.05	1.45	1.52
1	A	284	THR	N-CA	-6.05	1.38	1.46
1	A	48	THR	CB-CG2	-6.04	1.32	1.52
1	A	208	ARG	CZ-NH2	-6.04	1.25	1.33
1	A	266	LEU	CG-CD1	-6.04	1.32	1.52
1	B	151	SER	C-O	-6.04	1.15	1.24
1	A	137	GLN	C-O	-6.04	1.16	1.24
1	B	327	THR	C-O	-6.04	1.16	1.24
1	A	145	GLU	C-O	-6.04	1.15	1.24
1	A	304	GLN	C-O	-6.04	1.16	1.24
1	A	43	GLU	CA-CB	-6.04	1.44	1.53
1	B	64	GLU	N-CA	-6.03	1.39	1.46
1	A	36	LEU	CG-CD1	-6.03	1.32	1.52
1	B	243	MET	C-O	-6.03	1.16	1.24
1	B	209	LYS	N-CA	-6.03	1.38	1.46
1	A	323	PHE	C-O	-6.02	1.16	1.24
1	A	65	GLU	C-O	-6.02	1.17	1.24
1	B	36	LEU	C-O	-6.02	1.17	1.24
1	A	60	GLY	CA-C	-6.01	1.45	1.52
1	B	339	VAL	CA-C	-6.01	1.45	1.52
1	A	283	LEU	CA-C	-6.01	1.44	1.52
1	B	47	SER	C-O	-6.00	1.16	1.24
1	A	79	GLN	N-CA	-5.99	1.38	1.46
1	A	85	ILE	C-O	-5.99	1.17	1.24
1	A	91	LEU	CA-C	-5.99	1.44	1.52
1	A	143	SER	CA-C	-5.99	1.44	1.52
1	B	206	SER	C-O	-5.99	1.16	1.24
1	B	252	SER	N-CA	-5.99	1.37	1.45
2	C	7	HIS	C-O	-5.99	1.16	1.24
1	A	232	LEU	N-CA	-5.98	1.38	1.45
1	A	102	ASP	CA-C	-5.98	1.44	1.52
1	B	209	LYS	C-O	-5.97	1.16	1.24
1	B	314	LYS	CA-C	-5.97	1.44	1.52
1	A	332	VAL	C-O	-5.96	1.16	1.24
1	B	51	LYS	CA-C	-5.96	1.45	1.52
1	A	276	GLU	N-CA	-5.96	1.38	1.46
1	B	273	LEU	C-O	-5.96	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	ARG	C-O	-5.96	1.16	1.23
1	A	76	ASN	C-O	-5.96	1.16	1.24
1	A	53	MET	SD-CE	-5.96	1.64	1.79
1	A	216	GLU	C-O	-5.95	1.16	1.24
1	A	301	ALA	C-O	-5.95	1.16	1.24
1	A	135	GLY	C-O	-5.94	1.15	1.23
1	A	107	LEU	C-O	-5.94	1.17	1.24
1	B	262	THR	C-O	-5.94	1.16	1.24
1	A	128	LYS	N-CA	-5.93	1.38	1.46
1	B	197	LYS	N-CA	-5.92	1.39	1.46
1	B	244	HIS	N-CA	-5.92	1.38	1.46
1	B	259	PHE	C-O	-5.92	1.16	1.24
1	B	242	ARG	N-CA	-5.91	1.38	1.46
1	A	76	ASN	N-CA	-5.91	1.39	1.46
1	A	339	VAL	CA-CB	-5.91	1.46	1.54
1	A	109	VAL	CA-C	-5.91	1.45	1.52
1	A	268	LEU	CG-CD1	-5.91	1.33	1.52
1	B	197	LYS	C-O	-5.91	1.17	1.24
1	A	280	LYS	N-CA	-5.90	1.41	1.46
1	B	175	LEU	CA-C	-5.90	1.44	1.52
1	B	177	THR	C-O	-5.90	1.16	1.23
1	B	340	THR	CA-CB	-5.90	1.43	1.53
1	A	220	ALA	CA-C	-5.89	1.45	1.52
1	B	123	LEU	N-CA	-5.89	1.38	1.46
1	A	48	THR	CA-CB	-5.89	1.43	1.53
1	A	185	VAL	CB-CG2	-5.89	1.33	1.52
1	B	242	ARG	NE-CZ	-5.89	1.26	1.33
1	B	312	LYS	C-O	-5.89	1.15	1.24
1	A	170	THR	CA-C	-5.89	1.45	1.53
1	A	274	PHE	CE1-CZ	-5.89	1.21	1.38
1	A	100	ARG	NE-CZ	-5.88	1.26	1.33
1	A	205	ARG	N-CA	-5.88	1.38	1.46
1	B	162	ILE	CA-C	-5.88	1.45	1.53
1	B	327	THR	CA-CB	-5.88	1.44	1.53
1	A	246	SER	CA-C	-5.87	1.44	1.52
1	A	328	ASP	CA-C	-5.87	1.45	1.52
1	B	55	ILE	C-O	-5.87	1.17	1.24
1	B	227	LEU	N-CA	-5.87	1.38	1.46
1	B	221	ILE	CG1-CD1	-5.87	1.28	1.51
1	B	252	SER	C-O	-5.87	1.16	1.24
1	A	37	LEU	CA-C	-5.86	1.45	1.52
1	A	127	ILE	CB-CG2	-5.86	1.33	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	ILE	C-O	-5.86	1.16	1.23
1	A	150	ASP	N-CA	-5.86	1.38	1.46
1	B	190	THR	C-O	-5.86	1.16	1.23
1	B	208	ARG	C-O	-5.85	1.15	1.23
1	A	223	PHE	CE2-CZ	-5.85	1.21	1.38
1	A	252	SER	N-CA	-5.84	1.38	1.46
1	A	134	SER	C-O	-5.84	1.16	1.24
1	B	225	VAL	CA-C	-5.83	1.45	1.52
1	A	227	LEU	CA-C	-5.83	1.45	1.52
1	A	230	TYR	CE2-CZ	-5.83	1.24	1.38
1	A	56	ILE	CB-CG2	-5.83	1.33	1.52
1	A	176	ARG	NE-CZ	-5.83	1.26	1.33
1	A	208	ARG	CZ-NH1	-5.83	1.24	1.32
1	B	340	THR	C-O	-5.83	1.16	1.24
1	B	50	VAL	C-O	-5.82	1.17	1.24
1	A	270	LYS	N-CA	-5.82	1.38	1.46
1	A	315	ASP	CA-C	-5.82	1.47	1.52
1	B	282	PRO	CA-CB	-5.82	1.45	1.53
2	C	9	ILE	C-O	-5.82	1.18	1.24
2	D	11	VAL	N-CA	-5.82	1.39	1.46
1	A	299	ALA	CA-C	-5.82	1.44	1.52
1	B	274	PHE	CE2-CZ	-5.82	1.21	1.38
1	A	340	THR	C-O	-5.81	1.17	1.24
1	B	172	GLN	C-O	-5.80	1.16	1.24
1	A	144	ARG	CA-CB	-5.80	1.44	1.53
1	A	178	ARG	NE-CZ	-5.80	1.26	1.33
1	B	306	GLN	C-O	-5.80	1.16	1.24
1	A	158	ASP	CA-C	-5.79	1.44	1.53
1	A	280	LYS	CA-C	-5.78	1.46	1.52
1	A	272	ASP	CA-C	-5.78	1.44	1.52
1	A	109	VAL	N-CA	-5.78	1.39	1.46
1	B	292	GLY	C-O	-5.78	1.16	1.23
1	A	100	ARG	N-CA	-5.77	1.38	1.46
1	A	87	ALA	CA-C	-5.77	1.44	1.52
1	A	194	LEU	CA-C	-5.77	1.46	1.52
1	B	48	THR	C-O	-5.76	1.16	1.24
1	B	53	MET	CG-SD	-5.76	1.66	1.80
1	A	301	ALA	CA-C	-5.76	1.44	1.52
1	B	321	THR	C-O	-5.76	1.16	1.24
1	B	228	SER	C-O	-5.76	1.16	1.24
1	B	333	GLN	C-O	-5.76	1.16	1.24
1	A	55	ILE	C-O	-5.75	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	LEU	C-O	-5.75	1.17	1.24
1	B	319	ILE	CG1-CD1	-5.75	1.29	1.51
1	A	127	ILE	C-O	-5.75	1.17	1.23
1	B	46	LYS	C-O	-5.75	1.17	1.24
1	B	229	ASP	CA-C	-5.74	1.44	1.52
1	A	146	TYR	C-O	-5.74	1.17	1.23
1	A	258	TRP	CE3-CZ3	-5.74	1.21	1.38
1	B	172	GLN	N-CA	-5.74	1.39	1.46
1	B	229	ASP	C-O	-5.74	1.16	1.24
1	B	302	TYR	N-CA	-5.74	1.39	1.46
1	B	226	ALA	N-CA	-5.74	1.39	1.46
1	B	337	ASP	CA-C	-5.74	1.45	1.52
1	B	247	MET	C-O	-5.74	1.15	1.23
1	A	196	PHE	CA-C	-5.73	1.45	1.52
1	B	268	LEU	N-CA	-5.73	1.39	1.46
1	B	323	PHE	CE1-CZ	-5.73	1.21	1.38
1	B	323	PHE	CE2-CZ	-5.73	1.21	1.38
1	B	342	VAL	CB-CG2	-5.72	1.33	1.52
1	A	344	ILE	CA-C	-5.72	1.45	1.52
1	B	69	TYR	N-CA	-5.71	1.38	1.46
1	A	56	ILE	C-O	-5.71	1.17	1.24
1	A	92	LYS	CA-C	-5.71	1.45	1.52
1	A	294	ASN	C-O	-5.70	1.17	1.23
1	A	95	PHE	N-CA	-5.70	1.38	1.45
1	A	213	HIS	N-CA	-5.70	1.38	1.46
1	A	89	GLY	C-N	5.69	1.41	1.33
1	B	169	PRO	CA-C	-5.68	1.44	1.52
1	A	130	LEU	C-O	-5.68	1.16	1.23
1	A	164	GLN	CA-C	-5.68	1.45	1.52
1	B	148	LEU	C-O	-5.68	1.17	1.23
1	A	187	THR	C-O	-5.68	1.17	1.23
1	A	90	ARG	CA-C	-5.68	1.45	1.52
1	B	172	GLN	CA-C	-5.68	1.45	1.52
1	B	302	TYR	C-O	-5.67	1.17	1.24
1	B	68	GLN	CA-C	-5.67	1.45	1.52
1	B	248	LYS	N-CA	-5.67	1.38	1.46
1	A	267	PHE	CA-C	-5.67	1.45	1.52
1	A	269	ASN	CB-CG	-5.67	1.37	1.52
1	B	82	ILE	CA-C	-5.67	1.45	1.52
1	A	85	ILE	N-CA	-5.66	1.39	1.46
1	A	264	ILE	CB-CG2	-5.66	1.33	1.52
1	A	304	GLN	CA-C	-5.66	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	VAL	CB-CG1	-5.66	1.33	1.52
2	C	6	TYR	C-O	-5.66	1.15	1.23
1	A	85	ILE	CB-CG2	-5.66	1.33	1.52
1	B	212	ILE	CA-CB	-5.66	1.47	1.54
1	A	99	ALA	N-CA	-5.65	1.38	1.46
1	B	313	ARG	CA-C	-5.65	1.45	1.53
1	B	181	THR	CB-CG2	-5.64	1.33	1.52
1	A	167	TYR	CA-C	-5.64	1.45	1.52
1	B	41	ALA	C-N	-5.64	1.28	1.33
1	B	298	GLU	N-CA	-5.64	1.38	1.46
1	A	157	ASN	C-O	-5.64	1.16	1.23
1	A	342	VAL	CB-CG1	-5.64	1.33	1.52
1	B	191	PHE	C-O	-5.64	1.16	1.23
1	A	223	PHE	CG-CD2	-5.64	1.27	1.38
1	A	230	TYR	N-CA	-5.64	1.39	1.46
1	A	247	MET	SD-CE	-5.63	1.65	1.79
1	B	299	ALA	C-O	-5.63	1.16	1.24
2	D	9	ILE	CA-C	-5.63	1.46	1.52
1	A	273	LEU	N-CA	-5.63	1.38	1.46
1	B	52	GLN	CB-CG	-5.63	1.35	1.52
1	B	276	GLU	C-O	-5.63	1.16	1.24
1	B	227	LEU	CG-CD1	-5.63	1.33	1.52
1	B	297	GLU	CA-C	-5.63	1.44	1.52
2	C	11	VAL	C-O	-5.63	1.18	1.24
1	A	73	VAL	CA-C	-5.62	1.45	1.52
1	B	269	ASN	C-O	-5.62	1.16	1.23
1	A	82	ILE	CG1-CD1	-5.62	1.29	1.51
1	A	197	LYS	CA-C	-5.62	1.46	1.52
1	B	250	PHE	CE2-CZ	-5.62	1.21	1.38
1	B	272	ASP	N-CA	-5.62	1.39	1.46
1	B	197	LYS	CA-C	-5.62	1.46	1.52
1	A	232	LEU	CG-CD1	-5.62	1.34	1.52
1	B	284	THR	CA-C	-5.62	1.45	1.52
1	B	271	LYS	N-CA	-5.61	1.38	1.46
1	B	234	LEU	C-O	-5.61	1.16	1.23
1	A	82	ILE	CB-CG2	-5.61	1.34	1.52
1	A	225	VAL	CA-C	-5.61	1.45	1.52
1	B	34	VAL	C-O	-5.61	1.18	1.24
1	B	211	TRP	CA-C	-5.61	1.45	1.52
1	B	277	LYS	C-O	-5.61	1.17	1.24
1	A	101	ALA	CA-C	-5.60	1.45	1.52
1	B	198	MET	CA-C	-5.60	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	PRO	C-O	-5.60	1.16	1.24
1	B	223	PHE	CA-C	-5.60	1.46	1.52
1	B	34	VAL	CA-CB	-5.60	1.46	1.53
1	B	72	VAL	CA-C	-5.59	1.45	1.52
1	B	220	ALA	N-CA	-5.59	1.39	1.46
1	A	84	ILE	CA-C	-5.59	1.46	1.52
1	B	289	GLU	CA-C	-5.59	1.44	1.52
1	B	307	PHE	CE1-CZ	-5.59	1.21	1.38
1	B	64	GLU	CA-C	-5.59	1.46	1.52
1	B	344	ILE	CB-CG2	-5.59	1.34	1.52
1	A	65	GLU	CA-C	-5.59	1.46	1.52
1	B	253	ILE	CB-CG2	-5.58	1.34	1.52
1	A	295	THR	CA-CB	-5.58	1.43	1.54
1	A	237	ASP	N-CA	-5.58	1.39	1.46
1	A	165	PRO	CA-CB	-5.58	1.46	1.53
1	B	216	GLU	C-O	-5.58	1.17	1.24
1	B	50	VAL	CB-CG1	-5.57	1.34	1.52
1	B	149	ASN	N-CA	-5.57	1.38	1.46
1	B	319	ILE	CA-C	-5.57	1.46	1.52
1	A	222	ILE	N-CA	-5.57	1.38	1.46
1	B	176	ARG	C-O	-5.57	1.16	1.24
1	A	292	GLY	N-CA	-5.57	1.39	1.44
1	B	270	LYS	CA-CB	-5.57	1.45	1.53
1	A	242	ARG	CA-CB	-5.57	1.44	1.53
1	A	291	ALA	N-CA	-5.57	1.40	1.46
1	A	344	ILE	CB-CG2	-5.57	1.34	1.52
1	A	78	ILE	CA-C	-5.56	1.45	1.52
1	A	39	LEU	CG-CD1	-5.56	1.34	1.52
1	B	285	ILE	CA-C	-5.56	1.45	1.52
1	B	343	ILE	CG1-CD1	-5.56	1.30	1.51
1	A	145	GLU	N-CA	-5.56	1.39	1.46
1	B	199	PHE	CE1-CZ	-5.56	1.22	1.38
1	B	227	LEU	CA-C	-5.56	1.45	1.52
1	A	133	ASP	CB-CG	-5.55	1.38	1.52
1	B	52	GLN	C-O	-5.55	1.17	1.24
1	A	84	ILE	CB-CG2	-5.55	1.34	1.52
1	A	126	VAL	N-CA	-5.55	1.39	1.46
1	B	93	ILE	CA-C	-5.55	1.45	1.52
1	B	219	THR	C-O	-5.55	1.17	1.24
1	B	149	ASN	CA-C	-5.55	1.45	1.52
1	B	268	LEU	C-O	-5.55	1.17	1.24
1	A	287	TYR	CE2-CZ	-5.54	1.25	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	VAL	N-CA	-5.54	1.39	1.46
1	B	265	ILE	CB-CG2	-5.54	1.34	1.52
1	B	178	ARG	NE-CZ	-5.54	1.26	1.33
1	B	266	LEU	CG-CD1	-5.54	1.34	1.52
1	B	278	ILE	CB-CG2	-5.54	1.34	1.52
1	A	267	PHE	CE2-CZ	-5.54	1.22	1.38
1	B	151	SER	CA-C	-5.54	1.44	1.52
1	B	246	SER	N-CA	-5.54	1.38	1.46
1	A	211	TRP	C-O	-5.54	1.16	1.24
1	B	225	VAL	CB-CG2	-5.54	1.34	1.52
1	A	169	PRO	C-O	-5.53	1.17	1.23
1	A	189	PHE	CA-C	-5.53	1.45	1.52
1	B	101	ALA	CA-CB	-5.53	1.44	1.53
1	A	260	THR	C-O	-5.53	1.17	1.24
1	A	51	LYS	CA-C	-5.53	1.45	1.52
1	A	254	CYS	C-O	-5.53	1.17	1.24
1	B	173	ASP	CB-CG	-5.53	1.38	1.52
1	B	294	ASN	CA-C	-5.53	1.45	1.52
1	A	243	MET	C-O	-5.53	1.17	1.24
1	A	105	ARG	CA-C	-5.52	1.44	1.52
1	A	244	HIS	C-O	-5.52	1.17	1.24
1	B	297	GLU	C-O	-5.52	1.16	1.24
1	A	181	THR	CA-C	-5.52	1.46	1.52
1	B	137	GLN	CA-C	-5.51	1.45	1.52
1	B	300	ALA	N-CA	-5.51	1.38	1.46
1	A	43	GLU	C-O	-5.51	1.15	1.23
1	B	268	LEU	CA-C	-5.51	1.45	1.52
1	A	192	LYS	CA-C	-5.51	1.44	1.52
1	A	221	ILE	CG1-CD1	-5.51	1.30	1.51
1	A	287	TYR	N-CA	-5.51	1.40	1.46
1	B	56	ILE	CB-CG2	-5.50	1.34	1.52
1	B	191	PHE	CG-CD1	-5.50	1.27	1.38
1	B	185	VAL	CB-CG2	-5.50	1.34	1.52
1	A	77	THR	CB-CG2	-5.49	1.34	1.52
1	A	208	ARG	C-O	-5.49	1.17	1.24
1	A	317	LYS	C-O	-5.49	1.17	1.24
1	B	250	PHE	CE1-CZ	-5.49	1.22	1.38
1	B	45	GLY	CA-C	-5.49	1.44	1.51
1	B	218	VAL	CB-CG1	-5.49	1.34	1.52
1	B	279	LYS	C-O	-5.49	1.17	1.24
1	A	196	PHE	C-O	-5.48	1.17	1.23
1	A	342	VAL	C-O	-5.48	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	PHE	C-O	-5.48	1.17	1.24
1	B	154	TYR	C-O	-5.48	1.17	1.24
1	A	38	LEU	CG-CD1	-5.47	1.34	1.52
1	A	336	PHE	C-O	-5.47	1.16	1.24
1	A	136	VAL	N-CA	-5.47	1.38	1.46
1	A	75	SER	CA-C	-5.47	1.46	1.52
1	A	223	PHE	CE1-CZ	-5.47	1.22	1.38
1	A	257	LYS	N-CA	-5.47	1.38	1.46
1	B	308	GLU	CD-OE1	-5.47	1.15	1.25
1	B	222	ILE	CB-CG2	-5.46	1.34	1.52
1	A	249	LEU	CG-CD1	-5.46	1.34	1.52
1	A	72	VAL	CA-C	-5.46	1.46	1.52
1	B	170	THR	CB-CG2	-5.46	1.34	1.52
1	B	223	PHE	CA-CB	-5.46	1.46	1.53
1	A	85	ILE	CA-C	-5.45	1.45	1.52
1	A	170	THR	CB-CG2	-5.45	1.34	1.52
1	A	232	LEU	CA-C	-5.45	1.46	1.52
1	B	150	ASP	CA-C	-5.45	1.45	1.52
1	A	142	ARG	C-O	-5.45	1.15	1.23
1	A	231	ASP	CA-CB	-5.45	1.46	1.53
1	B	44	SER	CA-C	-5.44	1.45	1.52
1	A	233	VAL	CB-CG2	-5.44	1.34	1.52
1	B	309	ASP	C-O	-5.44	1.16	1.24
1	A	111	ALA	CA-CB	-5.44	1.34	1.52
1	A	283	LEU	N-CA	-5.43	1.39	1.46
1	B	316	THR	CB-CG2	-5.43	1.34	1.52
1	B	335	VAL	CB-CG1	-5.43	1.34	1.52
1	A	230	TYR	C-O	-5.43	1.17	1.24
1	B	270	LYS	CB-CG	-5.43	1.36	1.52
1	B	330	LYS	C-O	-5.42	1.17	1.24
1	B	83	ALA	CA-C	-5.42	1.45	1.52
1	A	132	LYS	CA-CB	-5.42	1.45	1.53
1	A	275	GLU	C-O	-5.42	1.16	1.24
1	B	191	PHE	CA-C	-5.42	1.46	1.52
1	B	339	VAL	CB-CG2	-5.42	1.34	1.52
1	A	260	THR	N-CA	-5.41	1.38	1.45
1	A	302	TYR	CE2-CZ	-5.41	1.25	1.38
1	B	247	MET	CA-C	-5.41	1.45	1.52
1	A	242	ARG	CA-C	-5.41	1.45	1.52
1	A	247	MET	CA-CB	-5.41	1.44	1.53
1	A	270	LYS	CA-C	-5.40	1.45	1.52
1	B	266	LEU	N-CA	-5.40	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	MET	N-CA	-5.40	1.35	1.46
1	A	46	LYS	CA-C	-5.40	1.45	1.52
1	A	208	ARG	N-CA	-5.40	1.38	1.46
1	A	250	PHE	CA-C	-5.40	1.45	1.52
1	B	245	GLU	N-CA	-5.40	1.39	1.46
1	A	88	MET	CA-C	-5.40	1.46	1.53
1	A	144	ARG	CB-CG	-5.39	1.36	1.52
1	A	201	VAL	CB-CG2	-5.39	1.34	1.52
1	B	175	LEU	C-O	-5.39	1.16	1.24
1	A	208	ARG	CG-CD	-5.39	1.36	1.52
2	D	9	ILE	N-CA	-5.39	1.40	1.46
1	A	277	LYS	CA-C	-5.39	1.45	1.52
1	A	281	SER	CA-C	-5.38	1.47	1.52
1	A	74	TYR	C-O	-5.38	1.16	1.23
1	A	302	TYR	CG-CD1	-5.38	1.28	1.39
2	D	9	ILE	CA-CB	-5.38	1.45	1.54
1	A	35	LYS	CA-C	-5.38	1.46	1.52
1	A	42	GLY	CA-C	-5.38	1.45	1.52
1	B	296	TYR	C-O	-5.37	1.17	1.24
1	A	88	MET	SD-CE	-5.37	1.66	1.79
1	A	174	VAL	CB-CG2	-5.37	1.34	1.52
1	A	281	SER	C-O	-5.37	1.16	1.24
1	B	157	ASN	C-O	-5.37	1.17	1.24
1	B	201	VAL	CB-CG1	-5.37	1.34	1.52
1	A	296	TYR	N-CA	-5.37	1.39	1.46
1	B	179	VAL	CB-CG1	-5.37	1.34	1.52
1	B	218	VAL	CB-CG2	-5.37	1.34	1.52
1	B	247	MET	SD-CE	-5.37	1.66	1.79
1	B	182	THR	CB-CG2	-5.37	1.34	1.52
1	B	305	CYS	CA-C	-5.37	1.45	1.52
1	A	128	LYS	CA-CB	-5.37	1.44	1.53
1	A	250	PHE	C-O	-5.37	1.18	1.24
1	A	43	GLU	N-CA	-5.36	1.38	1.46
1	B	232	LEU	C-O	-5.36	1.16	1.23
1	B	282	PRO	N-CA	-5.36	1.40	1.47
1	B	326	ALA	CA-C	-5.36	1.45	1.52
1	A	106	GLN	C-O	-5.36	1.17	1.24
2	C	11	VAL	CA-C	-5.36	1.45	1.52
1	A	285	ILE	CA-C	-5.36	1.45	1.53
1	A	285	ILE	CB-CG2	-5.36	1.34	1.52
1	B	53	MET	C-O	-5.36	1.16	1.24
1	A	244	HIS	N-CA	-5.35	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ALA	N-CA	-5.35	1.39	1.46
1	B	233	VAL	CB-CG2	-5.35	1.34	1.52
1	A	248	LYS	CA-CB	-5.35	1.45	1.53
1	A	327	THR	CB-CG2	-5.35	1.34	1.52
1	A	215	PHE	C-O	-5.34	1.16	1.23
1	B	182	THR	C-O	-5.34	1.17	1.23
1	A	79	GLN	CA-C	-5.34	1.45	1.52
1	A	101	ALA	C-O	-5.34	1.17	1.24
1	A	168	ILE	C-O	-5.34	1.17	1.24
1	A	194	LEU	C-O	-5.34	1.17	1.23
1	A	302	TYR	C-O	-5.34	1.18	1.24
1	B	285	ILE	C-O	-5.34	1.18	1.24
1	A	59	ALA	N-CA	-5.33	1.39	1.46
1	A	249	LEU	N-CA	-5.33	1.40	1.46
1	A	100	ARG	CA-CB	-5.33	1.44	1.53
1	B	184	ILE	C-O	-5.33	1.17	1.24
1	B	317	LYS	C-O	-5.33	1.18	1.23
1	B	330	LYS	CA-C	-5.33	1.45	1.52
1	A	69	TYR	CE1-CZ	-5.32	1.25	1.38
1	A	235	ALA	C-O	-5.32	1.17	1.24
1	A	174	VAL	CB-CG1	-5.32	1.35	1.52
1	A	253	ILE	CA-CB	-5.32	1.46	1.54
1	B	315	ASP	C-O	-5.32	1.17	1.24
1	B	73	VAL	N-CA	-5.31	1.38	1.46
1	B	93	ILE	N-CA	-5.31	1.39	1.46
1	B	199	PHE	CE2-CZ	-5.31	1.22	1.38
1	B	223	PHE	C-O	-5.31	1.17	1.24
1	B	257	LYS	N-CA	-5.31	1.38	1.46
1	A	199	PHE	CE2-CZ	-5.30	1.22	1.38
1	B	48	THR	CB-CG2	-5.30	1.35	1.52
1	B	303	ILE	CB-CG2	-5.30	1.35	1.52
1	A	102	ASP	C-O	-5.30	1.17	1.24
1	A	188	HIS	CA-C	-5.30	1.46	1.52
1	B	258	TRP	C-O	-5.30	1.17	1.24
1	B	327	THR	CA-C	-5.30	1.45	1.52
1	B	171	GLN	CA-CB	-5.29	1.44	1.53
1	A	156	LEU	C-O	-5.29	1.17	1.24
1	B	189	PHE	C-O	-5.29	1.18	1.23
1	B	312	LYS	CA-C	-5.29	1.45	1.52
2	D	12	GLY	C-O	-5.29	1.16	1.23
1	B	235	ALA	N-CA	-5.29	1.39	1.46
1	A	50	VAL	CB-CG2	-5.29	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	GLN	N-CA	-5.29	1.39	1.46
1	A	251	ASP	CA-C	-5.29	1.45	1.52
1	B	191	PHE	N-CA	-5.29	1.40	1.46
1	B	299	ALA	CA-C	-5.28	1.45	1.52
2	C	11	VAL	N-CA	-5.28	1.41	1.46
1	A	154	TYR	CE1-CZ	-5.28	1.25	1.38
1	A	196	PHE	CG-CD1	-5.28	1.27	1.38
1	A	232	LEU	CG-CD2	-5.28	1.35	1.52
1	A	145	GLU	CA-C	-5.27	1.45	1.52
1	B	154	TYR	CA-C	-5.27	1.45	1.52
1	A	69	TYR	C-O	-5.27	1.17	1.23
1	A	306	GLN	C-O	-5.27	1.17	1.24
1	A	75	SER	N-CA	-5.26	1.40	1.46
1	B	213	HIS	N-CA	-5.26	1.39	1.46
1	A	49	ILE	CG1-CD1	-5.26	1.31	1.51
1	B	68	GLN	CB-CG	-5.26	1.36	1.52
1	B	136	VAL	C-O	-5.25	1.19	1.24
1	B	208	ARG	CZ-NH2	-5.25	1.26	1.33
1	A	95	PHE	CE2-CZ	-5.25	1.23	1.38
1	B	290	TYR	CG-CD2	-5.25	1.28	1.39
1	A	77	THR	CA-CB	-5.25	1.45	1.53
1	B	290	TYR	CD1-CE1	-5.24	1.23	1.38
1	B	296	TYR	CA-C	-5.24	1.45	1.52
1	A	90	ARG	C-O	-5.23	1.17	1.24
1	B	238	GLU	CA-C	-5.23	1.45	1.52
1	B	143	SER	N-CA	-5.23	1.39	1.46
1	A	166	ASN	CA-C	-5.23	1.45	1.52
1	A	184	ILE	C-O	-5.23	1.18	1.24
1	A	240	MET	SD-CE	-5.23	1.66	1.79
1	A	274	PHE	CD2-CE2	-5.22	1.23	1.38
1	A	294	ASN	CA-CB	-5.22	1.46	1.53
1	B	241	ASN	N-CA	-5.22	1.39	1.46
1	A	324	THR	C-O	-5.22	1.17	1.23
1	B	134	SER	CA-C	-5.22	1.45	1.52
1	B	273	LEU	CG-CD1	-5.22	1.35	1.52
1	B	271	LYS	C-O	-5.22	1.17	1.24
1	B	237	ASP	CA-C	-5.21	1.47	1.53
1	B	80	SER	CA-C	-5.21	1.45	1.52
1	B	326	ALA	C-O	-5.21	1.17	1.24
1	A	341	ASP	C-N	-5.20	1.26	1.33
1	B	37	LEU	CA-C	-5.20	1.46	1.52
1	B	303	ILE	CA-C	-5.20	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	ASP	CA-C	-5.20	1.45	1.52
1	A	140	PHE	C-O	-5.20	1.16	1.23
1	A	179	VAL	N-CA	-5.20	1.39	1.46
1	B	138	ALA	CA-CB	-5.19	1.44	1.53
1	B	210	LYS	CA-C	-5.19	1.45	1.52
1	B	154	TYR	CE2-CZ	-5.19	1.25	1.38
1	B	62	SER	CA-C	-5.18	1.46	1.52
1	B	148	LEU	CG-CD1	-5.18	1.35	1.52
1	A	259	PHE	CG-CD1	-5.18	1.27	1.38
1	A	137	GLN	CG-CD	-5.17	1.39	1.52
1	A	168	ILE	N-CA	-5.17	1.40	1.46
1	A	221	ILE	CB-CG2	-5.17	1.35	1.52
1	B	323	PHE	CA-C	-5.17	1.46	1.52
1	A	310	LEU	N-CA	-5.17	1.39	1.46
1	A	34	VAL	C-O	-5.17	1.18	1.24
1	A	173	ASP	CA-C	-5.17	1.45	1.52
1	A	222	ILE	CB-CG2	-5.17	1.35	1.52
1	A	44	SER	CA-CB	-5.17	1.44	1.53
1	A	282	PRO	CA-CB	-5.17	1.46	1.53
1	B	342	VAL	C-N	-5.16	1.28	1.33
1	B	136	VAL	CA-CB	-5.16	1.48	1.54
1	A	206	SER	C-O	-5.16	1.17	1.24
1	A	265	ILE	N-CA	-5.16	1.40	1.46
1	B	335	VAL	CB-CG2	-5.16	1.35	1.52
1	B	46	LYS	N-CA	-5.16	1.40	1.46
1	A	218	VAL	CB-CG2	-5.16	1.35	1.52
1	A	193	ASP	C-O	-5.16	1.17	1.24
1	B	49	ILE	CG1-CD1	-5.16	1.31	1.51
1	B	257	LYS	CA-CB	-5.16	1.46	1.54
2	C	7	HIS	N-CA	-5.16	1.39	1.46
2	C	9	ILE	N-CA	-5.16	1.40	1.46
2	D	10	TRP	N-CA	-5.16	1.39	1.46
1	A	152	ALA	N-CA	-5.15	1.39	1.46
1	B	144	ARG	CA-C	-5.15	1.45	1.52
1	A	340	THR	N-CA	-5.15	1.40	1.46
1	A	272	ASP	C-O	-5.15	1.17	1.24
1	B	318	GLU	CA-C	-5.15	1.46	1.52
2	D	6	TYR	CA-CB	-5.15	1.47	1.53
1	A	311	ASN	CG-OD1	-5.15	1.13	1.23
1	B	180	LYS	C-O	-5.15	1.17	1.23
1	B	267	PHE	CE2-CZ	-5.14	1.23	1.38
1	A	273	LEU	CA-CB	-5.14	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	VAL	C-O	-5.14	1.18	1.24
1	A	161	ARG	NE-CZ	-5.13	1.27	1.33
1	B	290	TYR	CE1-CZ	-5.13	1.25	1.38
1	A	39	LEU	CA-C	-5.13	1.46	1.52
1	A	237	ASP	C-O	-5.12	1.17	1.24
1	A	67	LYS	C-O	-5.12	1.17	1.24
1	A	219	THR	CB-CG2	-5.12	1.35	1.52
1	B	243	MET	SD-CE	-5.12	1.66	1.79
1	A	267	PHE	CE1-CZ	-5.12	1.23	1.38
1	A	307	PHE	C-O	-5.12	1.16	1.23
1	A	332	VAL	CB-CG1	-5.12	1.35	1.52
1	B	37	LEU	CG-CD1	-5.12	1.35	1.52
1	A	291	ALA	C-N	-5.12	1.28	1.33
1	B	176	ARG	CZ-NH2	-5.11	1.26	1.33
1	A	96	GLY	C-O	-5.11	1.17	1.23
1	A	172	GLN	CD-NE2	-5.11	1.22	1.33
1	B	50	VAL	CA-C	-5.11	1.46	1.52
1	B	157	ASN	CA-C	-5.11	1.46	1.52
1	B	187	THR	CA-C	-5.11	1.46	1.52
1	B	260	THR	CB-CG2	-5.11	1.35	1.52
1	A	209	LYS	N-CA	-5.11	1.40	1.46
1	B	57	HIS	CA-C	-5.11	1.46	1.52
1	B	184	ILE	CG1-CD1	-5.11	1.31	1.51
1	B	278	ILE	CA-C	-5.11	1.46	1.52
1	A	46	LYS	N-CA	-5.11	1.40	1.46
1	B	272	ASP	CG-OD1	-5.10	1.15	1.25
1	B	68	GLN	CG-CD	-5.09	1.39	1.52
1	A	50	VAL	CB-CG1	-5.09	1.35	1.52
1	B	55	ILE	CG1-CD1	-5.09	1.31	1.51
1	B	321	THR	CA-CB	-5.09	1.44	1.53
1	A	210	LYS	C-O	-5.09	1.17	1.24
1	A	290	TYR	CE2-CZ	-5.09	1.26	1.38
1	A	234	LEU	CA-CB	-5.09	1.45	1.53
1	A	234	LEU	CG-CD1	-5.09	1.35	1.52
1	A	257	LYS	C-O	-5.09	1.17	1.24
1	A	345	LYS	CB-CG	-5.09	1.37	1.52
1	B	177	THR	CA-C	-5.09	1.46	1.52
1	A	290	TYR	CE1-CZ	-5.08	1.26	1.38
1	A	199	PHE	CG-CD2	-5.08	1.28	1.38
1	A	241	ASN	N-CA	-5.08	1.39	1.46
1	A	312	LYS	C-O	-5.08	1.17	1.23
1	B	230	TYR	CE2-CZ	-5.08	1.26	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	LEU	CG-CD2	-5.08	1.35	1.52
1	A	296	TYR	C-N	-5.08	1.27	1.33
1	A	124	ALA	C-O	-5.08	1.17	1.24
1	A	323	PHE	CE2-CZ	-5.07	1.23	1.38
1	B	194	LEU	N-CA	-5.07	1.39	1.45
1	B	298	GLU	C-O	-5.07	1.16	1.23
1	A	73	VAL	CB-CG2	-5.07	1.35	1.52
1	A	146	TYR	CD1-CE1	-5.07	1.23	1.38
1	A	321	THR	C-O	-5.07	1.17	1.24
2	D	9	ILE	CB-CG2	-5.07	1.35	1.52
1	B	290	TYR	CD2-CE2	-5.06	1.23	1.38
1	A	105	ARG	N-CA	-5.06	1.39	1.46
1	B	52	GLN	CA-C	-5.06	1.45	1.52
1	A	288	PRO	C-O	-5.06	1.17	1.24
1	A	335	VAL	C-O	-5.05	1.18	1.24
1	B	273	LEU	CG-CD2	-5.04	1.35	1.52
1	B	321	THR	CB-CG2	-5.04	1.35	1.52
1	B	289	GLU	C-O	-5.04	1.17	1.24
1	B	254	CYS	N-CA	-5.04	1.39	1.46
1	A	223	PHE	CD2-CE2	-5.04	1.23	1.38
1	A	250	PHE	CE1-CZ	-5.04	1.23	1.38
1	A	282	PRO	CA-C	-5.04	1.45	1.52
1	B	251	ASP	C-O	-5.04	1.17	1.24
1	A	219	THR	C-O	-5.03	1.16	1.23
1	B	161	ARG	NE-CZ	-5.03	1.27	1.33
1	B	231	ASP	CA-C	-5.03	1.46	1.52
1	A	92	LYS	N-CA	-5.03	1.39	1.46
1	B	146	TYR	C-O	-5.03	1.18	1.24
1	A	243	MET	CA-C	-5.02	1.46	1.52
1	B	279	LYS	CA-CB	-5.02	1.45	1.53
1	A	104	ALA	CA-C	-5.02	1.46	1.52
1	A	218	VAL	CB-CG1	-5.02	1.35	1.52
1	A	274	PHE	CD1-CE1	-5.02	1.23	1.38
1	B	190	THR	CB-CG2	-5.02	1.35	1.52
1	A	69	TYR	CE2-CZ	-5.01	1.26	1.38
1	B	319	ILE	N-CA	-5.01	1.40	1.46
1	A	65	GLU	N-CA	-5.01	1.40	1.46
1	B	196	PHE	CA-C	-5.01	1.46	1.52
1	A	273	LEU	C-O	-5.01	1.16	1.23
1	B	259	PHE	CE1-CZ	-5.01	1.23	1.38
1	A	230	TYR	CG-CD2	-5.01	1.28	1.39
1	A	294	ASN	CB-CG	-5.01	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	ILE	CB-CG2	-5.01	1.36	1.52
1	B	58	GLU	C-O	-5.01	1.18	1.23
1	A	302	TYR	CE1-CZ	-5.00	1.26	1.38
1	A	259	PHE	CE1-CZ	-5.00	1.23	1.38
1	B	191	PHE	CD1-CE1	-5.00	1.23	1.38
1	A	229	ASP	C-O	-5.00	1.17	1.24

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LEU	O-C-N	-77.33	40.38	123.13
1	A	109	VAL	CA-C-N	-54.51	10.61	123.99
1	A	109	VAL	C-N-CA	-54.51	10.61	123.99
1	B	95	PHE	CB-CA-C	-23.89	72.33	111.50
1	B	152	ALA	N-CA-C	20.39	136.77	111.69
1	B	81	ILE	N-CA-CB	-17.54	82.28	111.23
1	B	105	ARG	N-CA-C	17.05	147.12	110.80
1	A	341	ASP	CB-CA-C	-16.92	76.75	110.42
1	A	341	ASP	CA-C-N	16.86	152.32	121.97
1	A	341	ASP	C-N-CA	16.86	152.32	121.97
1	B	239	GLU	N-CA-CB	-16.49	83.53	110.40
1	B	95	PHE	N-CA-C	16.33	138.29	108.58
1	A	110	LEU	CA-C-N	16.14	150.75	121.70
1	A	110	LEU	C-N-CA	16.14	150.75	121.70
1	A	231	ASP	N-CA-C	15.67	133.96	111.87
1	A	50	VAL	N-CA-C	-15.66	99.21	111.90
1	B	126	VAL	N-CA-C	15.05	140.65	109.34
1	B	126	VAL	CB-CA-C	-14.98	86.72	111.29
1	B	183	GLY	N-CA-C	14.24	146.93	113.18
1	B	64	GLU	N-CA-C	-14.22	94.51	112.72
1	B	105	ARG	CB-CA-C	-13.90	82.77	110.42
1	B	81	ILE	CA-C-N	-13.78	97.16	121.97
1	B	81	ILE	C-N-CA	-13.78	97.16	121.97
1	A	109	VAL	O-C-N	-13.76	105.37	122.57
1	B	152	ALA	CB-CA-C	-13.52	85.97	110.70
1	B	139	CYS	N-CA-C	13.24	125.44	111.14
1	B	107	LEU	N-CA-C	12.73	137.93	110.80
1	B	257	LYS	N-CA-CB	-12.39	94.52	111.00
1	B	107	LEU	CB-CA-C	-12.35	85.85	110.42
1	A	273	LEU	N-CA-C	-11.83	99.33	113.88
1	A	103	ASP	N-CA-C	-11.72	99.00	113.18
2	C	7	HIS	N-CA-C	-11.66	85.97	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ALA	CB-CA-C	-11.60	87.33	110.42
1	A	140	PHE	N-CA-C	-11.33	99.95	113.88
1	B	89	GLY	N-CA-C	10.84	138.87	113.18
2	C	11	VAL	CB-CA-C	-10.77	100.09	110.65
1	B	82	ILE	CB-CA-C	-10.54	94.01	111.29
1	A	127	ILE	N-CA-C	-10.45	101.74	111.67
1	B	152	ALA	CA-C-N	10.38	137.70	121.19
1	B	152	ALA	C-N-CA	10.38	137.70	121.19
1	B	76	ASN	N-CA-C	-10.34	99.83	111.82
1	A	334	PHE	N-CA-C	10.33	132.81	110.80
1	B	127	ILE	N-CA-CB	-10.27	94.29	111.23
1	B	99	ALA	CA-C-N	-10.25	101.97	121.54
1	B	99	ALA	C-N-CA	-10.25	101.97	121.54
1	A	157	ASN	N-CA-C	-10.24	100.27	113.17
1	B	136	VAL	N-CA-C	-10.16	98.45	113.39
1	B	204	GLN	N-CA-C	-10.14	91.42	108.75
1	B	150	ASP	N-CA-C	-10.09	99.52	112.23
1	B	297	GLU	N-CA-C	-10.09	100.72	113.23
1	B	88	MET	N-CA-C	-10.08	98.72	111.02
1	A	181	THR	N-CA-C	-10.07	92.82	109.24
1	B	125	GLY	N-CA-C	-10.04	100.09	113.24
1	A	74	TYR	N-CA-C	-10.02	101.56	113.88
1	B	329	THR	N-CA-C	-10.01	101.07	113.28
1	A	264	ILE	CB-CA-C	-9.95	98.92	110.96
1	B	49	ILE	N-CA-C	-9.93	103.80	113.53
1	A	47	SER	N-CA-C	-9.90	100.96	113.23
1	B	80	SER	CB-CA-C	-9.85	92.40	110.63
1	B	298	GLU	N-CA-C	-9.85	101.77	113.88
1	A	344	ILE	O-C-N	-9.73	110.41	122.57
1	B	100	ARG	N-CA-C	9.72	131.50	110.80
1	A	231	ASP	N-CA-CB	-9.61	96.39	111.39
1	A	110	LEU	CB-CA-C	-9.58	102.42	114.40
1	A	49	ILE	N-CA-C	-9.57	103.30	112.29
1	A	62	SER	N-CA-C	-9.50	93.66	109.80
1	A	310	LEU	N-CA-C	-9.49	99.55	112.94
1	B	82	ILE	N-CA-C	9.48	129.07	109.34
1	B	139	CYS	N-CA-CB	-9.41	96.43	110.07
1	B	208	ARG	N-CA-C	-9.33	101.42	113.17
1	B	91	LEU	N-CA-C	-9.32	102.42	113.88
1	B	247	MET	N-CA-C	-9.22	102.53	113.88
1	B	138	ALA	N-CA-C	9.17	130.34	110.80
1	B	175	LEU	N-CA-C	-9.13	102.15	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	GLU	N-CA-C	9.10	123.94	113.02
1	A	205	ARG	N-CA-C	-9.09	100.99	112.90
1	A	152	ALA	CB-CA-C	-9.04	92.43	110.42
1	B	49	ILE	CB-CA-C	-8.98	101.85	110.65
1	B	101	ALA	N-CA-C	-8.97	102.51	113.19
1	B	72	VAL	CB-CA-C	-8.86	100.43	112.04
1	A	316	THR	N-CA-C	8.79	120.87	111.28
1	B	59	ALA	CB-CA-C	-8.79	106.43	116.54
1	A	110	LEU	N-CA-CB	-8.74	98.21	108.96
1	B	165	PRO	N-CD-CG	-8.74	90.09	103.20
1	B	310	LEU	N-CA-C	-8.72	102.19	112.92
1	A	91	LEU	N-CA-C	-8.72	102.18	113.17
1	A	239	GLU	N-CA-CB	-8.71	97.84	110.47
1	B	239	GLU	N-CA-C	8.69	123.66	112.89
1	A	99	ALA	N-CA-C	-8.64	102.44	113.16
1	A	147	GLN	N-CA-C	8.61	122.93	108.20
1	A	344	ILE	CB-CA-C	8.54	125.30	111.29
1	A	257	LYS	N-CA-C	-8.53	102.79	113.02
1	B	184	ILE	N-CA-C	8.47	126.96	109.34
1	B	334	PHE	N-CA-C	-8.43	101.60	112.23
1	B	255	ASN	N-CA-C	-8.38	102.25	114.39
1	A	335	VAL	N-CA-C	8.36	126.73	109.34
1	A	252	SER	N-CA-C	-8.34	103.24	113.50
1	B	133	ASP	N-CA-C	-8.28	100.23	110.41
1	A	89	GLY	CA-C-N	8.27	137.34	121.54
1	A	89	GLY	C-N-CA	8.27	137.34	121.54
1	A	296	TYR	N-CA-C	-8.22	102.32	111.28
1	A	64	GLU	N-CA-C	-8.19	103.29	113.28
1	B	86	ARG	N-CA-C	-8.11	101.37	111.75
1	A	300	ALA	N-CA-C	-8.02	102.75	112.54
1	B	236	GLU	N-CA-C	-8.01	103.45	113.55
1	B	341	ASP	N-CA-C	-7.92	101.95	111.69
1	A	139	CYS	N-CA-C	-7.92	102.67	112.88
1	A	208	ARG	N-CA-C	-7.84	103.60	113.01
1	B	148	LEU	N-CA-C	7.84	121.62	108.13
1	A	152	ALA	N-CA-C	7.83	127.47	110.80
1	B	59	ALA	CA-C-N	7.81	136.71	121.41
1	B	59	ALA	C-N-CA	7.81	136.71	121.41
1	A	233	VAL	CB-CA-C	-7.79	100.52	111.19
1	B	173	ASP	N-CA-C	-7.72	103.31	112.89
1	A	153	ALA	N-CA-C	7.72	122.46	112.89
1	B	343	ILE	N-CA-C	-7.71	102.97	112.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ALA	N-CA-C	-7.70	104.03	113.50
1	B	100	ARG	N-CA-CB	-7.68	97.51	110.49
1	A	100	ARG	N-CA-C	-7.68	103.50	113.17
1	A	34	VAL	CB-CA-C	7.67	123.86	111.29
1	B	99	ALA	N-CA-C	7.66	127.11	110.80
1	B	154	TYR	N-CA-C	-7.64	102.08	111.33
1	B	201	VAL	CB-CA-C	-7.59	99.58	110.82
1	B	180	LYS	N-CA-C	7.45	121.20	110.24
2	D	6	TYR	CA-C-N	-7.43	112.10	123.17
2	D	6	TYR	C-N-CA	-7.43	112.10	123.17
1	B	252	SER	N-CA-C	-7.41	104.08	113.72
1	B	104	ALA	N-CA-C	-7.38	97.08	108.00
1	B	34	VAL	CB-CA-C	-7.36	101.42	110.99
1	A	335	VAL	N-CA-CB	-7.36	99.09	111.23
1	A	150	ASP	N-CA-C	-7.34	103.94	113.12
1	A	345	LYS	N-CA-C	7.32	131.50	111.00
2	D	11	VAL	CB-CA-C	-7.26	99.38	111.29
1	B	59	ALA	N-CA-C	-7.24	97.31	108.31
1	B	97	ASP	N-CA-C	-7.22	95.41	110.80
2	D	8	GLY	N-CA-C	-7.17	104.95	115.63
1	A	50	VAL	CB-CA-C	-7.14	104.45	111.30
1	B	274	PHE	N-CA-C	-7.13	102.53	112.45
1	B	99	ALA	O-C-N	7.13	132.08	122.59
1	A	341	ASP	N-CA-C	-7.13	95.61	110.80
1	B	162	ILE	N-CA-C	-7.11	105.61	112.29
1	B	244	HIS	N-CA-C	-7.11	103.59	112.90
1	A	69	TYR	N-CA-C	-7.10	104.88	113.97
1	A	332	VAL	N-CA-C	-7.06	102.69	112.50
1	A	194	LEU	N-CA-CB	-7.03	99.61	110.85
1	A	334	PHE	CB-CA-C	-7.01	96.47	110.42
1	A	255	ASN	N-CA-C	-7.00	101.85	110.61
1	B	239	GLU	CB-CA-C	7.00	124.61	109.99
1	A	236	GLU	N-CA-C	-6.97	104.51	113.16
1	B	82	ILE	N-CA-CB	-6.96	99.74	111.23
1	B	213	HIS	N-CA-C	-6.95	104.79	113.20
1	B	109	VAL	CB-CA-C	-6.95	102.92	112.02
1	B	55	ILE	N-CA-C	6.84	117.54	110.36
1	B	134	SER	N-CA-C	-6.83	103.95	112.90
1	B	256	ASN	CB-CA-C	-6.80	95.36	110.19
1	A	60	GLY	N-CA-C	-6.78	102.14	112.84
1	B	161	ARG	N-CA-C	-6.75	104.92	113.43
1	B	103	ASP	O-C-N	-6.71	113.66	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	SER	N-CA-C	-6.69	105.25	113.41
1	B	225	VAL	CB-CA-C	-6.68	100.22	110.50
1	B	313	ARG	N-CA-C	6.59	117.83	108.54
1	B	188	HIS	N-CA-C	6.56	120.52	109.76
1	A	53	MET	N-CA-C	-6.56	104.32	113.37
1	A	167	TYR	N-CA-C	-6.55	98.73	109.40
1	B	110	LEU	N-CA-C	-6.51	104.03	112.23
1	A	188	HIS	N-CA-C	6.50	120.29	109.95
1	B	57	HIS	N-CA-C	-6.49	104.61	113.30
1	B	257	LYS	N-CA-C	-6.48	106.33	114.56
1	A	194	LEU	N-CA-C	6.44	120.19	109.95
1	A	254	CYS	N-CA-C	-6.41	105.18	112.87
1	B	183	GLY	CA-C-N	6.36	133.42	121.97
1	B	183	GLY	C-N-CA	6.36	133.42	121.97
1	B	52	GLN	N-CA-C	6.35	120.49	112.87
1	B	138	ALA	CB-CA-C	-6.34	97.79	110.42
1	A	282	PRO	N-CD-CG	-6.33	93.70	103.20
1	A	156	LEU	N-CA-C	-6.33	105.38	113.23
1	B	291	ALA	CB-CA-C	-6.32	97.85	110.42
1	A	279	LYS	N-CA-C	-6.31	104.85	113.30
1	B	47	SER	N-CA-C	-6.31	105.07	112.89
1	B	285	ILE	N-CA-C	6.28	117.03	110.62
1	B	74	TYR	N-CA-C	-6.26	103.03	112.04
1	A	108	PHE	CA-C-N	-6.25	110.71	121.97
1	A	108	PHE	C-N-CA	-6.25	110.71	121.97
1	A	260	THR	N-CA-C	-6.23	105.46	114.12
1	B	187	THR	CB-CA-C	-6.22	101.16	110.24
1	B	265	ILE	CG1-CB-CG2	-6.17	92.18	110.70
1	A	333	GLN	CB-CA-C	-6.09	100.56	110.79
1	B	304	GLN	N-CA-C	-6.07	104.58	111.07
1	A	190	THR	OG1-CB-CG2	-6.05	97.19	109.30
1	B	179	VAL	CB-CA-C	-6.05	101.89	110.12
1	B	72	VAL	N-CA-C	6.05	117.52	110.62
1	A	63	GLU	N-CA-CB	-6.01	101.31	110.33
1	A	261	ASP	N-CA-C	-5.97	103.52	112.54
1	A	66	CYS	CB-CA-C	5.95	122.26	110.42
1	A	144	ARG	N-CA-C	-5.95	105.21	112.88
1	B	54	LYS	N-CA-C	-5.94	105.12	112.72
1	A	271	LYS	N-CA-C	-5.92	105.88	113.23
1	B	78	ILE	CB-CA-C	-5.90	101.62	111.29
1	A	155	TYR	N-CA-C	-5.88	106.26	113.50
1	A	145	GLU	N-CA-C	-5.87	105.70	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ALA	N-CA-CB	5.87	125.98	111.30
1	A	340	THR	N-CA-C	-5.86	104.53	111.03
1	A	276	GLU	CB-CA-C	-5.84	100.90	110.08
1	B	214	CYS	N-CA-C	5.84	121.18	112.94
1	A	318	GLU	N-CA-C	5.84	119.60	110.32
1	A	221	ILE	CB-CA-C	-5.81	101.55	110.50
1	B	151	SER	N-CA-C	-5.78	106.84	112.97
1	A	341	ASP	O-C-N	-5.76	114.93	122.59
1	B	260	THR	N-CA-C	-5.75	105.93	113.12
1	A	184	ILE	N-CA-C	5.75	116.87	108.53
1	B	104	ALA	CB-CA-C	-5.71	108.34	116.34
1	B	166	ASN	N-CA-C	-5.69	103.54	111.39
1	A	184	ILE	CB-CA-C	-5.67	102.19	110.81
1	B	271	LYS	N-CA-C	-5.65	106.43	113.38
2	D	7	HIS	N-CA-C	-5.63	103.13	111.81
1	B	270	LYS	N-CA-C	5.62	119.60	111.56
1	A	90	ARG	N-CA-CB	-5.62	100.99	110.49
1	B	103	ASP	CA-C-N	-5.62	110.19	122.04
1	B	103	ASP	C-N-CA	-5.62	110.19	122.04
2	C	6	TYR	CA-C-N	-5.60	110.85	121.54
2	C	6	TYR	C-N-CA	-5.60	110.85	121.54
1	B	127	ILE	CB-CA-C	-5.58	102.15	111.29
1	A	202	GLY	N-CA-C	5.57	123.30	112.04
1	A	165	PRO	N-CA-C	-5.57	103.11	111.57
1	B	194	LEU	N-CA-C	5.57	118.62	109.72
1	B	316	THR	OG1-CB-CG2	-5.56	98.17	109.30
1	B	80	SER	CA-C-N	-5.52	112.03	121.97
1	B	80	SER	C-N-CA	-5.52	112.03	121.97
1	A	92	LYS	N-CA-C	5.50	122.51	110.80
1	B	73	VAL	N-CA-C	-5.47	104.01	111.89
1	B	206	SER	CA-C-N	-5.47	113.76	122.29
1	B	206	SER	C-N-CA	-5.47	113.76	122.29
1	A	284	THR	OG1-CB-CG2	-5.46	98.38	109.30
1	A	130	LEU	N-CA-C	-5.46	105.42	112.68
1	B	55	ILE	CB-CA-C	-5.45	104.91	111.88
1	A	302	TYR	N-CA-C	-5.45	104.58	111.11
1	A	230	TYR	N-CA-C	5.44	122.38	110.80
1	A	83	ALA	N-CA-C	-5.42	106.83	113.50
1	B	78	ILE	CA-C-N	5.42	127.99	120.29
1	B	78	ILE	C-N-CA	5.42	127.99	120.29
1	B	105	ARG	CA-C-N	5.41	127.47	120.44
1	B	105	ARG	C-N-CA	5.41	127.47	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	THR	OG1-CB-CG2	-5.40	98.50	109.30
1	B	282	PRO	N-CD-CG	-5.39	95.12	103.20
1	A	127	ILE	CB-CA-C	-5.36	105.47	111.80
1	B	79	GLN	CB-CA-C	-5.35	101.76	110.85
1	B	185	VAL	N-CA-C	5.34	115.55	107.80
1	B	324	THR	N-CA-C	5.33	118.14	109.24
1	B	290	TYR	N-CA-C	-5.33	99.46	110.80
1	B	138	ALA	CA-C-N	-5.32	113.20	120.44
1	B	138	ALA	C-N-CA	-5.32	113.20	120.44
1	B	238	GLU	N-CA-C	5.32	122.13	110.80
1	A	59	ALA	N-CA-CB	-5.32	102.15	110.44
1	A	219	THR	N-CA-C	-5.30	106.49	113.12
1	B	79	GLN	N-CA-C	-5.30	105.59	111.36
1	B	80	SER	N-CA-C	5.29	117.80	111.71
1	B	35	LYS	N-CA-C	5.27	117.33	108.96
1	B	164	GLN	CA-C-N	5.27	126.42	119.84
1	B	164	GLN	C-N-CA	5.27	126.42	119.84
1	B	232	LEU	N-CA-C	5.26	117.53	109.95
1	A	180	LYS	N-CA-C	5.24	118.04	110.28
1	B	229	ASP	N-CA-C	-5.23	106.49	112.92
1	B	55	ILE	O-C-N	-5.21	116.73	121.94
1	B	209	LYS	N-CA-C	-5.21	107.09	113.50
1	B	183	GLY	O-C-N	-5.20	115.94	122.70
1	B	260	THR	OG1-CB-CG2	-5.20	98.90	109.30
1	A	303	ILE	CB-CA-C	-5.19	105.06	112.22
1	B	251	ASP	N-CA-C	-5.19	105.11	111.75
1	B	262	THR	OG1-CB-CG2	-5.19	98.93	109.30
1	B	56	ILE	CB-CA-C	-5.18	105.23	112.02
1	B	122	GLU	CB-CA-C	-5.18	100.25	110.10
1	A	96	GLY	N-CA-C	5.18	118.94	112.73
1	B	276	GLU	N-CA-C	5.18	119.69	112.90
1	B	59	ALA	N-CA-CB	5.18	123.98	111.04
1	A	58	GLU	CA-C-N	-5.16	112.57	121.66
1	A	58	GLU	C-N-CA	-5.16	112.57	121.66
1	A	110	LEU	N-CA-C	5.16	116.57	109.29
1	B	329	THR	OG1-CB-CG2	-5.16	98.97	109.30
1	A	90	ARG	N-CA-C	5.16	121.78	110.80
1	A	98	SER	CA-C-N	-5.15	113.06	122.38
1	A	98	SER	C-N-CA	-5.15	113.06	122.38
2	D	9	ILE	CG1-CB-CG2	-5.15	95.26	110.70
1	B	189	PHE	N-CA-C	5.14	115.33	108.38
1	A	187	THR	OG1-CB-CG2	-5.14	99.02	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ALA	N-CA-C	-5.09	101.91	109.96
1	B	55	ILE	N-CA-CB	-5.09	104.86	110.51
2	C	12	GLY	N-CA-C	5.09	118.38	111.72
1	A	84	ILE	N-CA-C	5.08	115.20	110.42
1	A	84	ILE	CB-CA-C	-5.07	105.33	111.87
1	A	243	MET	N-CA-C	-5.07	107.27	113.50
1	A	178	ARG	N-CA-C	5.06	117.15	108.90
1	B	218	VAL	CB-CA-C	-5.04	104.07	110.98
1	A	88	MET	N-CA-C	-5.01	104.83	112.04
1	A	159	LEU	N-CA-C	-5.01	106.86	113.12

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	VAL	Peptide,Mainchain
1	A	110	LEU	Mainchain
1	A	183	GLY	Peptide
1	A	230	TYR	Mainchain
1	A	238	GLU	Mainchain
1	A	254	CYS	Peptide
1	A	256	ASN	Peptide
1	A	268	LEU	Peptide
1	A	272	ASP	Peptide
1	A	304	GLN	Peptide
1	A	33	GLU	Peptide
1	A	330	LYS	Peptide
1	A	333	GLN	Peptide
1	A	341	ASP	Peptide,Mainchain
1	A	88	MET	Peptide
1	A	89	GLY	Peptide
1	B	100	ARG	Peptide
1	B	102	ASP	Peptide
1	B	103	ASP	Peptide
1	B	105	ARG	Peptide
1	B	124	ALA	Peptide
1	B	125	GLY	Peptide
1	B	131	TRP	Peptide
1	B	137	GLN	Peptide
1	B	152	ALA	Peptide
1	B	158	ASP	Peptide
1	B	159	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	164	GLN	Peptide
1	B	183	GLY	Peptide
1	B	251	ASP	Peptide
1	B	254	CYS	Peptide
1	B	256	ASN	Peptide
1	B	290	TYR	Peptide
1	B	296	TYR	Peptide
1	B	328	ASP	Peptide
1	B	330	LYS	Peptide
1	B	56	ILE	Peptide
1	B	59	ALA	Peptide
1	B	64	GLU	Peptide
1	B	66	CYS	Peptide
1	B	73	VAL	Peptide
1	B	78	ILE	Peptide
1	B	89	GLY	Peptide
1	B	92	LYS	Peptide
1	B	99	ALA	Mainchain
2	D	12	GLY	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	2450	0	2428	285	3
1	B	2450	0	2430	535	0
2	C	96	0	82	11	0
2	D	96	0	82	10	3
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	9	1	0
5	B	28	0	8	2	0
6	A	17	0	0	1	0
6	B	12	0	0	0	0
6	C	1	0	0	0	0
All	All	5190	0	5039	841	3

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 82.

All (841) 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:100:ARG:CZ	1:B:129:ARG:HD2	1.19	1.55
1:B:167:TYR:CE1	1:B:169:PRO:HG3	1.51	1.46
1:B:126:VAL:C	1:B:130:LEU:CD1	1.89	1.45
1:B:126:VAL:C	1:B:130:LEU:HD12	1.40	1.40
1:B:104:ALA:N	1:B:104:ALA:CA	1.86	1.39
1:A:110:LEU:O	1:A:110:LEU:HD23	1.24	1.34
1:B:108:PHE:O	1:B:111:ALA:HB2	1.28	1.33
1:B:100:ARG:HH22	1:B:129:ARG:CG	1.40	1.32
1:B:100:ARG:NH2	1:B:129:ARG:NE	1.79	1.29
1:B:64:GLU:O	1:B:67:LYS:HB2	1.34	1.28
1:A:33:GLU:C	1:A:34:VAL:HG23	1.51	1.27
1:A:345:LYS:HD3	1:A:345:LYS:N	1.39	1.25
1:B:162:ILE:HB	1:B:167:TYR:CE2	1.72	1.24
1:A:342:VAL:O	1:A:345:LYS:HG2	1.37	1.23
1:A:63:GLU:HB3	1:A:64:GLU:OE2	1.41	1.20
1:B:167:TYR:HD1	1:B:168:ILE:N	1.38	1.19
1:B:168:ILE:N	1:B:168:ILE:HD12	1.56	1.19
1:B:159:LEU:C	1:B:159:LEU:HD12	1.62	1.17
1:B:159:LEU:HD12	1:B:159:LEU:O	1.41	1.16
1:B:167:TYR:CZ	1:B:169:PRO:HG3	1.81	1.16
1:B:212:ILE:HD12	1:B:212:ILE:N	1.48	1.15
1:A:103:ASP:OD1	1:A:129:ARG:NH2	1.78	1.15
1:B:124:ALA:C	1:B:126:VAL:HG23	1.70	1.15
1:B:344:ILE:HG22	1:B:345:LYS:N	1.49	1.15
1:B:110:LEU:H	1:B:110:LEU:CD1	1.44	1.14
1:B:100:ARG:NH2	1:B:129:ARG:CG	2.04	1.14
1:B:162:ILE:CB	1:B:167:TYR:CE2	2.30	1.14
1:A:345:LYS:N	1:A:345:LYS:CD	1.96	1.14
1:B:126:VAL:O	1:B:130:LEU:HD11	1.44	1.14
1:B:162:ILE:CG2	1:B:167:TYR:CE2	2.30	1.14
1:B:63:GLU:HG2	1:B:64:GLU:OE2	1.47	1.12
1:B:108:PHE:C	1:B:111:ALA:HB2	1.73	1.11
1:A:165:PRO:O	1:A:166:ASN:HB2	1.50	1.10
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.00	1.10
1:B:126:VAL:O	1:B:130:LEU:CD1	0.81	1.10
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.04	1.10
1:B:110:LEU:N	1:B:110:LEU:HD12	1.67	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ALA:O	1:A:341:ASP:O	1.69	1.08
1:B:162:ILE:HG22	1:B:167:TYR:CE2	1.86	1.08
1:B:100:ARG:CZ	1:B:129:ARG:CD	1.95	1.07
1:B:81:ILE:HG23	1:B:82:ILE:N	1.60	1.07
1:B:159:LEU:C	1:B:161:ARG:H	1.62	1.07
1:B:167:TYR:CE1	1:B:169:PRO:CG	2.36	1.07
1:B:122:GLU:O	1:B:122:GLU:HG3	1.52	1.06
1:A:110:LEU:O	1:A:110:LEU:CD2	2.04	1.06
1:B:159:LEU:HG	1:B:160:ASP:H	1.15	1.06
1:B:167:TYR:CE1	1:B:168:ILE:C	2.34	1.05
1:B:97:ASP:OD2	1:B:99:ALA:HB3	1.55	1.05
1:B:86:ARG:HB3	1:B:86:ARG:NH1	1.73	1.04
1:B:78:ILE:HG22	1:B:79:GLN:N	1.68	1.04
1:B:54:LYS:O	1:B:58:GLU:O	1.75	1.04
1:B:108:PHE:O	1:B:111:ALA:CB	2.06	1.04
1:B:168:ILE:HD12	1:B:168:ILE:H	1.05	1.03
1:B:110:LEU:H	1:B:110:LEU:HD12	0.88	1.03
1:B:63:GLU:O	1:B:67:LYS:HG3	1.56	1.02
1:B:162:ILE:HB	1:B:167:TYR:HE2	1.09	1.02
1:B:212:ILE:H	1:B:212:ILE:CD1	1.59	1.02
1:A:33:GLU:C	1:A:34:VAL:CG2	2.30	1.01
1:B:100:ARG:O	1:B:103:ASP:HB2	1.61	1.01
1:B:81:ILE:CG2	1:B:82:ILE:H	1.71	1.00
1:A:137:GLN:O	1:A:141:ASN:ND2	1.94	1.00
1:B:105:ARG:O	1:B:109:VAL:CG2	2.09	1.00
1:B:167:TYR:CD1	1:B:168:ILE:N	2.30	1.00
1:A:52:GLN:O	1:A:56:ILE:HG13	1.62	0.99
1:A:344:ILE:C	1:A:345:LYS:HD3	1.87	0.99
1:B:71:ALA:O	1:B:74:TYR:HB2	1.63	0.99
1:B:81:ILE:HG23	1:B:82:ILE:H	0.85	0.98
1:B:68:GLN:HE21	1:B:68:GLN:N	1.60	0.98
1:B:100:ARG:HA	1:B:103:ASP:OD2	1.62	0.98
1:A:269:ASN:O	1:A:270:LYS:HB2	1.62	0.98
1:B:167:TYR:CD1	1:B:167:TYR:C	2.38	0.98
1:A:96:GLY:N	1:A:133:ASP:OD2	1.96	0.97
1:A:74:TYR:O	1:A:78:ILE:HG13	1.64	0.97
1:A:228:SER:O	1:A:277:LYS:NZ	1.97	0.96
1:B:124:ALA:O	1:B:127:ILE:N	1.98	0.96
1:B:78:ILE:HG22	1:B:79:GLN:CA	1.96	0.95
1:B:86:ARG:NH1	1:B:86:ARG:CB	2.29	0.95
1:B:100:ARG:NH2	1:B:129:ARG:HD3	1.38	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:O	1:B:130:LEU:CG	2.15	0.94
1:B:159:LEU:HG	1:B:160:ASP:N	1.72	0.94
1:A:103:ASP:CG	1:A:129:ARG:HH21	1.75	0.94
1:B:124:ALA:O	1:B:126:VAL:HG23	1.64	0.94
1:A:245:GLU:O	1:A:245:GLU:HG3	1.65	0.94
1:B:167:TYR:HE1	1:B:168:ILE:C	1.71	0.94
1:A:62:SER:OG	1:A:65:GLU:HB2	1.68	0.94
1:B:86:ARG:HH11	1:B:86:ARG:CB	1.81	0.94
1:B:131:TRP:NE1	1:B:157:ASN:OD1	2.01	0.94
1:B:344:ILE:HG22	1:B:345:LYS:H	1.24	0.93
1:A:52:GLN:C	1:A:54:LYS:H	1.76	0.92
1:A:62:SER:H	1:A:65:GLU:HB2	1.35	0.92
1:B:85:ILE:HA	1:B:88:MET:HG3	1.49	0.91
1:A:70:LYS:HE3	1:A:167:TYR:O	1.71	0.91
1:A:108:PHE:O	1:A:109:VAL:O	1.87	0.91
1:B:332:VAL:O	1:B:332:VAL:HG12	1.69	0.90
1:A:139:CYS:O	1:A:146:TYR:OH	1.88	0.90
2:D:6:TYR:CE2	2:D:7:HIS:ND1	2.39	0.90
1:B:167:TYR:HD1	1:B:167:TYR:C	1.76	0.89
1:B:100:ARG:HH21	1:B:129:ARG:NE	1.51	0.89
1:B:100:ARG:HH22	1:B:129:ARG:HD3	0.90	0.89
1:A:57:HIS:O	1:A:58:GLU:HG2	1.73	0.87
1:B:162:ILE:HG22	1:B:167:TYR:CZ	2.07	0.87
1:A:283:LEU:C	1:A:285:ILE:H	1.82	0.87
1:A:33:GLU:O	1:A:34:VAL:HG23	1.73	0.87
1:B:93:ILE:O	1:B:93:ILE:HG22	1.73	0.87
1:B:102:ASP:O	1:B:105:ARG:HB2	1.75	0.87
1:B:142:ARG:HH21	1:B:145:GLU:CD	1.82	0.87
1:B:82:ILE:O	1:B:82:ILE:HG22	1.68	0.86
1:B:170:THR:O	1:B:173:ASP:N	2.07	0.86
1:B:159:LEU:CG	1:B:160:ASP:N	2.33	0.86
1:B:129:ARG:HG3	1:B:129:ARG:NH1	1.76	0.86
1:B:174:VAL:HG12	1:B:174:VAL:O	1.75	0.86
1:B:78:ILE:HG22	1:B:79:GLN:HA	1.58	0.86
1:B:256:ASN:OD1	1:B:257:LYS:N	2.08	0.85
1:A:63:GLU:O	1:A:67:LYS:HG3	1.75	0.85
1:A:278:ILE:O	1:A:278:ILE:HG13	1.75	0.85
1:B:159:LEU:C	1:B:161:ARG:N	2.28	0.85
2:D:11:VAL:HG23	2:D:12:GLY:O	1.77	0.85
1:B:167:TYR:CD1	1:B:168:ILE:C	2.55	0.85
1:B:52:GLN:O	1:B:56:ILE:CG1	2.25	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HD23	1:B:198:MET:HG3	1.59	0.85
1:B:87:ALA:O	1:B:91:LEU:HB2	1.77	0.85
1:B:81:ILE:CG2	1:B:82:ILE:N	2.30	0.84
1:A:299:ALA:O	1:A:303:ILE:HG13	1.77	0.84
1:A:49:ILE:HG22	1:A:49:ILE:O	1.77	0.84
1:A:192:LYS:O	1:A:193:ASP:HB2	1.77	0.84
1:A:303:ILE:C	1:A:305:CYS:H	1.86	0.83
1:B:134:SER:O	1:B:138:ALA:CB	2.26	0.83
1:B:167:TYR:CE1	1:B:168:ILE:O	2.30	0.83
1:B:228:SER:O	1:B:277:LYS:NZ	2.10	0.83
1:B:73:VAL:HG12	1:B:73:VAL:O	1.74	0.83
1:B:99:ALA:HB3	1:B:100:ARG:HD2	1.58	0.83
1:B:104:ALA:O	1:B:107:LEU:HB2	1.78	0.83
1:B:97:ASP:OD2	1:B:100:ARG:HD2	1.77	0.83
1:B:168:ILE:H	1:B:168:ILE:CD1	1.85	0.83
1:B:62:SER:O	1:B:65:GLU:HB2	1.79	0.82
1:B:100:ARG:HD2	1:B:100:ARG:N	1.95	0.82
1:B:307:PHE:C	1:B:309:ASP:H	1.87	0.82
1:B:97:ASP:CG	1:B:99:ALA:HB3	2.04	0.82
1:B:282:PRO:O	1:B:285:ILE:HG13	1.80	0.82
1:B:126:VAL:C	1:B:130:LEU:HD13	1.77	0.82
1:B:57:HIS:O	1:B:58:GLU:HG2	1.79	0.82
1:B:102:ASP:O	1:B:104:ALA:HB3	1.80	0.81
1:B:103:ASP:C	1:B:104:ALA:CA	2.52	0.81
1:B:126:VAL:O	1:B:130:LEU:HD12	1.03	0.81
1:B:123:LEU:O	1:B:126:VAL:CG2	2.29	0.81
1:B:343:ILE:HG22	1:B:343:ILE:O	1.81	0.81
2:D:11:VAL:HG23	2:D:11:VAL:O	1.76	0.81
1:B:105:ARG:O	1:B:109:VAL:HG23	1.81	0.80
1:B:162:ILE:CB	1:B:167:TYR:HE2	1.78	0.80
1:B:162:ILE:HA	1:B:167:TYR:CD2	2.17	0.80
1:B:52:GLN:O	1:B:56:ILE:HG13	1.81	0.80
1:B:162:ILE:HB	1:B:167:TYR:CD2	2.16	0.80
1:B:57:HIS:O	1:B:58:GLU:CG	2.29	0.80
1:A:283:LEU:O	1:A:285:ILE:N	2.14	0.80
1:B:97:ASP:OD2	1:B:99:ALA:CB	2.30	0.80
1:B:100:ARG:O	1:B:103:ASP:CB	2.30	0.80
1:B:124:ALA:HA	1:B:127:ILE:HG13	1.63	0.80
1:A:62:SER:OG	1:A:65:GLU:CG	2.30	0.80
1:B:59:ALA:CB	1:B:60:GLY:O	2.30	0.80
1:B:66:CYS:O	1:B:169:PRO:HD2	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG12	1:A:110:LEU:CA	2.12	0.80
1:A:313:ARG:C	1:A:315:ASP:H	1.87	0.80
1:B:59:ALA:HB1	1:B:60:GLY:O	1.80	0.79
1:B:100:ARG:HH22	1:B:129:ARG:CD	0.21	0.79
1:B:124:ALA:O	1:B:126:VAL:CG2	2.30	0.79
1:A:97:ASP:C	1:A:99:ALA:H	1.87	0.79
1:B:100:ARG:CA	1:B:103:ASP:OD2	2.29	0.79
1:A:122:GLU:O	1:A:122:GLU:HG2	1.79	0.79
1:B:167:TYR:HE1	1:B:169:PRO:N	1.81	0.79
1:B:97:ASP:OD2	1:B:100:ARG:CD	2.30	0.79
1:A:62:SER:OG	1:A:65:GLU:CB	2.30	0.79
1:B:124:ALA:O	1:B:126:VAL:CB	2.30	0.79
1:A:57:HIS:O	1:A:58:GLU:CG	2.30	0.79
1:A:343:ILE:O	1:A:344:ILE:C	2.23	0.79
1:B:124:ALA:O	1:B:127:ILE:CG1	2.30	0.79
1:B:343:ILE:O	1:B:343:ILE:CG2	2.30	0.78
1:A:122:GLU:O	1:A:122:GLU:CG	2.30	0.78
1:B:68:GLN:N	1:B:68:GLN:NE2	2.30	0.78
1:B:124:ALA:O	1:B:126:VAL:CA	2.30	0.78
1:B:130:LEU:O	1:B:136:VAL:HG21	1.84	0.78
1:B:332:VAL:O	1:B:332:VAL:CG1	2.30	0.78
1:B:134:SER:O	1:B:138:ALA:HB2	1.83	0.78
1:B:61:TYR:HB2	1:B:171:GLN:NE2	1.99	0.77
1:A:63:GLU:CB	1:A:64:GLU:OE2	2.29	0.77
1:B:167:TYR:HE1	1:B:169:PRO:CG	1.92	0.77
1:B:63:GLU:CG	1:B:64:GLU:OE2	2.30	0.77
1:B:72:VAL:C	1:B:74:TYR:H	1.89	0.77
1:B:342:VAL:C	1:B:344:ILE:H	1.91	0.77
1:B:104:ALA:O	1:B:107:LEU:CB	2.33	0.77
1:B:107:LEU:O	1:B:111:ALA:HA	1.85	0.77
1:A:101:ALA:O	1:A:105:ARG:HG3	1.85	0.77
2:C:6:TYR:HD2	2:C:6:TYR:O	1.68	0.76
1:A:93:ILE:HG22	1:A:94:ASP:H	1.49	0.76
1:B:103:ASP:N	1:B:106:GLN:HG3	1.99	0.76
1:B:167:TYR:HE1	1:B:169:PRO:CA	1.98	0.76
1:A:123:LEU:O	1:A:127:ILE:HG13	1.84	0.76
1:A:243:MET:HE1	1:A:303:ILE:HD13	1.65	0.76
1:A:33:GLU:O	1:A:34:VAL:CG2	2.30	0.76
1:B:134:SER:C	1:B:136:VAL:H	1.89	0.76
1:B:162:ILE:CA	1:B:167:TYR:CD2	2.69	0.76
1:B:124:ALA:O	1:B:127:ILE:HG13	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:O	1:B:126:VAL:HG23	1.86	0.76
1:B:282:PRO:O	1:B:282:PRO:HG2	1.85	0.76
1:B:58:GLU:O	1:B:59:ALA:C	2.26	0.75
1:B:63:GLU:C	1:B:64:GLU:OE2	2.29	0.75
1:B:174:VAL:O	1:B:174:VAL:CG1	2.33	0.75
1:B:63:GLU:O	1:B:67:LYS:CG	2.33	0.75
1:B:77:THR:O	1:B:78:ILE:C	2.29	0.75
1:B:192:LYS:O	1:B:193:ASP:HB2	1.86	0.75
1:B:257:LYS:HG2	1:B:258:TRP:N	1.92	0.75
1:B:86:ARG:HH12	1:B:90:ARG:NH1	1.84	0.75
1:A:260:THR:O	1:A:260:THR:CG2	2.29	0.74
1:B:68:GLN:HE21	1:B:68:GLN:H	1.35	0.74
1:B:97:ASP:HB3	1:B:100:ARG:HG2	1.67	0.74
1:B:311:ASN:O	1:B:314:LYS:HE3	1.87	0.74
1:B:62:SER:C	1:B:64:GLU:H	1.94	0.74
1:B:103:ASP:O	1:B:104:ALA:C	2.31	0.74
1:B:162:ILE:CB	1:B:167:TYR:CD2	2.70	0.74
1:B:110:LEU:O	1:B:111:ALA:C	2.30	0.74
1:B:234:LEU:HD23	1:B:242:ARG:HG2	1.69	0.74
1:A:234:LEU:HD23	1:A:242:ARG:HG2	1.69	0.74
1:A:52:GLN:O	1:A:56:ILE:CG1	2.35	0.74
1:B:100:ARG:C	1:B:102:ASP:H	1.93	0.74
1:A:52:GLN:C	1:A:54:LYS:N	2.34	0.73
1:A:82:ILE:HG22	1:A:82:ILE:O	1.80	0.73
1:B:294:ASN:CG	1:B:294:ASN:O	2.30	0.73
1:B:167:TYR:HD1	1:B:168:ILE:CA	2.00	0.73
1:B:125:GLY:O	1:B:129:ARG:HB2	1.87	0.73
1:A:207:GLU:C	1:A:209:LYS:H	1.95	0.73
1:B:212:ILE:HD12	1:B:212:ILE:H	0.67	0.73
1:B:85:ILE:C	1:B:87:ALA:N	2.37	0.73
1:B:100:ARG:NH2	1:B:129:ARG:CD	0.80	0.73
1:B:73:VAL:O	1:B:73:VAL:CG1	2.31	0.73
1:B:237:ASP:OD1	1:B:237:ASP:C	2.30	0.73
1:A:332:VAL:HG12	1:A:332:VAL:O	1.85	0.72
1:B:54:LYS:O	1:B:58:GLU:C	2.32	0.72
1:B:85:ILE:O	1:B:86:ARG:C	2.30	0.72
1:B:87:ALA:O	1:B:88:MET:C	2.30	0.72
1:B:167:TYR:CD1	1:B:168:ILE:O	2.42	0.72
1:A:165:PRO:O	1:A:166:ASN:CB	2.30	0.72
1:B:125:GLY:N	1:B:126:VAL:HG23	2.05	0.71
1:B:247:MET:HE1	1:B:287:TYR:HE1	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:CG1	1:A:126:VAL:O	2.34	0.71
1:B:61:TYR:HA	1:B:65:GLU:OE1	1.90	0.71
1:B:69:TYR:O	1:B:70:LYS:C	2.31	0.71
1:B:97:ASP:HB3	1:B:100:ARG:CG	2.20	0.71
1:A:269:ASN:O	1:A:270:LYS:CB	2.30	0.71
1:A:294:ASN:C	1:A:295:THR:HG23	2.14	0.71
1:B:57:HIS:C	1:B:58:GLU:HG3	2.14	0.71
1:B:283:LEU:HG	1:B:283:LEU:O	1.88	0.71
1:B:314:LYS:O	1:B:315:ASP:C	2.30	0.71
1:A:303:ILE:C	1:A:305:CYS:N	2.45	0.71
1:B:52:GLN:O	1:B:56:ILE:HG12	1.89	0.71
1:B:103:ASP:O	1:B:104:ALA:O	2.08	0.71
1:B:247:MET:HE2	1:B:287:TYR:OH	1.89	0.71
1:B:108:PHE:CA	1:B:111:ALA:HB2	2.19	0.71
1:A:272:ASP:OD2	5:A:355:GDP:N2	2.15	0.71
1:B:191:PHE:C	1:B:193:ASP:H	1.98	0.71
1:B:124:ALA:CA	1:B:127:ILE:HG13	2.21	0.70
1:B:154:TYR:OH	1:B:173:ASP:OD1	2.08	0.70
1:A:126:VAL:O	1:A:126:VAL:HG12	1.85	0.70
1:B:301:ALA:O	1:B:302:TYR:C	2.29	0.70
1:B:91:LEU:O	1:B:92:LYS:HB2	1.91	0.70
1:A:343:ILE:O	1:A:345:LYS:N	2.25	0.70
1:B:34:VAL:HG12	1:B:34:VAL:O	1.90	0.70
1:B:61:TYR:HB2	1:B:171:GLN:HE22	1.56	0.70
1:B:159:LEU:C	1:B:159:LEU:CD1	2.28	0.70
1:B:289:GLU:C	1:B:290:TYR:O	2.29	0.70
1:A:82:ILE:O	1:A:82:ILE:CG2	2.33	0.70
1:B:110:LEU:CD1	1:B:110:LEU:N	2.29	0.70
1:B:167:TYR:CD1	1:B:168:ILE:CA	2.74	0.70
2:C:6:TYR:O	2:C:6:TYR:CD2	2.44	0.69
1:B:52:GLN:NE2	1:B:326:ALA:O	2.23	0.69
1:B:47:SER:OG	5:B:355:GDP:O3B	2.10	0.69
1:A:57:HIS:C	1:A:58:GLU:CG	2.65	0.69
1:A:49:ILE:O	1:A:49:ILE:CG2	2.37	0.69
1:B:57:HIS:C	1:B:58:GLU:CG	2.64	0.69
1:B:123:LEU:O	1:B:124:ALA:C	2.33	0.69
1:B:247:MET:HE1	1:B:287:TYR:CE1	2.28	0.69
1:B:104:ALA:N	1:B:104:ALA:C	2.49	0.69
1:B:97:ASP:HB3	1:B:100:ARG:CD	2.24	0.68
1:B:251:ASP:O	1:B:255:ASN:HB2	1.92	0.68
1:A:333:GLN:HG2	1:A:334:PHE:N	2.04	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:THR:HG22	1:B:329:THR:O	1.93	0.68
1:B:148:LEU:O	1:B:149:ASN:C	2.30	0.68
1:A:72:VAL:O	1:A:73:VAL:C	2.30	0.68
1:A:343:ILE:C	1:A:345:LYS:N	2.51	0.68
1:B:100:ARG:HH21	1:B:129:ARG:CD	1.33	0.68
1:B:97:ASP:O	1:B:100:ARG:HG2	1.93	0.68
1:B:53:MET:HG3	1:B:198:MET:HE1	1.75	0.68
1:B:49:ILE:O	1:B:49:ILE:HG22	1.85	0.68
1:A:253:ILE:C	1:A:255:ASN:H	2.00	0.68
1:A:260:THR:O	1:A:260:THR:HG22	1.90	0.67
1:B:159:LEU:O	1:B:161:ARG:N	2.24	0.67
1:B:307:PHE:O	1:B:309:ASP:N	2.28	0.67
1:B:142:ARG:O	1:B:143:SER:C	2.36	0.67
1:B:153:ALA:O	1:B:154:TYR:C	2.29	0.67
1:B:253:ILE:O	1:B:254:CYS:C	2.30	0.67
1:B:82:ILE:O	1:B:82:ILE:CG2	2.36	0.67
1:A:93:ILE:HG22	1:A:94:ASP:N	2.09	0.67
1:B:167:TYR:OH	1:B:169:PRO:HB3	1.94	0.67
1:A:54:LYS:HG3	1:A:54:LYS:O	1.95	0.66
1:B:81:ILE:O	1:B:82:ILE:C	2.32	0.66
1:B:86:ARG:HH12	1:B:90:ARG:HH12	1.40	0.66
1:B:126:VAL:CA	1:B:130:LEU:HD12	2.25	0.66
1:B:140:PHE:CG	1:B:140:PHE:O	2.48	0.66
1:B:72:VAL:C	1:B:74:TYR:N	2.43	0.66
1:B:85:ILE:O	1:B:87:ALA:N	2.28	0.66
1:B:105:ARG:O	1:B:109:VAL:HG21	1.92	0.66
1:A:64:GLU:OE2	1:A:64:GLU:N	2.29	0.66
1:B:124:ALA:O	1:B:126:VAL:N	2.29	0.66
1:B:135:GLY:C	1:B:138:ALA:HB3	2.21	0.66
1:B:127:ILE:O	1:B:130:LEU:N	2.29	0.66
1:A:84:ILE:O	1:A:85:ILE:C	2.30	0.66
1:B:64:GLU:OE2	1:B:64:GLU:N	2.29	0.66
1:B:109:VAL:HB	1:B:110:LEU:HD12	1.78	0.66
1:B:156:LEU:O	1:B:158:ASP:N	2.29	0.66
1:A:277:LYS:C	1:A:279:LYS:H	2.04	0.66
1:A:97:ASP:C	1:A:99:ALA:N	2.53	0.65
1:A:294:ASN:C	1:A:295:THR:CG2	2.66	0.65
1:B:53:MET:O	1:B:57:HIS:HB2	1.95	0.65
1:B:64:GLU:HA	1:B:67:LYS:HG3	1.78	0.65
1:B:101:ALA:O	1:B:104:ALA:CB	2.45	0.65
1:B:142:ARG:NH2	1:B:145:GLU:OE2	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ASN:OD1	1:B:312:LYS:N	2.29	0.65
1:B:62:SER:O	1:B:64:GLU:N	2.30	0.65
1:B:85:ILE:C	1:B:87:ALA:H	2.03	0.65
1:B:95:PHE:O	1:B:96:GLY:C	2.36	0.65
1:B:139:CYS:O	1:B:141:ASN:N	2.29	0.65
1:B:142:ARG:O	1:B:144:ARG:N	2.29	0.65
1:B:159:LEU:O	1:B:162:ILE:N	2.29	0.65
1:B:49:ILE:O	1:B:49:ILE:CG2	2.34	0.65
1:A:65:GLU:O	1:A:66:CYS:C	2.40	0.65
1:B:102:ASP:OD1	1:B:105:ARG:NH1	2.30	0.65
1:A:85:ILE:O	1:A:87:ALA:N	2.30	0.65
1:A:130:LEU:O	1:A:132:LYS:N	2.30	0.65
1:A:249:LEU:O	1:A:250:PHE:C	2.36	0.65
1:A:313:ARG:O	1:A:315:ASP:N	2.30	0.65
1:B:65:GLU:C	1:B:67:LYS:H	2.03	0.65
1:B:63:GLU:N	1:B:64:GLU:OE2	2.30	0.65
1:B:65:GLU:O	1:B:67:LYS:N	2.28	0.65
1:B:191:PHE:O	1:B:193:ASP:N	2.30	0.65
1:B:311:ASN:OD1	1:B:311:ASN:C	2.33	0.65
1:B:142:ARG:NH2	1:B:145:GLU:OE1	2.30	0.64
1:B:342:VAL:O	1:B:344:ILE:N	2.30	0.64
1:A:303:ILE:O	1:A:305:CYS:N	2.30	0.64
1:B:64:GLU:O	1:B:68:GLN:NE2	2.31	0.64
1:A:329:THR:HG22	1:A:329:THR:O	1.98	0.64
1:A:65:GLU:O	1:A:67:LYS:N	2.29	0.64
1:B:85:ILE:O	1:B:88:MET:N	2.30	0.64
1:B:134:SER:C	1:B:136:VAL:N	2.45	0.64
1:B:134:SER:O	1:B:136:VAL:N	2.30	0.64
1:A:72:VAL:O	1:A:74:TYR:N	2.30	0.64
1:A:160:ASP:O	1:A:164:GLN:HG3	1.97	0.64
1:B:48:THR:HG22	1:B:48:THR:O	1.98	0.64
1:B:158:ASP:OD2	1:B:161:ARG:NH2	2.30	0.64
1:B:162:ILE:CG2	1:B:167:TYR:CZ	2.76	0.64
1:B:277:LYS:O	1:B:279:LYS:N	2.31	0.64
1:A:52:GLN:O	1:A:54:LYS:N	2.30	0.63
1:A:62:SER:HG	1:A:65:GLU:CD	2.04	0.63
1:B:78:ILE:HG23	1:B:82:ILE:HG13	1.79	0.63
1:B:156:LEU:C	1:B:158:ASP:H	2.06	0.63
1:B:272:ASP:CG	1:B:273:LEU:H	2.05	0.63
1:B:344:ILE:O	1:B:345:LYS:C	2.30	0.63
1:B:100:ARG:O	1:B:102:ASP:N	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:HB	1:B:110:LEU:CD1	2.29	0.63
2:C:6:TYR:HD2	2:C:7:HIS:HD1	1.45	0.63
1:A:340:THR:OG1	1:A:341:ASP:N	2.30	0.63
1:B:100:ARG:N	1:B:100:ARG:CD	2.50	0.63
1:B:164:GLN:C	1:B:165:PRO:O	2.39	0.63
1:A:161:ARG:HH11	1:A:161:ARG:CG	2.12	0.63
1:B:158:ASP:OD2	1:B:161:ARG:NE	2.30	0.63
1:B:167:TYR:CZ	1:B:169:PRO:CG	2.70	0.63
1:B:170:THR:O	1:B:171:GLN:C	2.40	0.63
1:B:293:SER:OG	1:B:294:ASN:N	2.30	0.63
1:B:163:ALA:O	1:B:164:GLN:C	2.39	0.63
1:A:52:GLN:NE2	1:A:326:ALA:O	2.30	0.63
1:B:96:GLY:O	1:B:98:SER:N	2.32	0.63
1:B:331:ASN:O	1:B:333:GLN:N	2.32	0.63
1:B:134:SER:O	1:B:138:ALA:HB3	1.97	0.62
1:B:143:SER:O	1:B:145:GLU:N	2.31	0.62
1:A:294:ASN:OD1	1:A:294:ASN:N	2.29	0.62
1:B:102:ASP:C	1:B:104:ALA:HB3	2.24	0.62
1:B:130:LEU:C	1:B:132:LYS:H	2.07	0.62
1:B:100:ARG:NH1	1:B:129:ARG:CD	2.58	0.62
1:A:302:TYR:O	1:A:305:CYS:HB3	1.99	0.62
1:B:139:CYS:C	1:B:141:ASN:H	2.05	0.62
1:A:272:ASP:OD1	1:A:272:ASP:N	2.31	0.62
1:A:136:VAL:HG12	1:A:136:VAL:O	1.99	0.62
1:B:127:ILE:O	1:B:130:LEU:HB2	2.00	0.62
1:A:191:PHE:C	1:A:193:ASP:H	2.06	0.62
1:B:207:GLU:OE1	1:B:210:LYS:NZ	2.30	0.62
1:B:42:GLY:N	1:B:203:GLY:O	2.32	0.62
1:A:130:LEU:O	1:A:131:TRP:C	2.37	0.62
1:B:88:MET:HE1	1:B:95:PHE:CD1	2.35	0.61
1:B:63:GLU:O	1:B:63:GLU:HG3	2.01	0.61
1:B:139:CYS:C	1:B:141:ASN:N	2.54	0.61
1:A:62:SER:OG	1:A:65:GLU:HG3	1.99	0.61
1:A:264:ILE:O	1:A:264:ILE:HG22	1.88	0.61
1:A:264:ILE:HD13	1:A:264:ILE:N	2.14	0.61
1:A:161:ARG:NH2	1:A:173:ASP:OD1	2.33	0.61
1:A:234:LEU:O	1:A:237:ASP:C	2.43	0.61
1:A:302:TYR:O	1:A:305:CYS:CB	2.48	0.61
1:B:126:VAL:HG12	1:B:130:LEU:HD11	1.83	0.61
1:B:127:ILE:O	1:B:131:TRP:N	2.30	0.61
1:A:57:HIS:C	1:A:58:GLU:HG3	2.25	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:C	1:A:209:LYS:N	2.46	0.61
1:A:133:ASP:C	1:A:135:GLY:H	2.09	0.61
1:B:129:ARG:CG	1:B:129:ARG:NH1	2.53	0.61
1:B:278:ILE:O	1:B:278:ILE:HG13	1.98	0.61
1:A:149:ASN:N	1:A:149:ASN:OD1	2.29	0.61
1:A:325:CYS:O	1:A:327:THR:N	2.33	0.61
1:B:308:GLU:HG3	1:B:319:ILE:HB	1.83	0.61
1:B:124:ALA:O	1:B:127:ILE:HG12	2.00	0.60
1:A:277:LYS:O	1:A:279:LYS:N	2.34	0.60
1:A:241:ASN:HB3	1:A:244:HIS:HB2	1.82	0.60
1:B:62:SER:C	1:B:64:GLU:N	2.57	0.60
1:B:191:PHE:O	1:B:192:LYS:C	2.44	0.60
1:A:109:VAL:HG12	1:A:110:LEU:HA	1.79	0.60
1:B:91:LEU:O	1:B:92:LYS:CB	2.49	0.60
1:B:96:GLY:O	1:B:97:ASP:C	2.41	0.60
1:B:59:ALA:HB1	1:B:60:GLY:C	2.25	0.60
1:A:221:ILE:HG22	1:A:222:ILE:N	2.17	0.60
1:A:313:ARG:C	1:A:315:ASP:N	2.51	0.60
1:B:123:LEU:C	1:B:126:VAL:HG23	2.27	0.60
1:A:33:GLU:CA	1:A:34:VAL:HG23	2.28	0.60
1:A:81:ILE:HG13	1:A:81:ILE:O	2.02	0.60
1:B:97:ASP:CG	1:B:99:ALA:CB	2.74	0.60
1:B:124:ALA:C	1:B:127:ILE:HG13	2.27	0.60
1:B:342:VAL:C	1:B:344:ILE:N	2.46	0.60
1:A:203:GLY:O	1:A:204:GLN:C	2.39	0.59
1:B:100:ARG:C	1:B:103:ASP:OD2	2.45	0.59
1:B:212:ILE:N	1:B:212:ILE:CD1	2.29	0.59
1:A:130:LEU:C	1:A:132:LYS:N	2.59	0.59
1:A:36:LEU:HD22	1:A:37:LEU:N	2.18	0.59
1:A:133:ASP:C	1:A:135:GLY:N	2.52	0.59
1:A:133:ASP:O	1:A:134:SER:C	2.40	0.59
1:A:61:TYR:HB2	1:A:171:GLN:NE2	2.18	0.59
1:B:78:ILE:CG2	1:B:82:ILE:HG13	2.31	0.59
1:B:163:ALA:O	1:B:165:PRO:CD	2.51	0.59
1:A:203:GLY:C	1:A:204:GLN:O	2.35	0.59
1:A:275:GLU:HB2	1:A:296:TYR:CD1	2.38	0.59
1:B:81:ILE:HA	1:B:84:ILE:HG13	1.84	0.59
2:D:13:GLU:H	2:D:13:GLU:CD	2.08	0.59
1:A:191:PHE:C	1:A:193:ASP:N	2.57	0.59
1:B:97:ASP:OD2	1:B:100:ARG:HD3	2.02	0.58
1:A:70:LYS:CE	1:A:167:TYR:O	2.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ARG:NH1	1:B:86:ARG:HB2	2.18	0.58
1:B:191:PHE:C	1:B:193:ASP:N	2.52	0.58
2:C:7:HIS:O	2:C:9:ILE:HG13	2.03	0.58
1:B:250:PHE:O	1:B:251:ASP:C	2.41	0.58
1:B:67:LYS:C	1:B:68:GLN:HE21	2.11	0.58
1:A:37:LEU:HD12	1:A:199:PHE:HB2	1.85	0.58
1:B:59:ALA:HB3	1:B:60:GLY:O	2.02	0.58
1:B:88:MET:HB3	1:B:93:ILE:HG21	1.84	0.58
1:B:123:LEU:O	1:B:123:LEU:HD12	2.03	0.58
1:A:178:ARG:C	1:A:179:VAL:HG23	2.28	0.58
1:A:336:PHE:O	1:A:340:THR:HG23	2.03	0.58
1:B:143:SER:C	1:B:145:GLU:H	2.11	0.58
1:B:71:ALA:HA	1:B:74:TYR:HD2	1.69	0.58
1:B:328:ASP:C	1:B:328:ASP:OD1	2.41	0.57
1:B:54:LYS:O	1:B:58:GLU:N	2.36	0.57
1:A:104:ALA:C	1:A:106:GLN:H	2.12	0.57
1:B:88:MET:HB3	1:B:93:ILE:CG2	2.35	0.57
2:D:13:GLU:OE2	2:D:13:GLU:N	2.30	0.57
1:A:163:ALA:O	1:A:164:GLN:C	2.46	0.57
1:B:102:ASP:O	1:B:105:ARG:CB	2.52	0.57
1:B:142:ARG:NH2	1:B:145:GLU:CD	2.59	0.57
1:A:61:TYR:H	1:A:171:GLN:HE22	1.53	0.57
1:B:100:ARG:HH21	1:B:129:ARG:HD2	0.94	0.57
1:B:107:LEU:O	1:B:107:LEU:HD12	2.04	0.57
1:B:336:PHE:O	1:B:340:THR:OG1	2.19	0.57
1:A:190:THR:HA	1:A:194:LEU:O	2.04	0.57
1:B:128:LYS:O	1:B:129:ARG:C	2.43	0.57
1:A:69:TYR:O	1:A:70:LYS:C	2.44	0.57
1:A:203:GLY:O	1:A:208:ARG:NE	2.37	0.57
1:A:42:GLY:O	1:A:43:GLU:HB2	2.04	0.57
1:B:88:MET:HE3	1:B:93:ILE:CG2	2.33	0.57
1:B:63:GLU:CA	1:B:64:GLU:OE2	2.52	0.57
1:B:101:ALA:C	1:B:104:ALA:CB	2.78	0.57
1:B:126:VAL:HB	1:B:127:ILE:HG12	1.87	0.57
1:B:167:TYR:C	1:B:168:ILE:HD12	2.28	0.57
1:A:301:ALA:O	1:A:305:CYS:HB2	2.05	0.56
1:A:48:THR:O	1:A:48:THR:HG22	2.06	0.56
1:A:109:VAL:HG12	1:A:110:LEU:CB	2.30	0.56
1:A:253:ILE:O	1:A:255:ASN:N	2.37	0.56
1:B:127:ILE:CA	1:B:130:LEU:HB2	2.35	0.56
1:B:250:PHE:C	1:B:252:SER:N	2.59	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLU:HG2	1:B:64:GLU:CD	2.26	0.56
2:C:11:VAL:HG23	2:C:12:GLY:N	2.21	0.56
1:B:131:TRP:HE3	1:B:131:TRP:HA	1.70	0.56
1:B:170:THR:OG1	1:B:173:ASP:CG	2.48	0.56
1:B:54:LYS:NZ	1:B:59:ALA:CB	2.68	0.56
1:B:123:LEU:O	1:B:126:VAL:HG21	2.03	0.56
1:B:142:ARG:NE	1:B:145:GLU:OE2	2.36	0.56
1:A:104:ALA:C	1:A:106:GLN:N	2.60	0.56
1:A:237:ASP:C	1:A:237:ASP:OD1	2.46	0.56
1:B:156:LEU:C	1:B:158:ASP:N	2.61	0.55
1:B:134:SER:O	1:B:135:GLY:C	2.46	0.55
1:B:62:SER:N	1:B:65:GLU:OE1	2.40	0.55
1:B:100:ARG:HH21	1:B:129:ARG:HE	1.47	0.55
1:A:127:ILE:O	1:A:128:LYS:C	2.46	0.55
1:A:332:VAL:O	1:A:332:VAL:CG1	2.46	0.55
1:A:342:VAL:HG12	1:A:343:ILE:N	2.19	0.55
1:B:131:TRP:HA	1:B:131:TRP:CE3	2.39	0.55
1:A:161:ARG:HH22	1:A:173:ASP:CG	2.14	0.55
1:B:100:ARG:CZ	1:B:129:ARG:HD3	2.01	0.55
1:A:85:ILE:O	1:A:86:ARG:C	2.49	0.55
1:A:128:LYS:O	1:A:129:ARG:C	2.46	0.55
1:B:124:ALA:O	1:B:126:VAL:C	2.49	0.55
1:B:218:VAL:O	1:B:262:THR:OG1	2.23	0.55
1:B:100:ARG:NH2	1:B:129:ARG:CB	2.70	0.55
1:B:253:ILE:O	1:B:255:ASN:N	2.40	0.55
1:B:253:ILE:C	1:B:255:ASN:H	2.14	0.55
1:A:54:LYS:HG2	1:A:55:ILE:N	2.20	0.54
1:B:108:PHE:HA	1:B:111:ALA:HB2	1.89	0.54
1:B:84:ILE:O	1:B:87:ALA:HB3	2.06	0.54
1:B:127:ILE:HA	1:B:130:LEU:HB2	1.88	0.54
1:B:72:VAL:O	1:B:73:VAL:C	2.42	0.54
1:B:250:PHE:C	1:B:252:SER:H	2.14	0.54
1:A:178:ARG:C	1:A:179:VAL:CG2	2.80	0.54
1:A:69:TYR:O	1:A:71:ALA:N	2.41	0.54
1:A:153:ALA:O	1:A:157:ASN:HB2	2.08	0.54
1:B:102:ASP:O	1:B:103:ASP:O	2.26	0.54
1:B:167:TYR:CE1	1:B:169:PRO:CA	2.87	0.54
1:A:53:MET:HG3	1:A:198:MET:HE1	1.89	0.54
1:A:253:ILE:C	1:A:255:ASN:N	2.56	0.54
1:B:64:GLU:CA	1:B:67:LYS:HG3	2.37	0.54
1:B:155:TYR:OH	1:B:173:ASP:O	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG12	1:B:226:ALA:N	2.09	0.54
1:B:69:TYR:O	1:B:71:ALA:N	2.41	0.54
1:B:97:ASP:HB3	1:B:100:ARG:HD3	1.90	0.54
1:A:62:SER:O	1:A:66:CYS:SG	2.66	0.53
1:A:340:THR:O	1:A:342:VAL:N	2.41	0.53
1:B:329:THR:O	1:B:329:THR:CG2	2.55	0.53
1:A:66:CYS:HB3	1:A:169:PRO:O	2.07	0.53
1:A:72:VAL:C	1:A:74:TYR:N	2.62	0.53
1:B:52:GLN:C	1:B:54:LYS:H	2.15	0.53
1:A:85:ILE:C	1:A:87:ALA:H	2.16	0.53
1:B:57:HIS:O	1:B:58:GLU:HG3	2.05	0.53
1:B:67:LYS:O	1:B:70:LYS:HB2	2.07	0.53
1:B:103:ASP:C	1:B:104:ALA:C	2.75	0.53
1:A:62:SER:HG	1:A:65:GLU:CG	2.22	0.53
1:A:192:LYS:O	1:A:193:ASP:CB	2.49	0.53
1:B:277:LYS:C	1:B:279:LYS:N	2.64	0.53
1:B:82:ILE:O	1:B:86:ARG:HG3	2.09	0.53
1:B:162:ILE:CG2	1:B:167:TYR:HE2	1.99	0.53
1:A:72:VAL:C	1:A:74:TYR:H	2.16	0.53
1:A:187:THR:C	1:A:188:HIS:HD2	2.16	0.53
1:B:95:PHE:O	1:B:97:ASP:O	2.26	0.53
1:B:126:VAL:CA	1:B:130:LEU:CD1	2.82	0.53
1:B:164:GLN:OE1	1:B:164:GLN:N	2.30	0.53
1:B:36:LEU:CD2	1:B:198:MET:HG3	2.37	0.53
1:A:80:SER:O	1:A:84:ILE:HG13	2.09	0.53
1:B:142:ARG:C	1:B:144:ARG:N	2.66	0.53
1:B:86:ARG:CB	1:B:86:ARG:CZ	2.86	0.53
1:B:167:TYR:CE1	1:B:169:PRO:CD	2.91	0.53
1:A:329:THR:O	1:A:329:THR:CG2	2.55	0.52
1:B:65:GLU:C	1:B:67:LYS:N	2.63	0.52
1:B:135:GLY:O	1:B:138:ALA:HB3	2.09	0.52
1:B:137:GLN:N	1:B:138:ALA:HB3	2.23	0.52
1:B:253:ILE:C	1:B:255:ASN:N	2.60	0.52
1:B:127:ILE:O	1:B:128:LYS:C	2.50	0.52
1:B:344:ILE:CG2	1:B:345:LYS:H	2.01	0.52
1:B:192:LYS:O	1:B:193:ASP:CB	2.55	0.52
2:D:11:VAL:C	2:D:12:GLY:O	2.46	0.52
1:B:143:SER:C	1:B:145:GLU:N	2.66	0.52
1:B:92:LYS:O	1:B:93:ILE:HG12	2.10	0.52
1:B:167:TYR:OH	1:B:169:PRO:CB	2.58	0.52
1:B:142:ARG:O	1:B:145:GLU:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ILE:O	1:B:222:ILE:HG22	2.02	0.52
1:B:272:ASP:OD1	1:B:272:ASP:N	2.30	0.51
1:B:170:THR:C	1:B:172:GLN:N	2.67	0.51
1:B:272:ASP:CG	1:B:273:LEU:N	2.61	0.51
1:A:245:GLU:O	1:A:245:GLU:CG	2.45	0.51
1:B:342:VAL:O	1:B:343:ILE:C	2.52	0.51
1:B:170:THR:H	1:B:173:ASP:HB2	1.76	0.51
1:B:245:GLU:C	1:B:247:MET:H	2.19	0.51
1:B:308:GLU:OE2	1:B:319:ILE:O	2.27	0.51
1:A:159:LEU:O	1:A:160:ASP:C	2.51	0.51
1:A:36:LEU:CD2	1:A:37:LEU:H	2.24	0.51
1:A:260:THR:O	1:A:260:THR:HG23	2.07	0.51
1:B:289:GLU:O	1:B:290:TYR:C	2.50	0.51
1:A:36:LEU:HD22	1:A:37:LEU:H	1.75	0.51
1:A:85:ILE:C	1:A:87:ALA:N	2.67	0.51
1:A:158:ASP:OD2	1:A:161:ARG:NE	2.43	0.51
1:B:100:ARG:O	1:B:103:ASP:OD2	2.29	0.51
1:A:193:ASP:O	1:A:194:LEU:HD23	2.11	0.50
1:B:86:ARG:O	1:B:89:GLY:C	2.54	0.50
1:B:309:ASP:OD1	1:B:309:ASP:O	2.29	0.50
1:A:102:ASP:OD1	1:A:102:ASP:O	2.30	0.50
1:A:161:ARG:CG	1:A:161:ARG:NH1	2.72	0.50
1:A:162:ILE:HB	1:A:167:TYR:CZ	2.46	0.50
1:B:148:LEU:O	1:B:149:ASN:O	2.30	0.50
1:B:163:ALA:O	1:B:165:PRO:N	2.45	0.50
1:A:188:HIS:O	1:A:189:PHE:HB3	2.10	0.50
1:A:191:PHE:O	1:A:193:ASP:N	2.45	0.50
1:B:128:LYS:C	1:B:130:LEU:N	2.66	0.50
1:B:237:ASP:OD1	1:B:237:ASP:O	2.30	0.50
1:A:133:ASP:O	1:A:135:GLY:N	2.44	0.50
1:A:136:VAL:O	1:A:136:VAL:CG1	2.58	0.50
1:A:207:GLU:O	1:A:209:LYS:N	2.45	0.50
1:A:191:PHE:O	1:A:192:LYS:C	2.52	0.50
1:B:153:ALA:C	1:B:155:TYR:N	2.66	0.50
1:B:296:TYR:O	1:B:300:ALA:HB2	2.11	0.50
1:A:69:TYR:C	1:A:71:ALA:N	2.64	0.50
1:B:277:LYS:C	1:B:279:LYS:H	2.19	0.50
1:A:64:GLU:N	1:A:64:GLU:CD	2.70	0.50
1:A:161:ARG:NH1	1:A:161:ARG:HG2	2.27	0.50
1:B:101:ALA:C	1:B:104:ALA:HB2	2.37	0.50
1:B:134:SER:OG	1:B:135:GLY:N	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:CG1	1:B:226:ALA:N	2.59	0.50
1:B:284:THR:HA	1:B:287:TYR:O	2.12	0.50
1:A:243:MET:HE1	1:A:303:ILE:CD1	2.37	0.49
1:B:295:THR:O	1:B:296:TYR:C	2.55	0.49
1:A:143:SER:O	1:A:146:TYR:O	2.30	0.49
1:B:294:ASN:O	1:B:294:ASN:OD1	2.29	0.49
1:A:203:GLY:O	1:A:204:GLN:O	2.29	0.49
1:B:124:ALA:C	1:B:126:VAL:N	2.60	0.49
1:A:299:ALA:C	1:A:301:ALA:N	2.65	0.49
1:B:123:LEU:C	1:B:126:VAL:CG2	2.84	0.49
1:B:164:GLN:H	1:B:164:GLN:CD	2.11	0.49
1:A:109:VAL:CG1	1:A:110:LEU:HA	2.40	0.49
1:B:125:GLY:O	1:B:129:ARG:N	2.30	0.49
1:B:159:LEU:O	1:B:163:ALA:N	2.44	0.49
1:A:109:VAL:CB	1:A:110:LEU:HB2	2.43	0.49
1:B:110:LEU:O	1:B:111:ALA:O	2.30	0.49
1:B:132:LYS:C	1:B:133:ASP:O	2.50	0.49
1:B:344:ILE:O	1:B:345:LYS:O	2.30	0.49
2:D:11:VAL:O	2:D:12:GLY:O	2.29	0.49
1:A:97:ASP:OD2	1:A:99:ALA:HB2	2.13	0.49
1:A:81:ILE:O	1:A:85:ILE:HG12	2.12	0.49
1:A:276:GLU:O	1:A:279:LYS:HB2	2.13	0.49
1:B:102:ASP:N	1:B:103:ASP:HB2	2.28	0.49
1:B:123:LEU:O	1:B:124:ALA:O	2.29	0.49
1:B:127:ILE:C	1:B:130:LEU:H	2.21	0.49
1:A:33:GLU:O	1:A:34:VAL:HG22	2.11	0.48
1:B:77:THR:O	1:B:78:ILE:O	2.30	0.48
1:B:87:ALA:O	1:B:88:MET:O	2.30	0.48
1:B:126:VAL:O	1:B:130:LEU:HD13	0.67	0.48
1:A:84:ILE:O	1:A:85:ILE:O	2.31	0.48
1:B:81:ILE:O	1:B:84:ILE:N	2.45	0.48
1:B:158:ASP:OD2	1:B:158:ASP:O	2.30	0.48
1:B:162:ILE:O	1:B:167:TYR:HD2	1.96	0.48
1:B:311:ASN:O	1:B:314:LYS:CE	2.60	0.48
1:A:63:GLU:C	1:A:64:GLU:OE2	2.56	0.48
1:A:69:TYR:C	1:A:71:ALA:H	2.21	0.48
1:A:130:LEU:C	1:A:132:LYS:H	2.20	0.48
1:A:165:PRO:O	1:A:165:PRO:HG2	2.13	0.48
1:B:86:ARG:NH1	1:B:90:ARG:HH12	2.11	0.48
1:A:253:ILE:O	1:A:254:CYS:C	2.53	0.48
1:A:337:ASP:O	1:A:338:ALA:C	2.50	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:O	1:A:130:LEU:N	2.47	0.48
1:B:167:TYR:OH	1:B:169:PRO:HG3	2.09	0.48
1:B:127:ILE:C	1:B:130:LEU:HB2	2.39	0.48
1:A:192:LYS:NZ	1:A:337:ASP:OD2	2.42	0.47
1:A:304:GLN:O	1:A:304:GLN:HG2	2.14	0.47
1:B:81:ILE:O	1:B:83:ALA:N	2.46	0.47
1:A:65:GLU:C	1:A:67:LYS:H	2.21	0.47
1:B:165:PRO:O	1:B:166:ASN:C	2.56	0.47
1:B:301:ALA:C	1:B:303:ILE:N	2.65	0.47
1:A:62:SER:N	1:A:65:GLU:HB2	2.17	0.47
1:B:211:TRP:C	1:B:213:HIS:H	2.20	0.47
1:B:146:TYR:N	1:B:146:TYR:CD1	2.82	0.47
1:A:65:GLU:C	1:A:67:LYS:N	2.71	0.47
1:B:164:GLN:HA	1:B:165:PRO:HD2	1.24	0.47
1:A:93:ILE:CG2	1:A:94:ASP:N	2.76	0.47
1:B:88:MET:HE3	1:B:93:ILE:HG21	1.97	0.47
1:B:101:ALA:O	1:B:104:ALA:HB3	2.14	0.47
1:B:54:LYS:HZ3	1:B:59:ALA:CB	2.28	0.47
1:B:88:MET:HE1	1:B:95:PHE:CE1	2.49	0.47
1:B:102:ASP:O	1:B:103:ASP:C	2.57	0.47
1:B:167:TYR:CE1	1:B:169:PRO:CB	2.95	0.47
1:B:243:MET:O	1:B:243:MET:HG3	2.14	0.47
1:B:72:VAL:O	1:B:72:VAL:HG12	2.15	0.47
1:B:140:PHE:O	1:B:140:PHE:CD1	2.67	0.47
1:A:36:LEU:CD2	1:A:37:LEU:N	2.78	0.47
1:A:159:LEU:C	1:A:161:ARG:N	2.69	0.47
1:A:102:ASP:C	1:A:104:ALA:N	2.66	0.47
1:A:256:ASN:OD1	1:A:257:LYS:N	2.48	0.47
1:B:64:GLU:C	1:B:67:LYS:HB2	2.27	0.47
1:B:303:ILE:O	1:B:304:GLN:C	2.56	0.47
1:B:72:VAL:O	1:B:74:TYR:N	2.46	0.46
1:B:78:ILE:HD12	1:B:78:ILE:HA	1.50	0.46
1:B:104:ALA:O	1:B:107:LEU:HB3	2.14	0.46
1:A:184:ILE:HG22	1:A:185:VAL:N	2.30	0.46
1:B:167:TYR:OH	1:B:169:PRO:CG	2.63	0.46
1:A:106:GLN:O	1:A:106:GLN:HG3	2.16	0.46
1:B:57:HIS:NE2	1:B:191:PHE:CD1	2.80	0.46
1:B:102:ASP:O	1:B:104:ALA:C	2.59	0.46
1:B:102:ASP:O	1:B:105:ARG:N	2.48	0.46
1:B:135:GLY:C	1:B:138:ALA:CB	2.89	0.46
1:A:231:ASP:N	1:A:231:ASP:OD1	2.38	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:VAL:O	1:A:343:ILE:C	2.57	0.46
1:B:331:ASN:O	1:B:332:VAL:C	2.56	0.46
1:A:97:ASP:O	1:A:99:ALA:N	2.49	0.46
1:A:243:MET:CE	1:A:303:ILE:HD13	2.42	0.46
1:A:172:GLN:O	1:A:173:ASP:C	2.58	0.46
1:A:299:ALA:C	1:A:301:ALA:H	2.24	0.46
1:B:86:ARG:HH12	1:B:90:ARG:CZ	2.28	0.46
1:B:204:GLN:O	1:B:205:ARG:C	2.55	0.46
1:B:52:GLN:C	1:B:54:LYS:N	2.74	0.46
2:C:6:TYR:CD2	2:C:6:TYR:C	2.92	0.46
1:A:73:VAL:O	1:A:73:VAL:HG12	2.09	0.45
1:A:109:VAL:HG12	1:A:110:LEU:HB2	1.98	0.45
1:A:222:ILE:O	1:A:222:ILE:HG22	2.14	0.45
1:A:335:VAL:O	1:A:338:ALA:HB3	2.16	0.45
1:B:124:ALA:O	1:B:126:VAL:HB	2.16	0.45
1:A:247:MET:HE2	1:A:287:TYR:OH	2.16	0.45
1:B:158:ASP:OD2	1:B:161:ARG:CZ	2.64	0.45
1:A:131:TRP:CE3	1:A:156:LEU:HD13	2.51	0.45
1:A:276:GLU:O	1:A:277:LYS:C	2.55	0.45
1:A:278:ILE:O	1:A:278:ILE:CG1	2.52	0.45
1:A:305:CYS:C	1:A:307:PHE:N	2.71	0.45
1:A:325:CYS:O	1:A:326:ALA:C	2.56	0.45
1:B:62:SER:O	1:B:65:GLU:CB	2.60	0.45
1:A:172:GLN:HA	1:A:175:LEU:HD12	1.98	0.45
1:A:304:GLN:O	1:A:304:GLN:CG	2.65	0.45
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.66	0.45
1:B:107:LEU:O	1:B:111:ALA:CA	2.61	0.45
1:B:68:GLN:NE2	1:B:68:GLN:H	2.04	0.45
1:B:97:ASP:CB	1:B:100:ARG:CD	2.94	0.45
1:B:170:THR:C	1:B:173:ASP:H	2.17	0.45
1:B:341:ASP:O	1:B:344:ILE:HB	2.16	0.45
1:B:56:ILE:HD13	1:B:56:ILE:HG23	1.65	0.45
1:B:84:ILE:HG23	1:B:84:ILE:HD13	1.63	0.45
1:B:164:GLN:O	1:B:165:PRO:C	2.53	0.45
1:B:164:GLN:O	1:B:167:TYR:HB2	2.17	0.45
1:B:171:GLN:H	1:B:171:GLN:HG2	1.55	0.45
1:B:314:LYS:C	1:B:316:THR:N	2.69	0.45
1:A:241:ASN:HB3	1:A:244:HIS:CG	2.52	0.45
1:B:233:VAL:HB	1:B:238:GLU:O	2.17	0.45
1:A:303:ILE:O	1:A:304:GLN:C	2.57	0.44
1:B:130:LEU:C	1:B:132:LYS:N	2.67	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:CG2	1:A:94:ASP:H	2.25	0.44
1:A:139:CYS:O	1:A:139:CYS:SG	2.75	0.44
1:A:227:LEU:C	1:A:229:ASP:H	2.26	0.44
1:A:256:ASN:C	1:A:258:TRP:H	2.23	0.44
1:B:97:ASP:CB	1:B:100:ARG:HD3	2.45	0.44
1:B:100:ARG:NH1	1:B:129:ARG:HD3	2.26	0.44
1:A:330:LYS:HB3	1:A:330:LYS:HE2	1.75	0.44
2:C:5:TYR:HA	2:C:9:ILE:O	2.17	0.44
1:A:277:LYS:C	1:A:279:LYS:N	2.64	0.44
1:B:167:TYR:HE1	1:B:169:PRO:CD	2.27	0.44
1:A:170:THR:O	1:A:174:VAL:HG23	2.17	0.44
1:B:164:GLN:O	1:B:167:TYR:CB	2.66	0.44
1:B:226:ALA:O	1:B:229:ASP:HB2	2.18	0.44
1:B:49:ILE:HG23	1:B:49:ILE:HD13	1.59	0.44
1:A:54:LYS:O	1:A:58:GLU:HB2	2.18	0.44
1:A:193:ASP:C	1:A:194:LEU:HD23	2.43	0.44
1:B:88:MET:CE	1:B:95:PHE:CE1	3.00	0.44
1:B:168:ILE:N	1:B:168:ILE:CD1	2.29	0.43
1:B:168:ILE:HA	1:B:169:PRO:HD3	1.56	0.43
1:B:100:ARG:O	1:B:103:ASP:CG	2.61	0.43
1:B:170:THR:OG1	1:B:173:ASP:OD2	2.36	0.43
1:B:195:HIS:CE1	1:B:197:LYS:HE2	2.53	0.43
1:A:133:ASP:HB3	1:A:136:VAL:H	1.83	0.43
1:A:284:THR:H	1:A:284:THR:HG23	1.50	0.43
1:B:37:LEU:HD12	1:B:37:LEU:HA	1.73	0.43
1:A:122:GLU:O	1:A:122:GLU:HG3	2.16	0.43
1:B:156:LEU:O	1:B:157:ASN:C	2.60	0.43
1:B:247:MET:CE	1:B:287:TYR:CE1	3.00	0.43
1:A:53:MET:CG	1:A:198:MET:HE1	2.48	0.43
1:A:271:LYS:HG2	1:A:324:THR:O	2.19	0.43
1:A:283:LEU:C	1:A:285:ILE:N	2.41	0.43
1:B:42:GLY:C	1:B:43:GLU:HG3	2.42	0.43
1:B:48:THR:OG1	5:B:355:GDP:O1A	2.25	0.43
1:A:343:ILE:HD13	1:A:343:ILE:HG21	1.77	0.43
1:A:107:LEU:O	1:A:110:LEU:HB3	2.18	0.43
1:B:100:ARG:NH2	1:B:129:ARG:HD2	0.26	0.43
1:A:172:GLN:HE21	1:A:172:GLN:HB2	1.59	0.43
1:B:139:CYS:O	1:B:140:PHE:C	2.59	0.43
1:B:264:ILE:HG21	1:B:264:ILE:HD12	1.65	0.43
1:A:253:ILE:HG23	1:A:253:ILE:HD12	1.66	0.42
1:B:97:ASP:CG	1:B:100:ARG:CD	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:TYR:CE2	1:B:173:ASP:OD1	2.72	0.42
1:A:319:ILE:HG21	1:A:319:ILE:HD13	1.69	0.42
1:A:331:ASN:O	1:A:332:VAL:C	2.55	0.42
1:A:334:PHE:CD1	1:A:334:PHE:C	2.93	0.42
1:B:243:MET:HG2	1:B:286:CYS:SG	2.60	0.42
1:B:328:ASP:OD1	1:B:329:THR:N	2.52	0.42
1:A:238:GLU:HG2	1:A:239:GLU:HG2	2.01	0.42
1:B:88:MET:CB	1:B:93:ILE:HG21	2.49	0.42
1:B:137:GLN:H	1:B:138:ALA:HB3	1.84	0.42
1:B:209:LYS:O	1:B:212:ILE:HD11	2.19	0.42
1:A:221:ILE:HG21	1:A:221:ILE:HD13	1.50	0.42
1:B:149:ASN:OD1	1:B:149:ASN:N	2.29	0.42
1:B:68:GLN:H	1:B:68:GLN:HG2	1.54	0.42
1:A:56:ILE:HG23	1:A:56:ILE:HD13	1.57	0.42
1:A:73:VAL:O	1:A:73:VAL:CG1	2.63	0.42
1:B:162:ILE:HG21	1:B:162:ILE:HD12	1.80	0.42
1:B:187:THR:O	1:B:187:THR:HG22	2.05	0.42
1:A:57:HIS:O	1:A:58:GLU:HG3	2.12	0.42
1:A:251:ASP:O	1:A:255:ASN:HB2	2.20	0.42
1:A:303:ILE:HD13	1:A:303:ILE:HG23	1.78	0.42
1:B:103:ASP:O	1:B:106:GLN:N	2.52	0.42
1:A:178:ARG:NH2	1:A:180:LYS:HG3	2.34	0.41
1:A:274:PHE:C	1:A:276:GLU:H	2.27	0.41
1:B:247:MET:CE	1:B:287:TYR:OH	2.63	0.41
1:B:250:PHE:O	1:B:252:SER:N	2.51	0.41
2:C:5:TYR:CD1	2:C:5:TYR:N	2.88	0.41
1:A:188:HIS:CD2	1:A:188:HIS:N	2.83	0.41
1:A:257:LYS:H	1:A:257:LYS:HG3	1.38	0.41
2:C:7:HIS:H	2:C:9:ILE:H	1.66	0.41
1:B:64:GLU:O	1:B:67:LYS:CB	2.30	0.41
1:B:127:ILE:HB	1:B:128:LYS:H	1.44	0.41
2:D:9:ILE:HD13	2:D:9:ILE:HG21	1.50	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.81	0.41
1:B:88:MET:HE1	1:B:95:PHE:HD1	1.82	0.41
1:B:126:VAL:HG12	1:B:130:LEU:CD1	2.48	0.41
2:D:11:VAL:H	2:D:11:VAL:HG22	1.61	0.41
1:B:184:ILE:H	1:B:184:ILE:HG13	1.48	0.41
1:B:272:ASP:O	1:B:273:LEU:C	2.60	0.41
1:B:319:ILE:HG21	1:B:319:ILE:HD13	1.65	0.41
2:C:9:ILE:HG22	2:C:10:TRP:N	2.35	0.41
1:A:49:ILE:HD13	1:A:49:ILE:HG23	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:N	6:A:3:HOH:O	2.53	0.41
1:B:98:SER:O	1:B:100:ARG:N	2.54	0.41
1:B:102:ASP:H	1:B:103:ASP:HB2	1.84	0.41
1:B:264:ILE:O	1:B:264:ILE:HG22	2.17	0.41
1:A:49:ILE:HG21	1:A:49:ILE:HD12	1.68	0.41
1:A:144:ARG:HH11	1:A:144:ARG:HD3	1.55	0.41
1:B:55:ILE:O	1:B:56:ILE:C	2.60	0.41
1:B:202:GLY:HA2	3:B:359:ALF:F3	2.10	0.41
1:B:245:GLU:C	1:B:247:MET:N	2.73	0.40
1:A:56:ILE:HG21	1:A:56:ILE:HD12	1.69	0.40
1:A:143:SER:HA	1:A:146:TYR:CE1	2.55	0.40
1:A:162:ILE:O	1:A:162:ILE:HG13	2.21	0.40
1:A:325:CYS:C	1:A:327:THR:N	2.79	0.40
2:D:6:TYR:CD2	2:D:7:HIS:ND1	2.81	0.40
1:A:85:ILE:HD12	1:A:85:ILE:HG23	1.88	0.40
1:B:55:ILE:HD13	1:B:55:ILE:HG21	1.52	0.40
1:B:124:ALA:O	1:B:125:GLY:C	2.61	0.40
1:B:142:ARG:CZ	1:B:145:GLU:OE2	2.70	0.40
1:A:274:PHE:C	1:A:276:GLU:N	2.79	0.40
1:B:76:ASN:HD22	1:B:76:ASN:HA	1.65	0.40
1:B:81:ILE:C	1:B:81:ILE:HD12	2.46	0.40
1:B:91:LEU:HA	1:B:91:LEU:HD23	0.95	0.40
1:A:78:ILE:HD12	1:A:78:ILE:HG21	1.86	0.40
1:B:319:ILE:HG22	1:B:320:TYR:N	2.35	0.40
2:C:11:VAL:H	2:C:11:VAL:HG22	1.53	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASP:OD2	2:D:6:TYR:O[2_455]	1.40	0.80
1:A:97:ASP:CG	2:D:6:TYR:O[2_455]	2.07	0.13
1:A:97:ASP:OD1	2:D:6:TYR:O[2_455]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/313 (96%)	240 (80%)	43 (14%)	16 (5%)	1	4
1	B	299/313 (96%)	232 (78%)	41 (14%)	26 (9%)	0	1
2	C	9/11 (82%)	8 (89%)	1 (11%)	0	100	100
2	D	9/11 (82%)	5 (56%)	4 (44%)	0	100	100
All	All	616/648 (95%)	485 (79%)	89 (14%)	42 (7%)	1	2

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	GLY
1	B	93	ILE
1	B	105	ARG
1	B	138	ALA
1	B	160	ASP
1	B	165	PRO
1	B	184	ILE
1	B	291	ALA
1	A	66	CYS
1	A	131	TRP
1	A	230	TYR
1	A	284	THR
1	A	326	ALA
1	A	344	ILE
1	B	82	ILE
1	B	92	LYS
1	B	99	ALA
1	B	126	VAL
1	B	143	SER
1	B	157	ASN
1	B	169	PRO
1	B	238	GLU
1	A	152	ALA
1	A	304	GLN
1	B	273	LEU
1	A	166	ASN
1	B	66	CYS
1	B	193	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	193	ASP
1	B	124	ALA
1	B	164	GLN
1	B	290	TYR
1	B	331	ASN
1	A	34	VAL
1	A	85	ILE
1	B	95	PHE
1	B	131	TRP
1	A	73	VAL
1	A	109	VAL
1	B	78	ILE
1	A	343	ILE
1	B	278	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/272 (98%)	211 (79%)	56 (21%)	1	4
1	B	267/272 (98%)	182 (68%)	85 (32%)	0	1
2	C	8/8 (100%)	7 (88%)	1 (12%)	4	15
2	D	8/8 (100%)	7 (88%)	1 (12%)	4	15
All	All	550/560 (98%)	407 (74%)	143 (26%)	0	2

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	43	GLU
1	A	44	SER
1	A	46	LYS
1	A	49	ILE
1	A	51	LYS
1	A	56	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	62	SER
1	A	63	GLU
1	A	64	GLU
1	A	70	LYS
1	A	74	TYR
1	A	75	SER
1	A	78	ILE
1	A	82	ILE
1	A	88	MET
1	A	94	ASP
1	A	102	ASP
1	A	127	ILE
1	A	128	LYS
1	A	143	SER
1	A	149	ASN
1	A	158	ASP
1	A	161	ARG
1	A	162	ILE
1	A	167	TYR
1	A	168	ILE
1	A	177	THR
1	A	185	VAL
1	A	193	ASP
1	A	206	SER
1	A	212	ILE
1	A	214	CYS
1	A	228	SER
1	A	234	LEU
1	A	243	MET
1	A	246	SER
1	A	247	MET
1	A	249	LEU
1	A	257	LYS
1	A	258	TRP
1	A	260	THR
1	A	264	ILE
1	A	279	LYS
1	A	280	LYS
1	A	285	ILE
1	A	289	GLU
1	A	294	ASN
1	A	303	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	313	ARG
1	A	315	ASP
1	A	316	THR
1	A	317	LYS
1	A	331	ASN
1	A	344	ILE
1	A	345	LYS
1	B	36	LEU
1	B	37	LEU
1	B	49	ILE
1	B	50	VAL
1	B	52	GLN
1	B	56	ILE
1	B	64	GLU
1	B	67	LYS
1	B	68	GLN
1	B	74	TYR
1	B	78	ILE
1	B	81	ILE
1	B	82	ILE
1	B	84	ILE
1	B	86	ARG
1	B	90	ARG
1	B	91	LEU
1	B	92	LYS
1	B	93	ILE
1	B	106	GLN
1	B	107	LEU
1	B	110	LEU
1	B	122	GLU
1	B	126	VAL
1	B	127	ILE
1	B	128	LYS
1	B	129	ARG
1	B	130	LEU
1	B	131	TRP
1	B	132	LYS
1	B	133	ASP
1	B	139	CYS
1	B	141	ASN
1	B	142	ARG
1	B	143	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	144	ARG
1	B	149	ASN
1	B	151	SER
1	B	159	LEU
1	B	162	ILE
1	B	164	GLN
1	B	167	TYR
1	B	168	ILE
1	B	170	THR
1	B	177	THR
1	B	187	THR
1	B	193	ASP
1	B	194	LEU
1	B	204	GLN
1	B	206	SER
1	B	212	ILE
1	B	213	HIS
1	B	216	GLU
1	B	221	ILE
1	B	232	LEU
1	B	233	VAL
1	B	236	GLU
1	B	238	GLU
1	B	239	GLU
1	B	240	MET
1	B	246	SER
1	B	247	MET
1	B	249	LEU
1	B	257	LYS
1	B	258	TRP
1	B	260	THR
1	B	262	THR
1	B	264	ILE
1	B	276	GLU
1	B	279	LYS
1	B	280	LYS
1	B	282	PRO
1	B	285	ILE
1	B	289	GLU
1	B	294	ASN
1	B	297	GLU
1	B	304	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	313	ARG
1	B	316	THR
1	B	317	LYS
1	B	329	THR
1	B	331	ASN
1	B	343	ILE
1	B	344	ILE
1	B	345	LYS
2	C	7	HIS
2	D	7	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	164	GLN
1	A	171	GLN
1	A	188	HIS
1	A	269	ASN
1	A	304	GLN
1	B	68	GLN
1	B	171	GLN
1	B	172	GLN
1	B	195	HIS
1	B	304	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GDP	A	355	4,3	29,30,30	4.05	22 (75%)	45,47,47	2.75	26 (57%)
3	ALF	B	359	4,5,1	4,4,4	0.63	0	-		
3	ALF	A	357	4,5,1	4,4,4	0.68	0	-		
5	GDP	B	355	4,3	29,30,30	3.53	20 (68%)	45,47,47	2.95	21 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	A	355	4,3	-	4/16/32/32	0/3/3/3
5	GDP	B	355	4,3	-	1/16/32/32	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	355	GDP	PA-O3A	-8.73	1.50	1.59
5	B	355	GDP	C6-N1	-8.66	1.22	1.38
5	A	355	GDP	C6-N1	-8.21	1.23	1.38
5	B	355	GDP	C5-N7	-6.58	1.25	1.39
5	A	355	GDP	C5-N7	-5.72	1.27	1.39
5	A	355	GDP	PB-O2B	-5.67	1.33	1.54
5	A	355	GDP	C2-N1	-5.06	1.25	1.37
5	A	355	GDP	PB-O1B	-5.04	1.34	1.50
5	B	355	GDP	PB-O2B	-4.82	1.36	1.54
5	A	355	GDP	C8-N9	-4.79	1.26	1.37
5	B	355	GDP	PA-O3A	-4.74	1.54	1.59
5	A	355	GDP	PA-O1A	-4.60	1.34	1.50
5	A	355	GDP	PA-O2A	-4.57	1.34	1.55
5	B	355	GDP	C8-N9	-4.46	1.27	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	355	GDP	C2-N1	-4.40	1.26	1.37
5	A	355	GDP	O2'-C2'	-4.10	1.32	1.43
5	A	355	GDP	C4-N9	-4.05	1.27	1.38
5	A	355	GDP	C2'-C3'	-4.05	1.42	1.53
5	B	355	GDP	PB-O3B	-4.04	1.39	1.54
5	B	355	GDP	PA-O2A	-3.88	1.37	1.55
5	B	355	GDP	PA-O1A	-3.75	1.37	1.50
5	B	355	GDP	PA-O5'	-3.64	1.45	1.59
5	A	355	GDP	C2'-C1'	-3.59	1.42	1.53
5	B	355	GDP	C2'-C3'	-3.49	1.43	1.53
5	A	355	GDP	PA-O5'	-3.42	1.46	1.59
5	B	355	GDP	O3'-C3'	-3.41	1.34	1.43
5	B	355	GDP	C4-N9	-3.40	1.29	1.38
5	A	355	GDP	C3'-C4'	-3.38	1.44	1.53
5	A	355	GDP	O4'-C4'	-3.36	1.37	1.45
5	A	355	GDP	O3'-C3'	-3.34	1.34	1.43
5	B	355	GDP	O2'-C2'	-3.02	1.35	1.43
5	A	355	GDP	O4'-C1'	-3.01	1.35	1.42
5	B	355	GDP	O4'-C4'	-2.87	1.38	1.45
5	B	355	GDP	C2-N2	-2.82	1.27	1.34
5	B	355	GDP	C3'-C4'	-2.78	1.45	1.53
5	B	355	GDP	C2'-C1'	-2.72	1.44	1.53
5	A	355	GDP	O6-C6	-2.65	1.18	1.23
5	A	355	GDP	O5'-C5'	-2.34	1.35	1.44
5	A	355	GDP	C2-N3	-2.30	1.27	1.33
5	B	355	GDP	O6-C6	-2.30	1.19	1.23
5	A	355	GDP	C2-N2	-2.05	1.29	1.34
5	B	355	GDP	C4-N3	-2.03	1.29	1.34

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	355	GDP	C5-C4-N3	-8.29	115.19	128.39
5	A	355	GDP	O3B-PB-O3A	6.10	125.11	104.64
5	A	355	GDP	C5-C4-N3	-6.10	118.69	128.39
5	B	355	GDP	N9-C4-N3	5.65	137.25	125.95
5	B	355	GDP	O2B-PB-O3A	-5.38	86.59	104.64
5	B	355	GDP	O5'-PA-O1A	-5.16	88.50	108.94
5	B	355	GDP	O2A-PA-O3A	5.14	121.17	107.27
5	A	355	GDP	O2A-PA-O3A	4.94	120.62	107.27
5	A	355	GDP	O4'-C1'-C2'	-4.85	96.24	106.62
5	B	355	GDP	O3A-PA-O1A	4.81	125.17	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	355	GDP	N9-C4-N3	4.65	135.25	125.95
5	A	355	GDP	C2-N3-C4	4.36	119.81	112.30
5	B	355	GDP	O3'-C3'-C4'	-4.06	99.42	111.08
5	A	355	GDP	O2B-PB-O1B	-4.06	95.03	110.83
5	B	355	GDP	O4'-C4'-C5'	3.74	121.30	109.33
5	B	355	GDP	O2A-PA-O5'	-3.71	90.75	107.57
5	A	355	GDP	O5'-C5'-C4'	3.70	121.58	108.99
5	B	355	GDP	O5'-C5'-C4'	3.69	121.55	108.99
5	B	355	GDP	O4'-C4'-C3'	-3.63	97.94	105.15
5	A	355	GDP	C6-C5-N7	3.63	136.90	130.29
5	B	355	GDP	C4-C5-N7	-3.56	105.03	110.67
5	B	355	GDP	O3'-C3'-C2'	-3.31	101.20	111.82
5	A	355	GDP	O4'-C4'-C5'	3.23	119.67	109.33
5	B	355	GDP	O2'-C2'-C3'	-3.11	101.84	111.82
5	A	355	GDP	O6-C6-N1	-3.08	114.33	120.11
5	A	355	GDP	O4'-C1'-N9	-3.01	101.53	108.36
5	B	355	GDP	C8-N7-C5	3.00	109.61	104.26
5	B	355	GDP	C2-N3-C4	2.99	117.46	112.30
5	B	355	GDP	O4'-C1'-C2'	-2.95	100.30	106.62
5	B	355	GDP	C6-C5-C4	2.86	123.14	118.83
5	A	355	GDP	O2'-C2'-C3'	-2.84	102.71	111.82
5	A	355	GDP	O3A-PB-O1B	-2.79	96.36	111.04
5	A	355	GDP	C5-C6-N1	2.74	120.22	113.25
5	A	355	GDP	O5'-PA-O1A	-2.71	98.19	108.94
5	A	355	GDP	O3B-PB-O1B	2.58	120.87	110.83
5	A	355	GDP	C3'-C2'-C1'	2.54	106.28	101.46
5	B	355	GDP	N1-C2-N3	2.45	127.80	123.32
5	A	355	GDP	O3A-PA-O1A	-2.42	103.42	110.70
5	B	355	GDP	C4'-O4'-C1'	2.39	114.75	109.47
5	A	355	GDP	C2-N1-C6	-2.23	121.07	125.11
5	A	355	GDP	C4'-O4'-C1'	2.19	114.30	109.47
5	B	355	GDP	O3A-PB-O1B	2.14	122.32	111.04
5	A	355	GDP	C4-C5-N7	-2.12	107.31	110.67
5	A	355	GDP	C2'-C3'-C4'	-2.05	98.65	102.61
5	A	355	GDP	O3B-PB-O2B	2.04	115.46	107.80
5	A	355	GDP	O2B-PB-O3A	-2.04	97.81	104.64
5	A	355	GDP	C6-C5-C4	-2.03	115.77	118.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

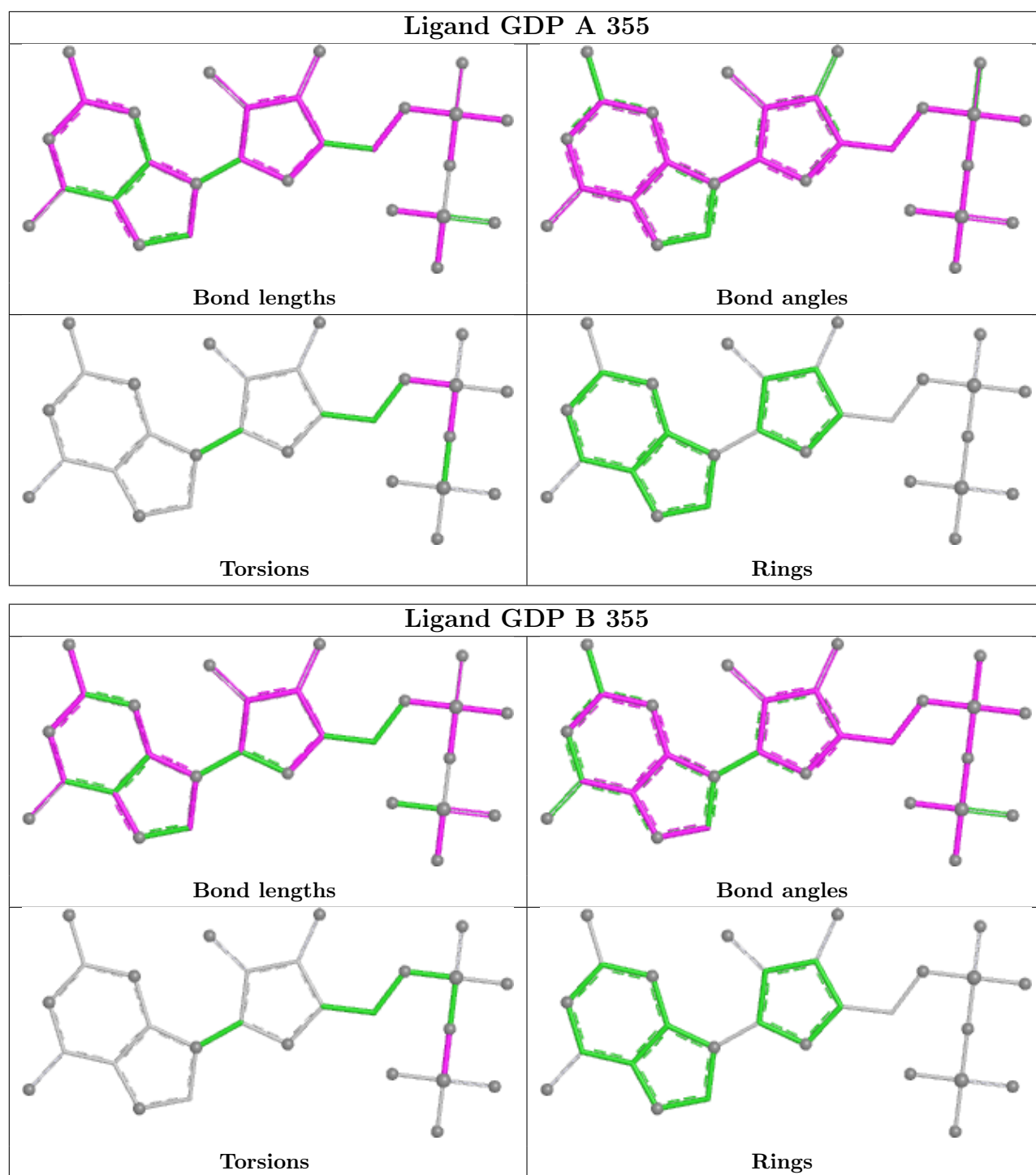
Mol	Chain	Res	Type	Atoms
5	A	355	GDP	C5'-O5'-PA-O3A
5	A	355	GDP	C5'-O5'-PA-O1A
5	A	355	GDP	C5'-O5'-PA-O2A
5	A	355	GDP	PB-O3A-PA-O2A
5	B	355	GDP	PA-O3A-PB-O2B

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	355	GDP	1	0
3	B	359	ALF	1	0
5	B	355	GDP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	103:ASP	C	104:ALA	N	1.18
1	A	344:ILE	C	345:LYS	N	1.15
1	A	110:LEU	C	111:ALA	N	0.86
1	A	109:VAL	C	110:LEU	N	0.73

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	303/313 (96%)	0.20	13 (4%) 40 31	27, 50, 84, 124	0
1	B	303/313 (96%)	0.46	18 (5%) 28 21	29, 57, 110, 151	0
2	C	11/11 (100%)	1.08	2 (18%) 3 2	47, 66, 107, 109	0
2	D	11/11 (100%)	0.86	2 (18%) 3 2	45, 53, 80, 103	0
All	All	628/648 (96%)	0.36	35 (5%) 30 23	27, 53, 104, 151	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	SER	4.7
1	A	89	GLY	4.1
1	B	183	GLY	4.1
1	A	166	ASN	3.4
1	A	160	ASP	3.4
1	B	123	LEU	3.3
1	B	128	LYS	3.2
2	D	3	ARG	3.2
1	B	168	ILE	3.0
1	A	195	HIS	2.9
1	B	345	LYS	2.8
2	C	6	TYR	2.7
1	B	239	GLU	2.7
1	A	122	GLU	2.7
1	A	289	GLU	2.6
1	A	79	GLN	2.6
1	A	209	LYS	2.6
1	B	195	HIS	2.6
1	A	345	LYS	2.6
1	A	102	ASP	2.5
1	A	212	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	108	PHE	2.4
1	B	80	SER	2.3
1	B	99	ALA	2.2
2	D	13	GLU	2.2
1	B	166	ASN	2.2
1	B	63	GLU	2.2
1	B	95	PHE	2.2
1	B	152	ALA	2.2
1	B	70	LYS	2.1
1	B	33	GLU	2.1
2	C	4	GLY	2.1
1	A	111	ALA	2.1
1	A	203	GLY	2.1
1	B	276	GLU	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.

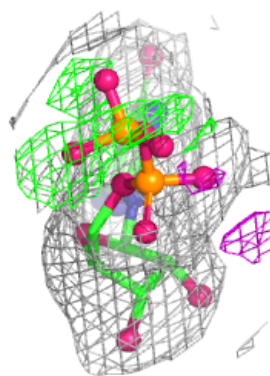
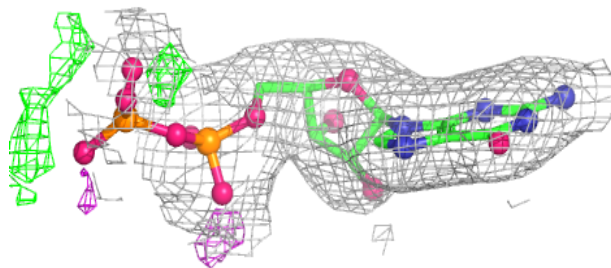
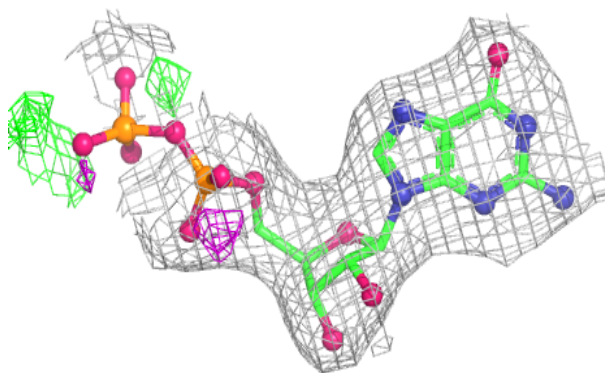
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ALF	B	359	5/5	0.88	0.13	59,61,63,65	0
4	MG	B	358	1/1	0.94	0.07	45,45,45,45	0
5	GDP	A	355	28/28	0.95	0.07	30,33,39,40	0
3	ALF	A	357	5/5	0.96	0.15	53,53,55,56	0
5	GDP	B	355	28/28	0.96	0.07	38,42,45,48	0
4	MG	A	356	1/1	0.97	0.08	29,29,29,29	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.

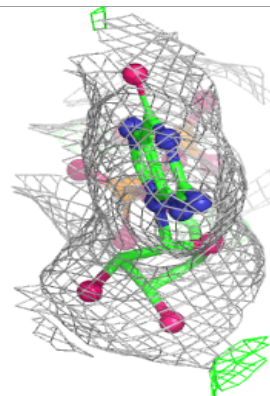
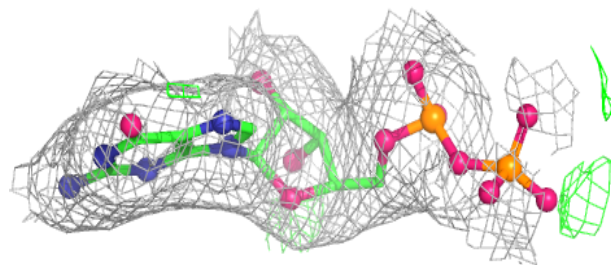
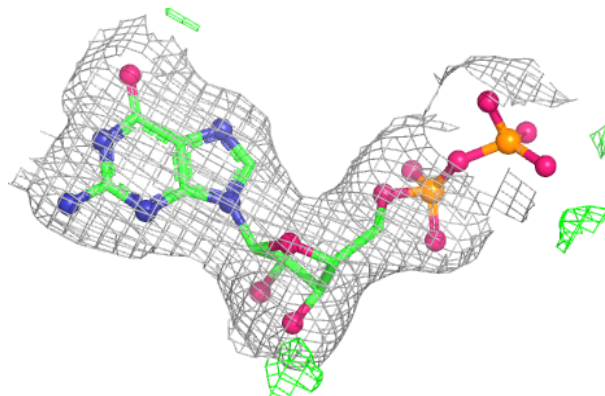
Electron density around GDP A 355:

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



Electron density around GDP B 355:

$2mF_o-DF_c$ (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.