



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:32 PM UTC

PDB ID : 3A5C / pdb_00003a5c
Title : Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase
Authors : Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.
Deposited on : 2009-08-06
Resolution : 4.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

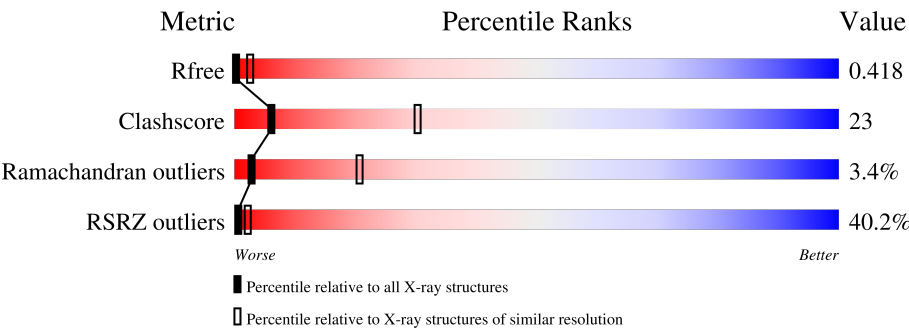
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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	1131 (5.14-3.90)
Clashscore	190562	1005 (5.10-3.94)
Ramachandran outliers	187476	1061 (5.12-3.90)
RSRZ outliers	180081	1126 (5.14-3.90)

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	578	40% 80% 13% ...
1	B	578	25% 82% 12% ...
1	C	578	45% 82% 12% ...
1	I	578	51% 79% 15% ...
1	J	578	25% 82% 13% ...
1	K	578	52% 80% 14% ...
2	D	478	32% 82% 10% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	478	41% 80% 12% 6%
2	F	478	48% 81% 11% 6%
2	L	478	28% 81% 10% 6%
2	M	478	39% 81% 11% 6%
2	N	478	52% 81% 11% 6%
3	G	223	7% 19% 29% 9% 42%
3	O	223	6% 17% 30% 9% 42%
4	H	104	44% 64% 32%
4	P	104	32% 64% 27% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32188 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	B	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	C	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	I	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	J	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	K	561	Total	C	N	O	0	0	0
			2752	1630	561	561			

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	E	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	F	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	L	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	M	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	N	450	Total	C	N	O	0	0	0
			2212	1312	450	450			

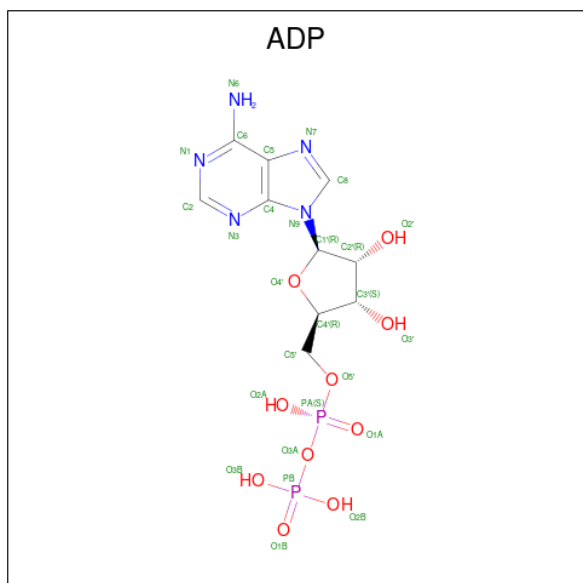
- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	0	0	0
			639	381	129	129			
3	O	129	Total	C	N	O	0	0	0
			639	381	129	129			

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total	C	N	O	0	0	0
			509	301	104	104			
4	P	104	Total	C	N	O	0	0	0
			509	301	104	104			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

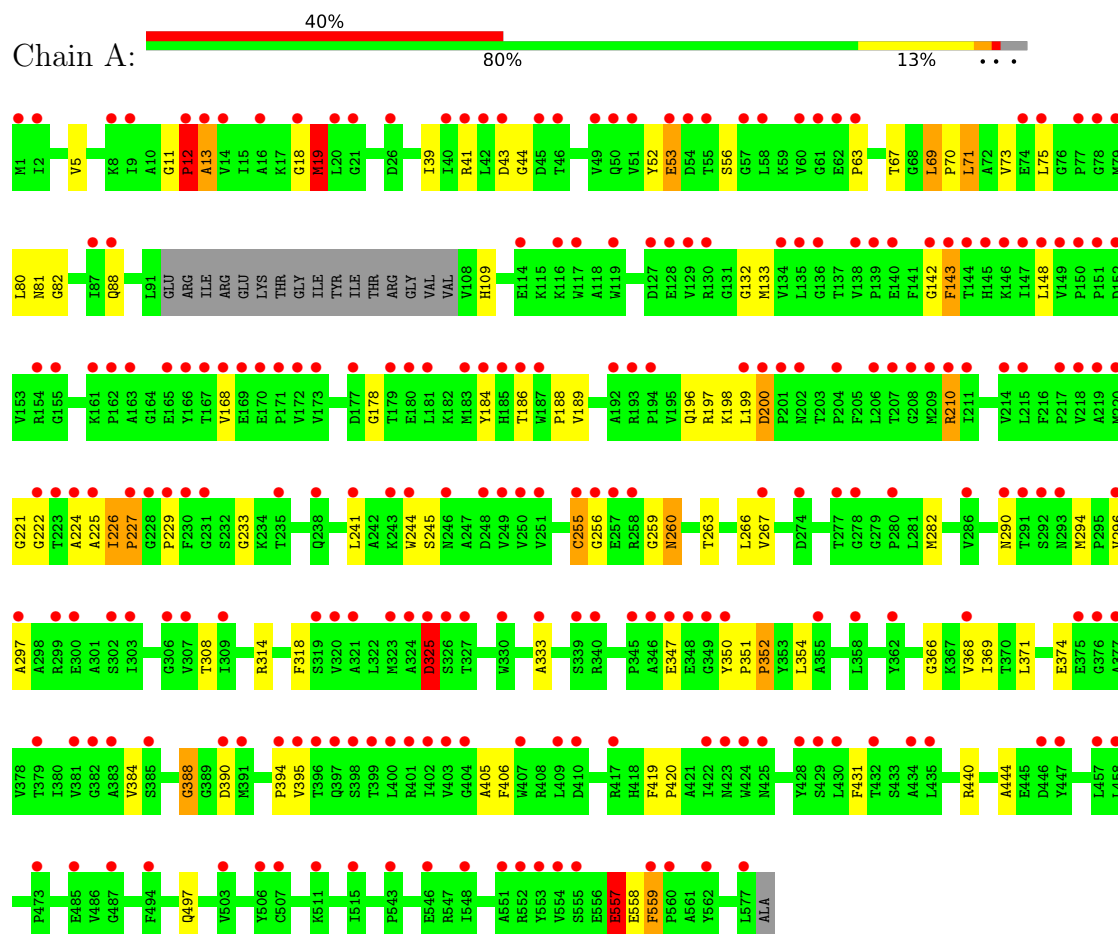


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

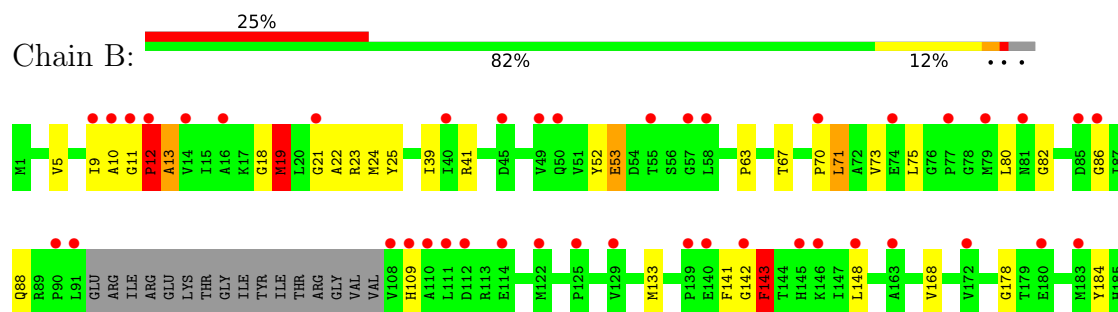
3 Residue-property plots [i](#)

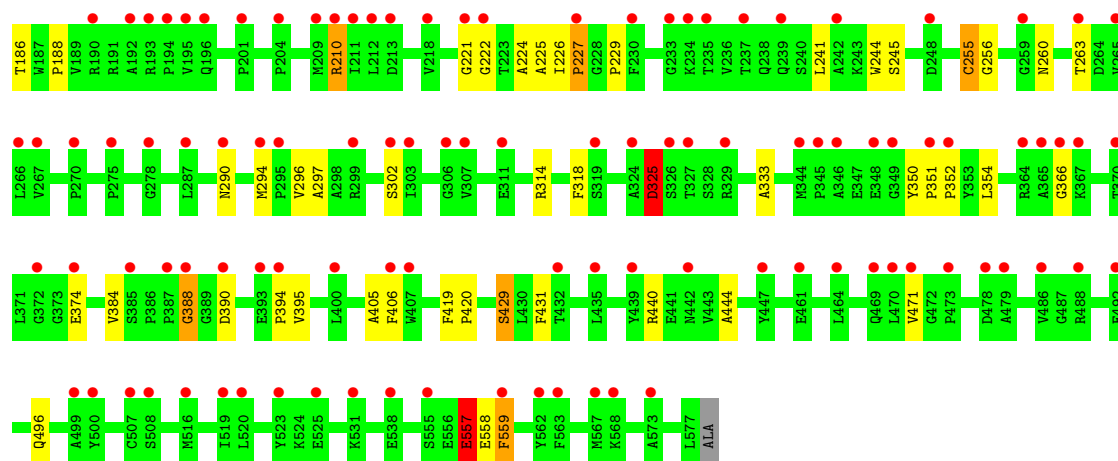
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: V-type ATP synthase alpha chain

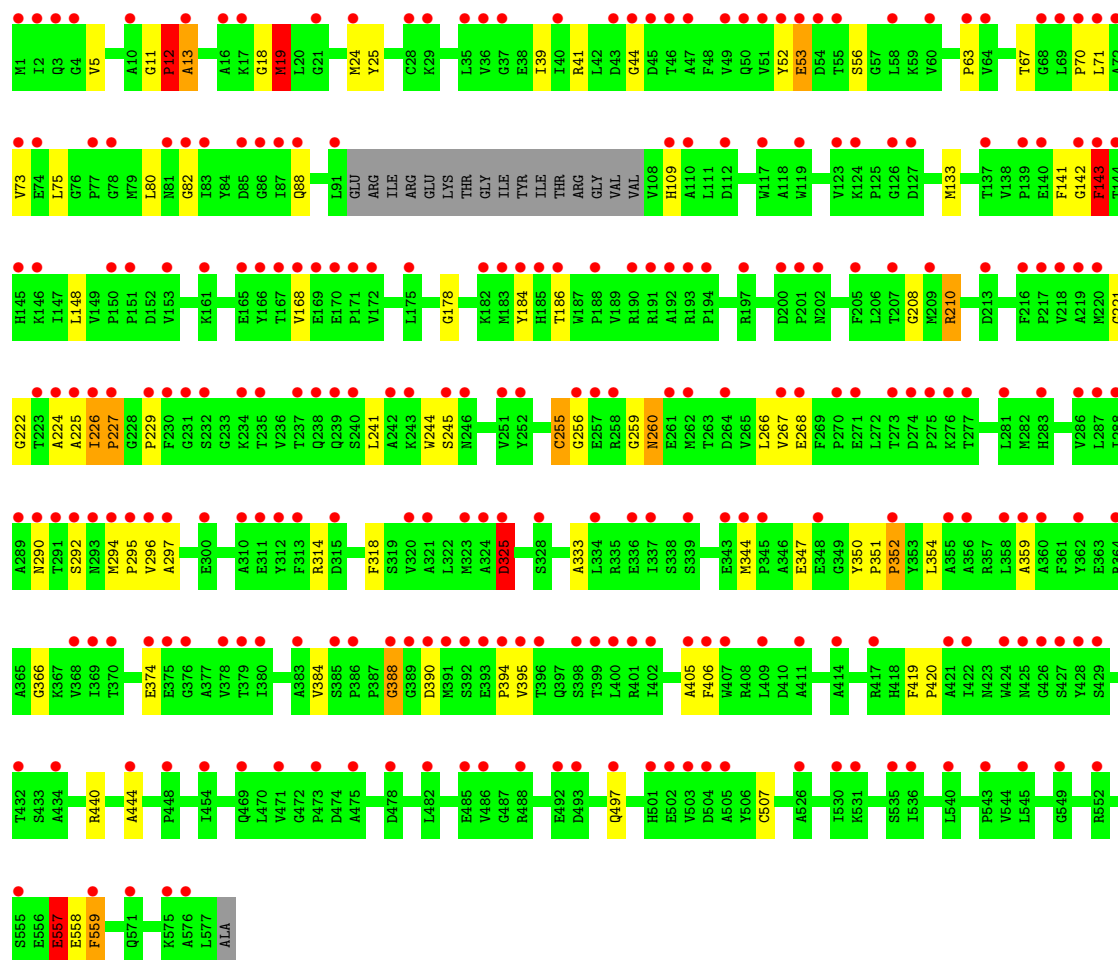
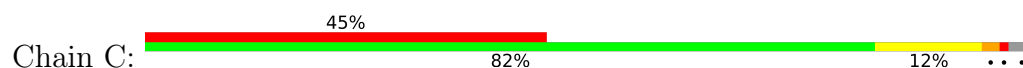


• Molecule 1: V-type ATP synthase alpha chain



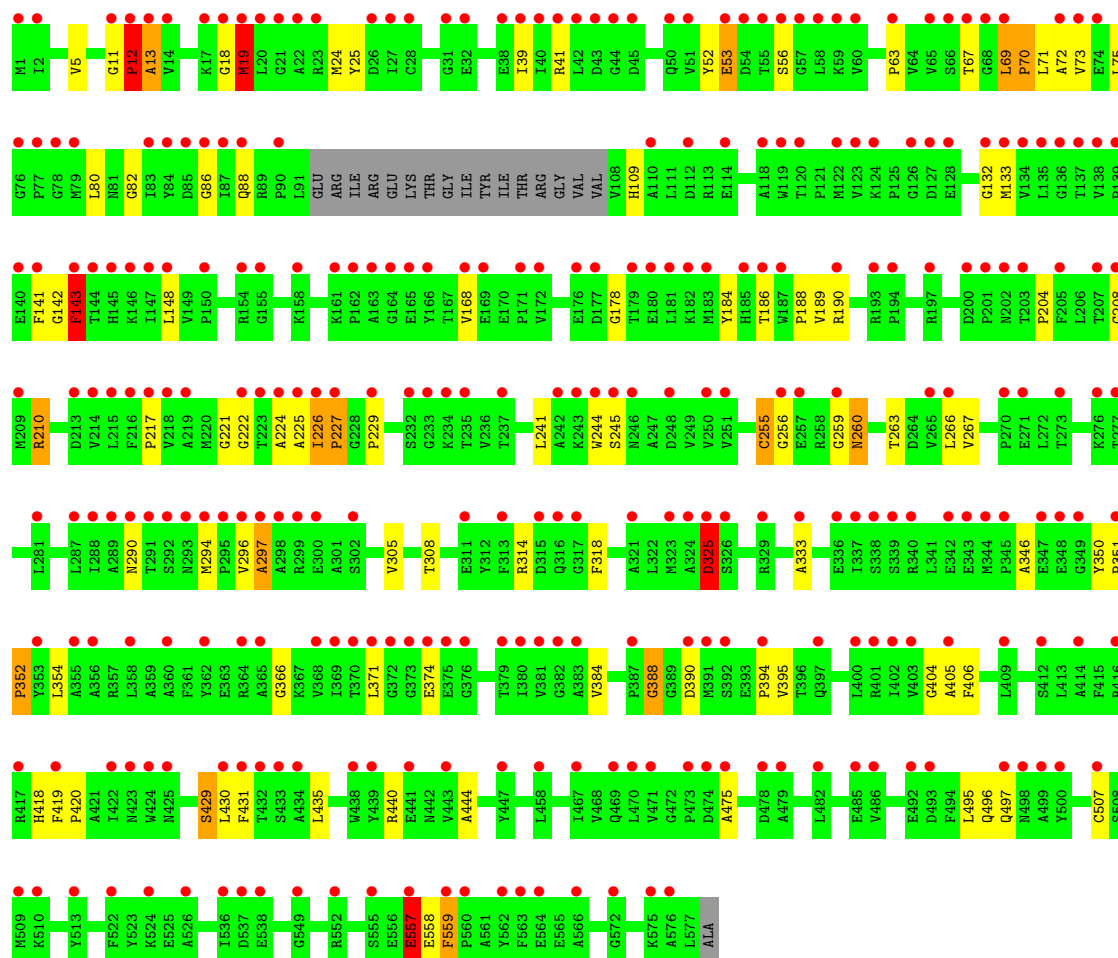


• Molecule 1: V-type ATP synthase alpha chain

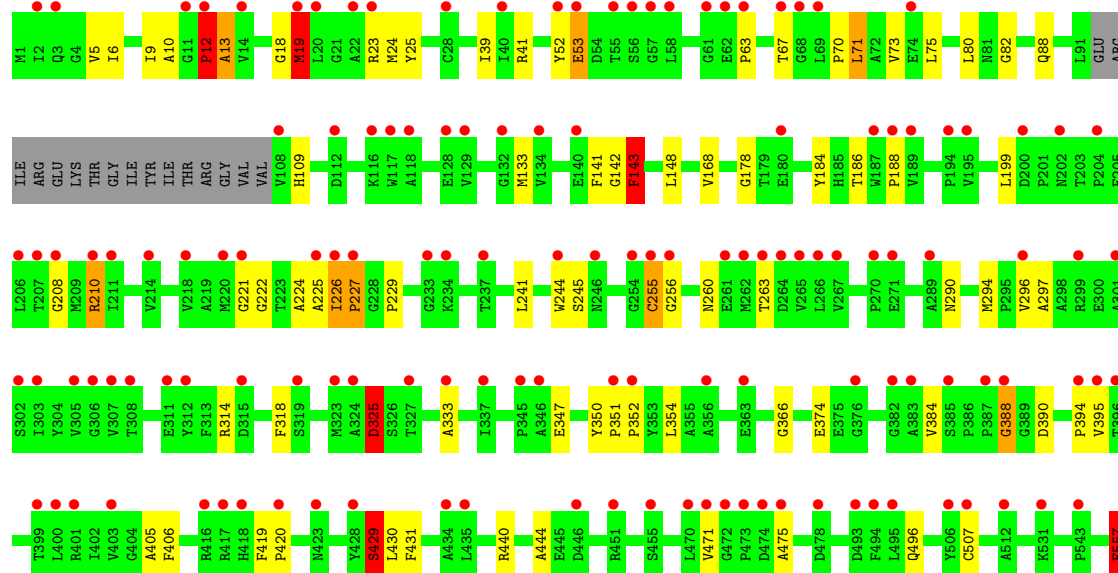
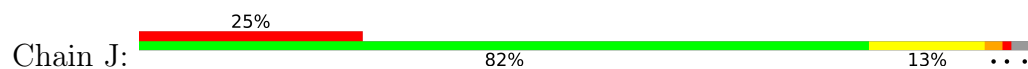


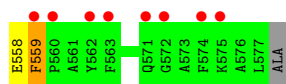
• Molecule 1: V-type ATP synthase alpha chain



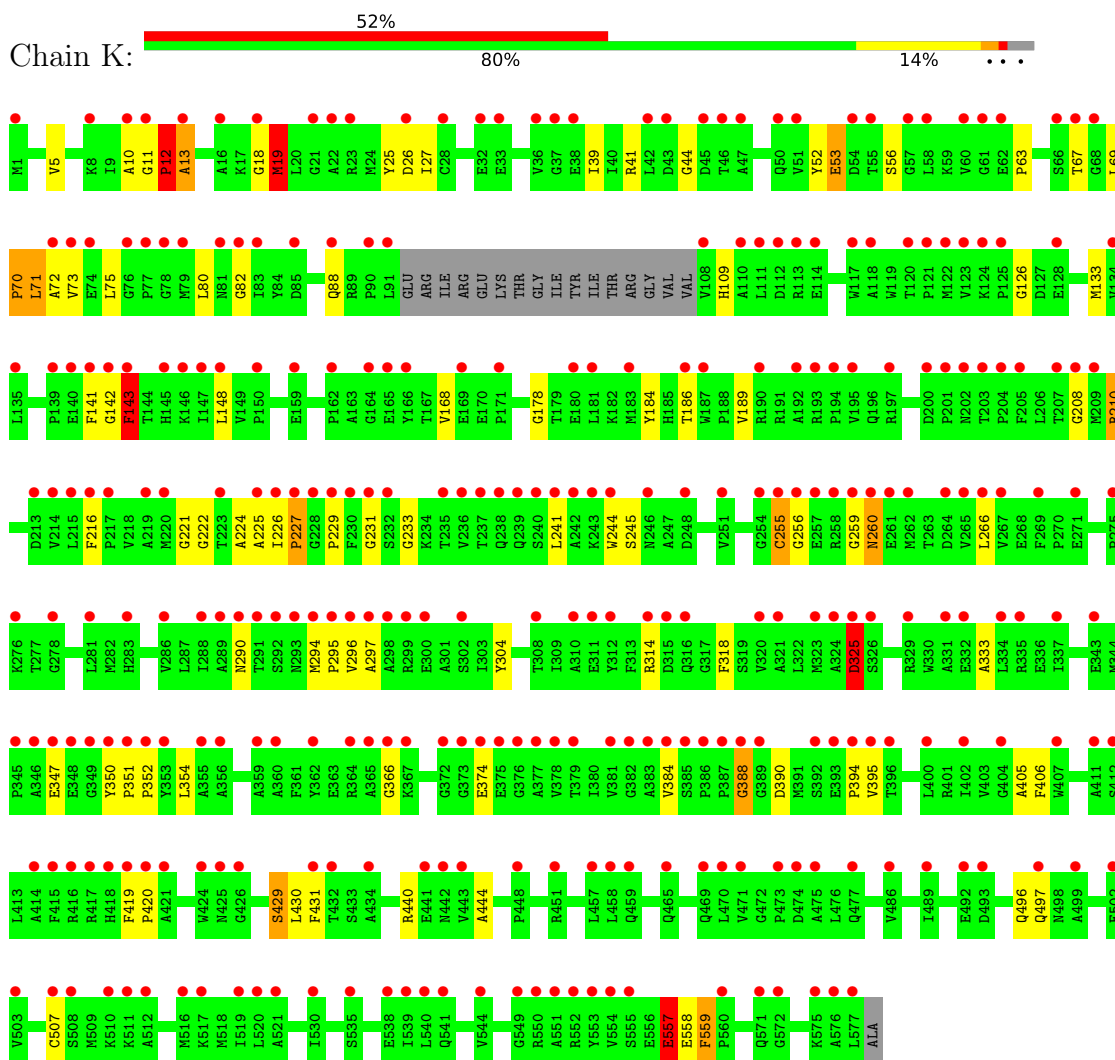


• Molecule 1: V-type ATP synthase alpha chain

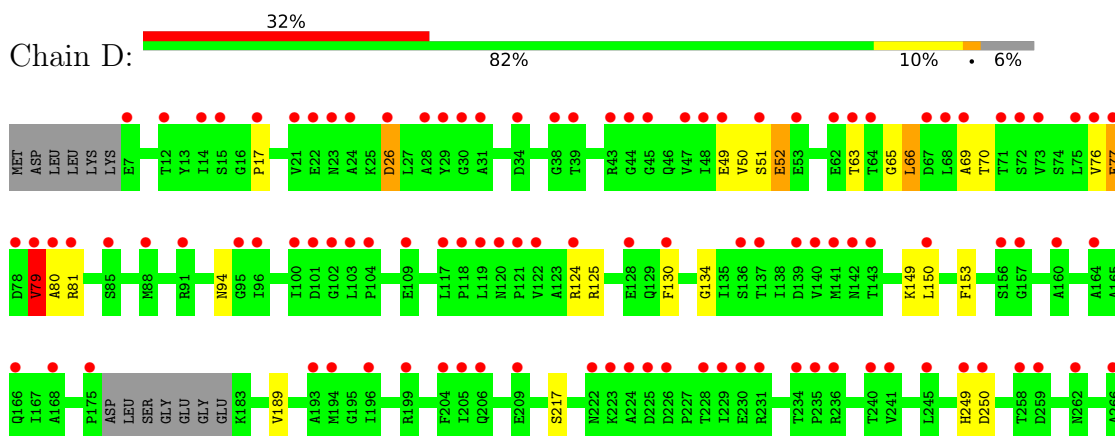


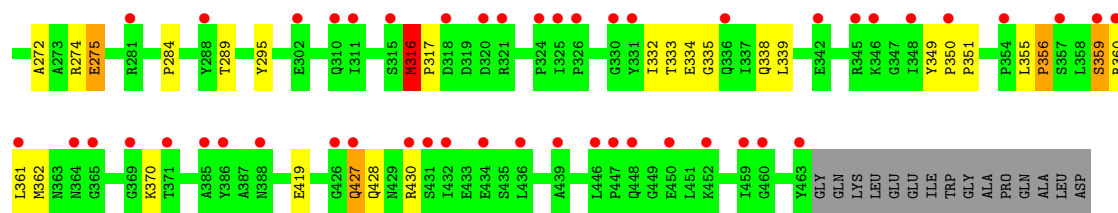


• Molecule 1: V-type ATP synthase alpha chain

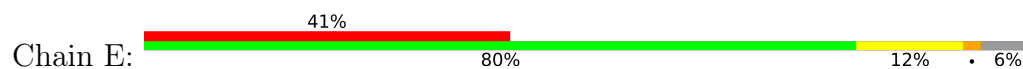


• Molecule 2: V-type ATP synthase beta chain

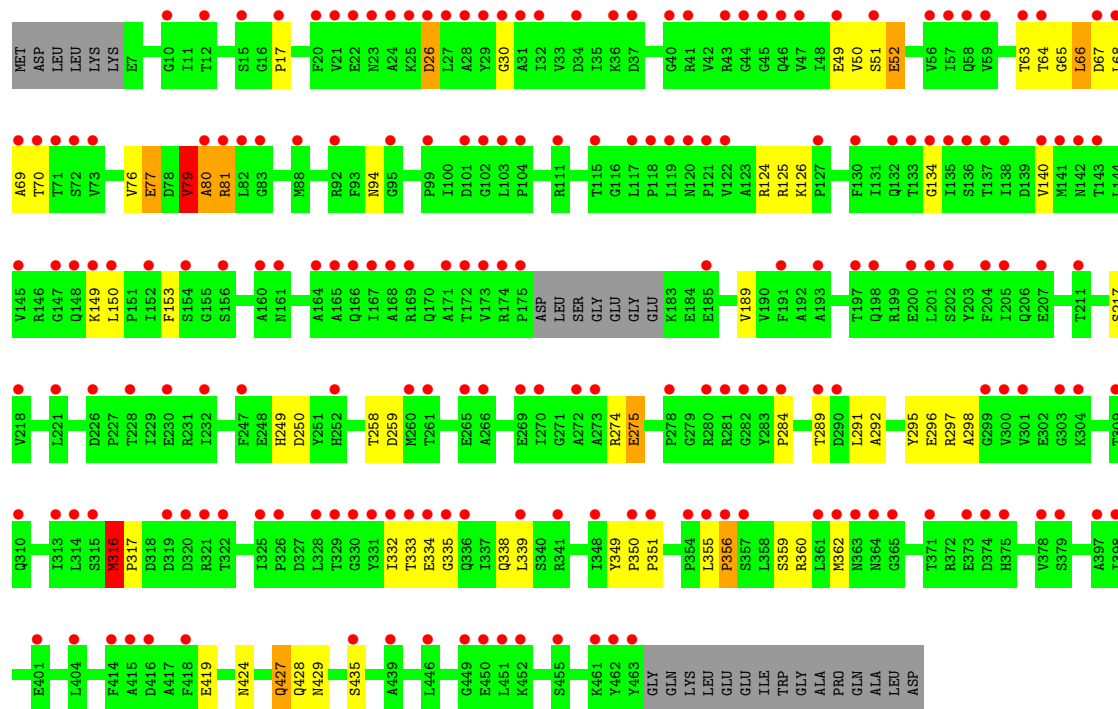




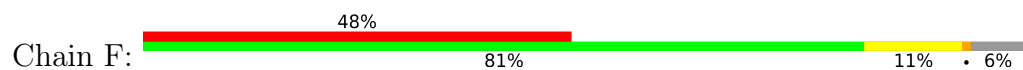
• Molecule 2: V-type ATP synthase beta chain



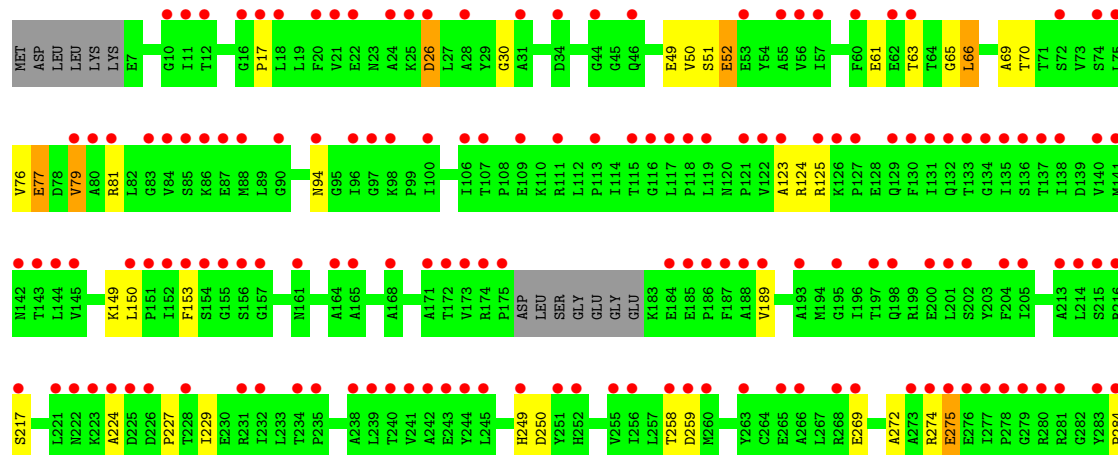
Chain E:

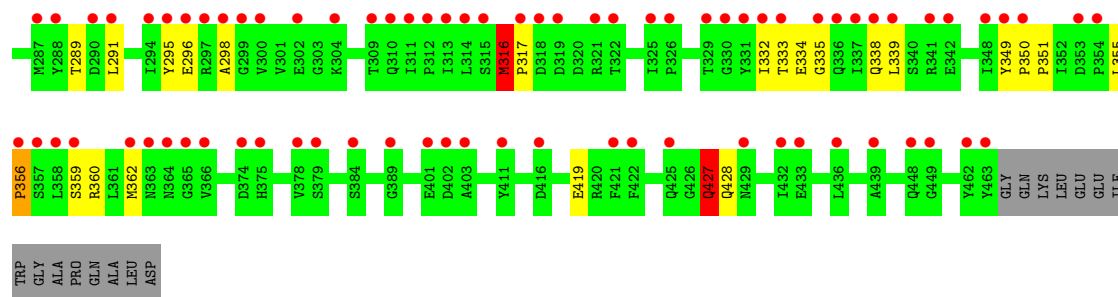


• Molecule 2: V-type ATP synthase beta chain

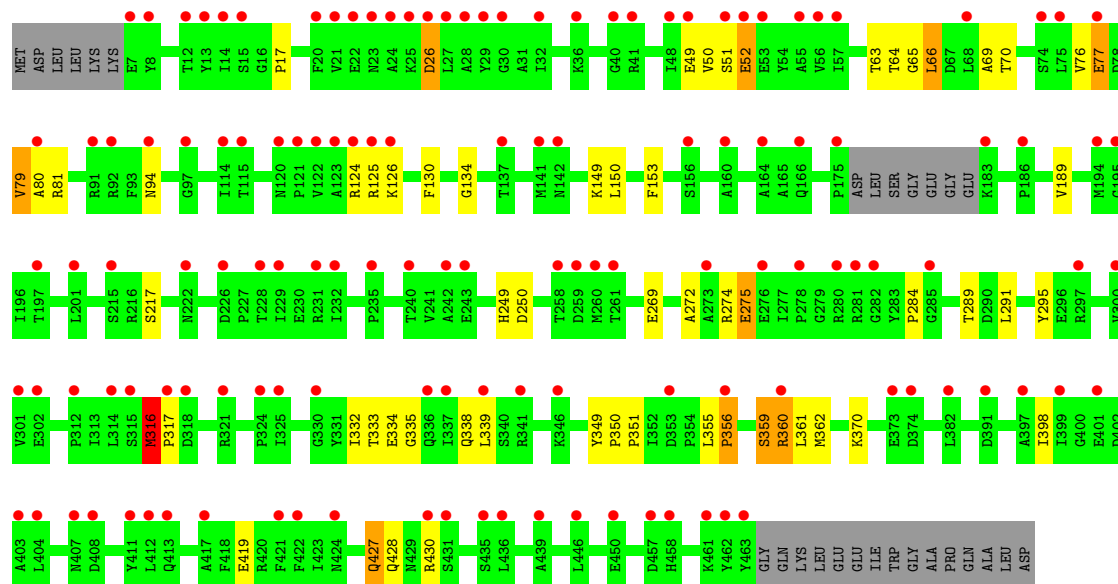
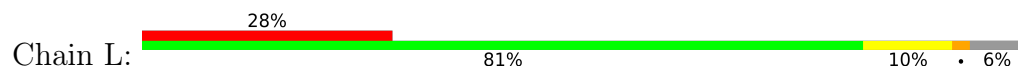


Chain F:

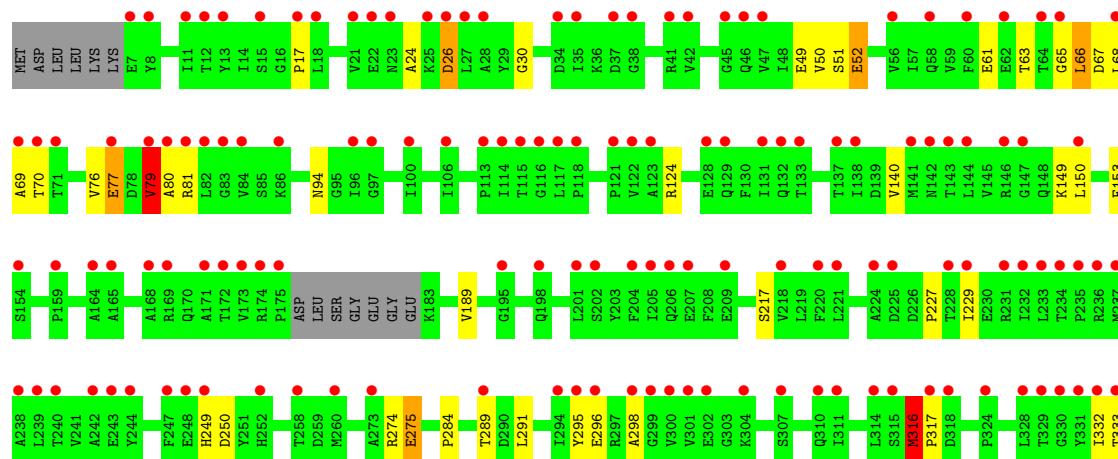
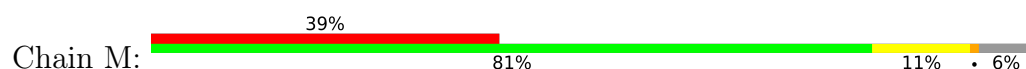


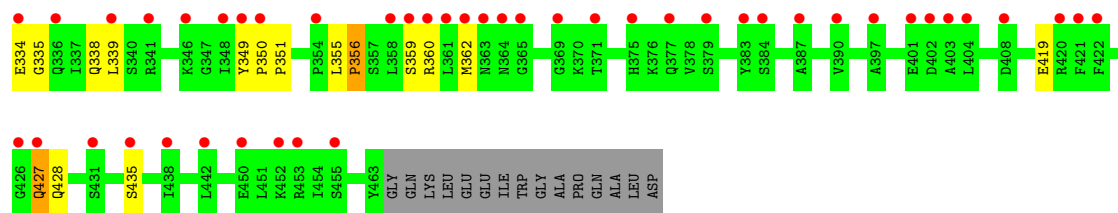


• Molecule 2: V-type ATP synthase beta chain

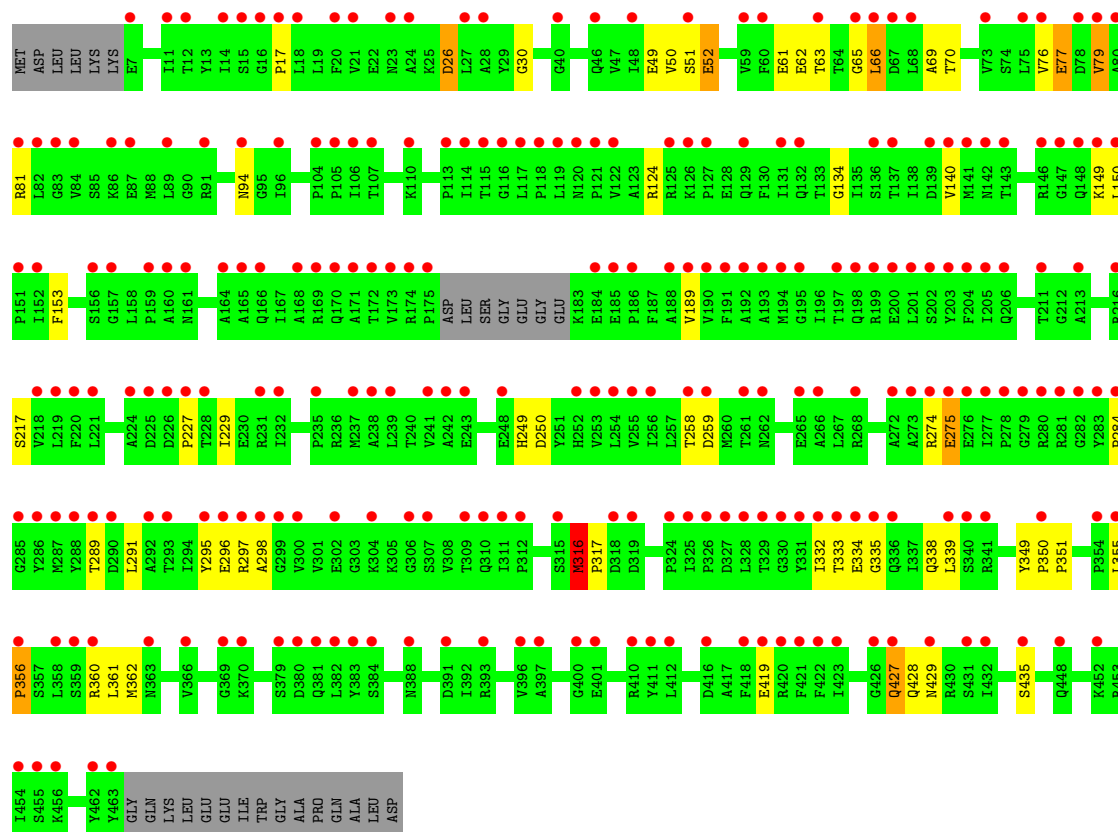
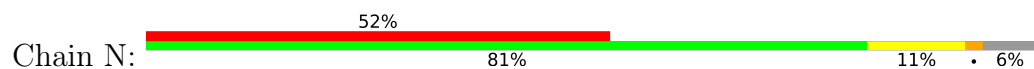


• Molecule 2: V-type ATP synthase beta chain

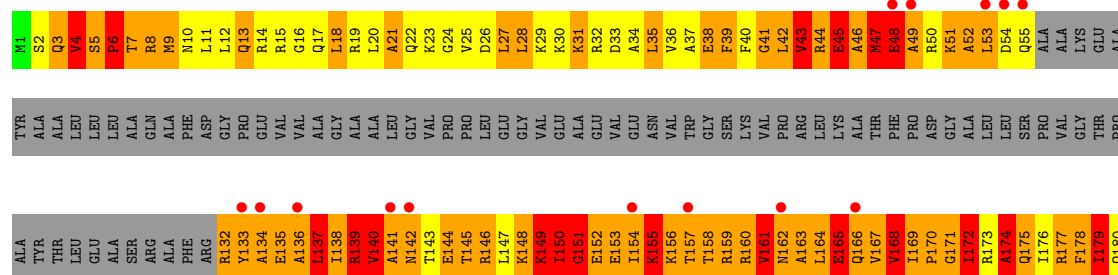


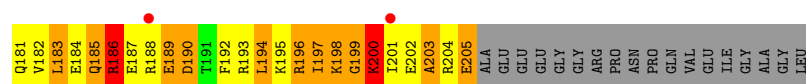


• Molecule 2: V-type ATP synthase beta chain

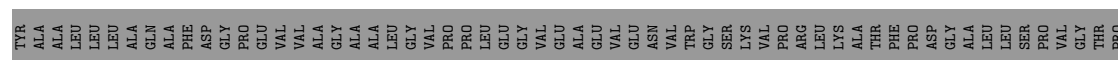


• Molecule 3: V-type ATP synthase subunit D

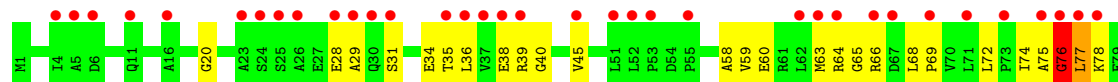
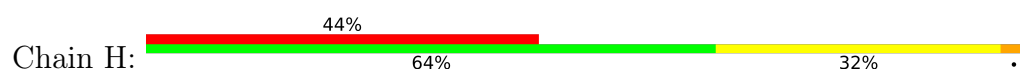




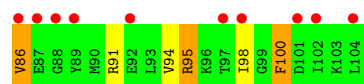
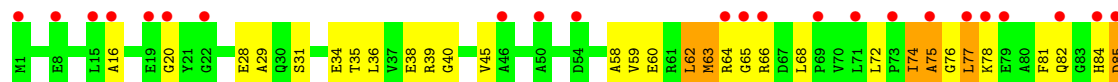
- Molecule 3: V-type ATP synthase subunit D



- Molecule 4: V-type ATP synthase subunit F



- Molecule 4: V-type ATP synthase subunit F



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	381.58Å 381.58Å 147.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 4.51 29.92 – 4.51	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.92-4.51) 96.5 (29.92-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 4.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.429 , 0.437 0.408 , 0.418	Depositor DCC
R_{free} test set	3589 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	145.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.08 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	32188	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.94	4/2750 (0.1%)	1.80	33/3815 (0.9%)
1	B	0.94	4/2750 (0.1%)	1.77	31/3815 (0.8%)
1	C	0.94	4/2750 (0.1%)	1.77	32/3815 (0.8%)
1	I	0.94	4/2750 (0.1%)	2.01	36/3815 (0.9%)
1	J	0.94	4/2750 (0.1%)	1.77	31/3815 (0.8%)
1	K	0.95	5/2750 (0.2%)	1.97	34/3815 (0.9%)
2	D	1.27	15/2210 (0.7%)	1.61	18/3068 (0.6%)
2	E	1.39	16/2210 (0.7%)	1.63	20/3068 (0.7%)
2	F	1.12	9/2210 (0.4%)	1.54	13/3068 (0.4%)
2	L	1.15	12/2210 (0.5%)	1.59	17/3068 (0.6%)
2	M	1.16	13/2210 (0.6%)	1.56	15/3068 (0.5%)
2	N	1.13	10/2210 (0.5%)	1.54	13/3068 (0.4%)
3	G	6.39	253/637 (39.7%)	4.09	159/885 (18.0%)
3	O	6.38	248/637 (38.9%)	4.09	160/885 (18.1%)
4	H	2.27	18/508 (3.5%)	2.35	20/703 (2.8%)
4	P	2.68	20/508 (3.9%)	3.37	28/703 (4.0%)
All	All	1.70	639/32050 (2.0%)	1.93	660/44474 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	5
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
2	F	0	3
2	L	0	4
2	M	0	3
2	N	0	3
4	H	0	3
4	P	0	2
All	All	0	60

All (639) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-32.26	0.98	1.53
3	G	47	MET	CA-CB	-32.17	0.99	1.53
3	G	196	ARG	CA-C	23.93	1.84	1.52
3	O	196	ARG	CA-C	23.85	1.84	1.52
3	G	167	VAL	CA-C	23.36	1.81	1.52
3	O	167	VAL	CA-C	23.25	1.81	1.52
4	P	75	ALA	CA-C	21.72	1.81	1.52
3	G	138	ILE	CA-CB	-21.61	1.27	1.54
4	P	75	ALA	N-CA	21.56	1.73	1.45
3	O	138	ILE	CA-CB	-21.55	1.27	1.54
2	E	80	ALA	CA-C	20.72	1.78	1.52
3	O	7	THR	CA-CB	20.38	1.86	1.53
2	E	81	ARG	CA-C	20.36	1.77	1.52
3	O	4	VAL	CA-C	20.19	1.78	1.52
3	G	7	THR	CA-CB	20.14	1.86	1.53
3	G	4	VAL	CA-C	20.14	1.78	1.52
3	O	27	LEU	CA-CB	19.81	1.87	1.53
3	G	27	LEU	CA-CB	19.77	1.87	1.53
3	O	31	LYS	N-CA	19.31	1.71	1.46
3	G	31	LYS	N-CA	18.96	1.70	1.46
2	E	81	ARG	N-CA	17.96	1.67	1.46
3	G	194	LEU	CA-C	17.32	1.75	1.52
3	O	194	LEU	CA-C	17.13	1.75	1.52
3	G	168	VAL	CA-CB	-16.92	1.31	1.54
4	H	34	GLU	C-O	16.83	1.43	1.24
4	P	34	GLU	C-O	16.79	1.43	1.24
3	O	168	VAL	CA-CB	-16.79	1.31	1.54
3	G	163	ALA	CA-C	16.45	1.75	1.52
2	D	80	ALA	CA-C	16.43	1.72	1.52
3	O	163	ALA	CA-C	16.25	1.74	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	19	ARG	N-CA	15.23	1.65	1.46
3	G	19	ARG	N-CA	15.19	1.65	1.46
2	E	80	ALA	N-CA	15.06	1.65	1.45
3	G	184	GLU	N-CA	14.90	1.64	1.46
2	D	81	ARG	CA-C	14.88	1.71	1.52
3	O	184	GLU	N-CA	14.85	1.64	1.46
3	O	20	LEU	CA-C	14.84	1.71	1.52
3	G	20	LEU	CA-C	14.84	1.71	1.52
3	G	16	GLY	CA-C	14.56	1.69	1.51
3	O	16	GLY	CA-C	14.55	1.69	1.51
3	O	52	ALA	CA-CB	14.46	1.75	1.53
3	G	52	ALA	CA-CB	14.40	1.75	1.53
3	O	38	GLU	N-CA	14.34	1.63	1.46
3	G	38	GLU	N-CA	14.24	1.63	1.46
3	G	32	ARG	C-O	14.19	1.40	1.24
3	G	189	GLU	CA-CB	14.19	1.76	1.53
3	O	32	ARG	C-O	14.18	1.40	1.24
3	O	142	ASN	CA-CB	14.07	1.75	1.53
3	O	189	GLU	CA-CB	14.04	1.76	1.53
3	G	142	ASN	CA-CB	14.01	1.75	1.53
3	G	156	LYS	CA-C	13.98	1.71	1.52
3	G	32	ARG	CA-C	13.95	1.71	1.52
3	O	156	LYS	CA-C	13.88	1.70	1.52
3	O	32	ARG	CA-C	13.86	1.70	1.52
3	G	167	VAL	CA-CB	13.36	1.70	1.54
3	G	164	LEU	C-O	13.29	1.40	1.24
3	O	164	LEU	C-O	13.21	1.40	1.24
3	G	6	PRO	C-O	13.19	1.41	1.24
3	G	189	GLU	CA-C	13.13	1.69	1.52
3	O	167	VAL	CA-CB	13.12	1.69	1.54
3	G	184	GLU	CA-CB	13.12	1.73	1.53
3	O	184	GLU	CA-CB	13.10	1.73	1.53
3	O	189	GLU	CA-C	12.99	1.69	1.52
3	O	163	ALA	C-O	12.92	1.40	1.24
3	O	6	PRO	C-O	12.81	1.40	1.24
3	G	163	ALA	C-O	12.79	1.40	1.24
2	D	81	ARG	N-CA	12.78	1.62	1.46
3	G	195	LYS	N-CA	12.74	1.62	1.46
3	O	195	LYS	N-CA	12.63	1.62	1.46
3	G	182	VAL	N-CA	12.61	1.62	1.46
3	O	205	GLU	CA-CB	12.60	1.78	1.53
3	O	155	LYS	N-CA	12.58	1.62	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	182	VAL	N-CA	12.58	1.62	1.46
3	G	155	LYS	N-CA	12.53	1.62	1.46
3	O	50	ARG	C-O	12.52	1.41	1.24
3	G	183	LEU	C-O	12.49	1.39	1.24
3	O	170	PRO	CA-C	12.47	1.68	1.52
3	O	183	LEU	C-O	12.37	1.39	1.24
3	O	169	ILE	C-O	12.36	1.40	1.24
3	G	205	GLU	CA-CB	12.33	1.78	1.53
3	G	33	ASP	N-CA	12.30	1.61	1.46
3	O	33	ASP	N-CA	12.30	1.61	1.46
3	G	169	ILE	C-O	12.29	1.40	1.24
3	O	9	MET	CA-C	-12.27	1.36	1.52
3	G	50	ARG	C-O	12.26	1.40	1.24
3	G	170	PRO	CA-C	12.22	1.68	1.52
3	G	28	LEU	CA-C	12.17	1.69	1.52
4	P	76	GLY	CA-C	12.16	1.71	1.52
3	G	9	MET	CA-C	-12.04	1.36	1.52
3	O	171	GLY	CA-C	11.98	1.68	1.51
3	G	169	ILE	CA-C	11.93	1.65	1.52
3	G	171	GLY	CA-C	11.92	1.68	1.51
3	O	28	LEU	CA-C	11.91	1.69	1.52
3	O	192	PHE	CA-C	11.91	1.69	1.52
3	G	192	PHE	CA-C	11.84	1.69	1.52
3	O	169	ILE	CA-C	11.73	1.65	1.52
3	O	52	ALA	N-CA	11.69	1.60	1.46
3	O	4	VAL	CA-CB	11.68	1.70	1.54
3	G	188	ARG	N-CA	11.66	1.60	1.46
3	G	4	VAL	CA-CB	11.66	1.70	1.54
3	O	188	ARG	N-CA	11.59	1.60	1.46
3	O	134	ALA	N-CA	11.55	1.61	1.46
3	G	52	ALA	N-CA	11.54	1.60	1.46
3	O	16	GLY	C-O	11.53	1.40	1.23
3	G	7	THR	CA-C	11.48	1.68	1.52
4	P	76	GLY	N-CA	11.46	1.60	1.45
3	O	187	GLU	CA-C	11.46	1.67	1.52
3	G	134	ALA	N-CA	11.45	1.60	1.46
3	O	7	THR	CA-C	11.45	1.68	1.52
3	G	193	ARG	N-CA	11.44	1.60	1.46
3	O	32	ARG	C-N	11.42	1.49	1.33
3	O	172	ILE	N-CA	11.42	1.60	1.46
3	O	185	GLN	C-O	11.40	1.38	1.24
3	O	193	ARG	N-CA	11.40	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	172	ILE	N-CA	11.35	1.60	1.46
3	O	53	LEU	N-CA	11.35	1.60	1.46
3	G	32	ARG	C-N	11.34	1.49	1.33
3	G	185	GLN	C-O	11.30	1.38	1.24
2	D	80	ALA	N-CA	11.19	1.59	1.45
3	G	16	GLY	C-O	11.16	1.39	1.23
3	O	198	LYS	C-O	11.12	1.38	1.24
3	G	53	LEU	N-CA	11.10	1.60	1.46
3	G	198	LYS	C-O	11.07	1.38	1.24
3	G	36	VAL	CA-C	11.03	1.67	1.52
3	G	187	GLU	CA-C	11.02	1.67	1.52
3	G	46	ALA	C-O	10.99	1.37	1.24
3	O	36	VAL	CA-C	10.88	1.67	1.52
4	P	40	GLY	C-O	10.88	1.36	1.24
3	O	46	ALA	C-O	10.87	1.37	1.24
3	O	51	LYS	C-O	10.78	1.37	1.24
3	G	14	ARG	N-CA	10.77	1.59	1.46
3	O	27	LEU	N-CA	10.75	1.60	1.46
4	H	40	GLY	C-O	10.69	1.36	1.24
3	G	24	GLY	CA-C	10.68	1.64	1.51
3	G	27	LEU	N-CA	10.67	1.60	1.46
3	G	192	PHE	C-O	10.64	1.37	1.24
3	G	154	ILE	C-O	10.63	1.36	1.24
3	O	49	ALA	CA-C	-10.62	1.39	1.52
3	O	169	ILE	N-CA	10.59	1.59	1.46
3	O	192	PHE	C-O	10.59	1.37	1.24
3	O	34	ALA	CA-CB	-10.59	1.35	1.53
3	G	34	ALA	CA-CB	-10.56	1.35	1.53
3	G	49	ALA	CA-C	-10.56	1.39	1.52
3	G	51	LYS	C-O	10.55	1.37	1.24
3	G	179	ILE	C-O	10.50	1.36	1.24
3	G	4	VAL	C-O	10.49	1.36	1.24
3	O	24	GLY	CA-C	10.47	1.64	1.51
3	G	22	GLN	C-O	10.46	1.37	1.24
3	G	169	ILE	N-CA	10.45	1.59	1.46
3	O	201	ILE	CA-CB	-10.41	1.41	1.54
3	O	14	ARG	N-CA	10.39	1.58	1.46
3	O	179	ILE	C-O	10.39	1.36	1.24
3	O	22	GLN	C-O	10.38	1.37	1.24
3	G	201	ILE	CA-CB	-10.37	1.41	1.54
3	G	204	ARG	N-CA	10.35	1.59	1.46
3	O	4	VAL	C-O	10.32	1.36	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	138	ILE	CA-C	-10.31	1.39	1.52
3	O	204	ARG	N-CA	10.28	1.59	1.46
3	O	154	ILE	C-O	10.26	1.36	1.24
4	H	75	ALA	CA-C	10.21	1.65	1.52
3	G	200	LYS	CA-C	10.18	1.66	1.52
2	L	289	THR	C-N	10.10	1.46	1.33
3	G	6	PRO	CA-CB	10.10	1.68	1.53
3	G	138	ILE	CA-C	-10.01	1.39	1.52
3	O	200	LYS	CA-C	10.00	1.66	1.52
3	O	6	PRO	CA-CB	9.90	1.67	1.53
2	M	289	THR	C-N	9.83	1.46	1.33
2	M	66	LEU	CA-CB	-9.80	1.42	1.54
3	G	14	ARG	C-O	9.79	1.35	1.24
3	O	146	ARG	CA-CB	9.79	1.70	1.53
2	N	66	LEU	CA-CB	-9.77	1.42	1.54
3	O	205	GLU	CA-C	9.77	1.73	1.52
2	N	289	THR	C-N	9.76	1.46	1.33
3	G	164	LEU	N-CA	9.75	1.58	1.46
2	E	289	THR	C-N	9.74	1.46	1.33
2	F	66	LEU	CA-CB	-9.74	1.42	1.54
3	G	146	ARG	CA-CB	9.74	1.70	1.53
2	F	289	THR	C-N	9.74	1.46	1.33
3	O	14	ARG	C-O	9.73	1.35	1.24
2	D	289	THR	C-N	9.72	1.46	1.33
3	G	205	GLU	CA-C	9.69	1.73	1.52
3	O	11	LEU	CA-CB	9.69	1.69	1.53
2	L	66	LEU	CA-CB	-9.67	1.42	1.54
3	O	164	LEU	N-CA	9.67	1.58	1.46
2	E	66	LEU	CA-CB	-9.66	1.42	1.54
3	G	11	LEU	CA-CB	9.63	1.69	1.53
2	D	66	LEU	CA-CB	-9.58	1.42	1.54
3	O	184	GLU	CA-C	9.56	1.65	1.52
3	G	184	GLU	CA-C	9.53	1.65	1.52
3	G	35	LEU	CA-C	9.52	1.65	1.52
3	O	35	LEU	CA-C	9.50	1.65	1.52
3	G	49	ALA	N-CA	9.42	1.57	1.46
3	G	50	ARG	CA-C	9.39	1.66	1.52
3	G	163	ALA	C-N	9.37	1.46	1.34
3	O	163	ALA	C-N	9.38	1.46	1.34
3	O	203	ALA	N-CA	-9.36	1.34	1.46
3	O	50	ARG	CA-C	9.35	1.65	1.52
3	G	17	GLN	CA-CB	-9.28	1.39	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	49	ALA	N-CA	9.18	1.57	1.46
3	O	5	SER	CA-C	-9.14	1.41	1.52
3	O	17	GLN	CA-CB	-9.14	1.39	1.53
3	O	31	LYS	C-O	9.07	1.35	1.24
3	G	203	ALA	N-CA	-9.03	1.34	1.46
3	O	194	LEU	C-O	9.00	1.34	1.24
3	O	196	ARG	CA-CB	8.99	1.68	1.53
3	G	23	LYS	N-CA	8.97	1.57	1.46
3	G	194	LEU	C-O	8.96	1.34	1.24
3	O	23	LYS	N-CA	8.96	1.57	1.46
3	G	5	SER	CA-C	-8.96	1.41	1.52
3	G	196	ARG	CA-CB	8.95	1.67	1.53
3	O	22	GLN	CA-C	8.94	1.64	1.52
3	G	158	THR	CA-CB	-8.91	1.38	1.53
3	O	51	LYS	CA-C	8.90	1.64	1.52
4	H	75	ALA	N-CA	8.85	1.56	1.46
3	O	18	LEU	CA-C	8.85	1.64	1.52
3	O	175	GLN	CA-CB	-8.84	1.39	1.53
3	G	31	LYS	C-O	8.82	1.35	1.24
2	M	81	ARG	CA-C	8.81	1.63	1.52
3	G	52	ALA	C-O	8.80	1.34	1.24
3	G	51	LYS	CA-C	8.79	1.64	1.52
3	O	52	ALA	C-O	8.77	1.34	1.24
3	G	18	LEU	CA-C	8.73	1.64	1.52
3	G	198	LYS	CA-C	8.71	1.64	1.52
3	O	45	GLU	C-O	8.71	1.34	1.24
3	G	22	GLN	CA-C	8.70	1.64	1.52
3	G	175	GLN	CA-CB	-8.65	1.39	1.53
3	G	134	ALA	CA-CB	8.64	1.68	1.53
3	O	158	THR	CA-CB	-8.63	1.39	1.53
3	O	14	ARG	CA-CB	8.61	1.66	1.53
3	O	193	ARG	CA-C	-8.61	1.41	1.52
3	O	36	VAL	CA-CB	8.60	1.65	1.54
3	G	22	GLN	C-N	8.58	1.45	1.34
3	G	45	GLU	C-O	8.55	1.34	1.24
3	O	134	ALA	CA-CB	8.54	1.67	1.53
3	O	166	GLN	CA-C	8.52	1.64	1.52
3	G	148	LYS	CA-CB	8.51	1.68	1.53
3	G	166	GLN	CA-C	8.51	1.64	1.52
3	G	193	ARG	CA-C	-8.50	1.41	1.52
3	O	148	LYS	CA-CB	8.48	1.68	1.53
3	O	22	GLN	C-N	8.47	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	164	LEU	CA-C	8.47	1.64	1.52
3	O	12	LEU	CA-C	-8.44	1.42	1.52
3	G	148	LYS	N-CA	8.42	1.57	1.46
3	G	143	THR	N-CA	8.41	1.56	1.46
3	O	148	LYS	N-CA	8.40	1.57	1.46
3	G	36	VAL	CA-CB	8.39	1.65	1.54
3	O	183	LEU	C-N	8.38	1.44	1.33
3	O	198	LYS	CA-C	8.36	1.64	1.52
3	G	164	LEU	CA-C	8.35	1.64	1.52
2	E	81	ARG	C-N	8.35	1.44	1.33
3	G	170	PRO	N-CA	8.34	1.56	1.47
3	O	24	GLY	C-O	8.34	1.33	1.23
3	O	143	THR	N-CA	8.34	1.56	1.46
2	E	80	ALA	C-N	8.33	1.44	1.33
3	G	183	LEU	C-N	8.31	1.44	1.33
3	G	14	ARG	CA-CB	8.31	1.66	1.53
3	G	25	VAL	N-CA	8.29	1.57	1.46
3	G	12	LEU	CA-C	-8.28	1.42	1.52
3	O	25	VAL	N-CA	8.28	1.57	1.46
3	O	48	GLU	CA-C	8.27	1.63	1.52
3	G	21	ALA	C-O	8.24	1.34	1.24
3	O	170	PRO	N-CA	8.20	1.56	1.47
3	O	7	THR	N-CA	8.18	1.56	1.46
1	J	13	ALA	CA-CB	-8.17	1.39	1.53
1	B	13	ALA	CA-CB	-8.16	1.39	1.53
3	G	149	LYS	CA-C	8.14	1.63	1.52
1	K	13	ALA	CA-CB	-8.14	1.39	1.53
1	C	13	ALA	CA-CB	-8.12	1.39	1.53
3	G	7	THR	N-CA	8.12	1.56	1.46
3	G	15	ARG	CA-CB	8.11	1.66	1.53
3	G	48	GLU	CA-C	8.10	1.63	1.52
1	A	13	ALA	CA-CB	-8.09	1.39	1.53
3	O	21	ALA	C-O	8.08	1.34	1.24
3	O	175	GLN	N-CA	-8.08	1.36	1.46
3	G	142	ASN	CA-C	8.06	1.63	1.52
1	I	13	ALA	CA-CB	-8.06	1.39	1.53
3	O	15	ARG	CA-CB	8.04	1.66	1.53
3	G	49	ALA	CA-CB	-8.03	1.40	1.53
3	O	142	ASN	CA-C	8.03	1.63	1.52
3	G	15	ARG	C-O	8.02	1.33	1.24
3	O	149	LYS	CA-C	8.01	1.63	1.52
3	O	165	GLU	N-CA	8.00	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	153	GLU	N-CA	7.99	1.56	1.46
3	G	175	GLN	N-CA	-7.99	1.36	1.46
3	O	153	GLU	N-CA	7.94	1.56	1.46
3	O	47	MET	C-O	7.93	1.33	1.24
3	G	47	MET	C-O	7.93	1.33	1.24
3	G	166	GLN	CA-CB	-7.92	1.40	1.53
3	G	24	GLY	C-O	7.91	1.33	1.23
3	O	166	GLN	CA-CB	-7.87	1.41	1.53
2	M	81	ARG	N-CA	7.86	1.55	1.46
3	G	195	LYS	CA-C	-7.85	1.42	1.52
3	O	136	ALA	N-CA	7.83	1.56	1.46
3	O	195	LYS	CA-C	-7.83	1.42	1.52
3	O	49	ALA	CA-CB	-7.82	1.41	1.53
2	N	77	GLU	CA-CB	-7.82	1.43	1.54
3	G	165	GLU	N-CA	7.81	1.56	1.46
1	I	352	PRO	CA-CB	-7.81	1.42	1.53
3	O	168	VAL	N-CA	7.80	1.56	1.46
3	G	17	GLN	N-CA	7.79	1.56	1.46
2	F	77	GLU	CA-CB	-7.76	1.43	1.54
3	O	15	ARG	C-O	7.76	1.33	1.24
2	M	77	GLU	CA-CB	-7.75	1.43	1.54
3	G	160	ARG	CA-C	7.75	1.63	1.52
3	O	160	ARG	CA-C	7.73	1.63	1.52
3	O	187	GLU	C-N	7.71	1.44	1.33
3	G	187	GLU	C-N	7.70	1.44	1.33
3	G	199	GLY	N-CA	7.67	1.56	1.45
1	A	352	PRO	CA-CB	-7.67	1.43	1.53
2	D	77	GLU	CA-CB	-7.67	1.44	1.54
3	O	183	LEU	CA-C	7.66	1.63	1.52
3	G	12	LEU	N-CA	7.64	1.55	1.46
3	G	168	VAL	N-CA	7.63	1.55	1.46
1	C	325	ASP	C-N	-7.63	1.23	1.33
1	I	325	ASP	C-N	-7.63	1.23	1.33
3	G	52	ALA	CA-C	7.63	1.62	1.52
2	E	77	GLU	CA-CB	-7.62	1.44	1.54
3	O	194	LEU	C-N	7.60	1.44	1.34
4	P	29	ALA	CA-CB	-7.60	1.41	1.53
3	G	201	ILE	C-O	7.58	1.33	1.24
3	G	136	ALA	N-CA	7.58	1.55	1.46
3	G	26	ASP	C-O	7.57	1.32	1.24
1	K	325	ASP	C-N	-7.57	1.23	1.33
1	A	325	ASP	C-N	-7.57	1.23	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	36	VAL	C-O	7.56	1.33	1.24
3	O	12	LEU	N-CA	7.55	1.55	1.46
3	G	183	LEU	CA-C	7.54	1.62	1.52
4	H	29	ALA	CA-CB	-7.53	1.41	1.53
3	O	196	ARG	C-O	7.53	1.33	1.24
3	O	201	ILE	C-O	7.53	1.33	1.24
3	O	17	GLN	N-CA	7.53	1.55	1.46
1	B	325	ASP	C-N	-7.51	1.24	1.33
3	G	194	LEU	C-N	7.50	1.44	1.34
2	L	77	GLU	CA-CB	-7.49	1.44	1.54
1	J	325	ASP	C-N	-7.49	1.24	1.33
3	O	19	ARG	CA-C	7.48	1.62	1.52
3	G	19	ARG	CA-C	7.48	1.62	1.52
3	G	7	THR	C-O	7.46	1.33	1.24
4	H	29	ALA	N-CA	-7.46	1.37	1.46
3	G	196	ARG	C-O	7.45	1.33	1.24
3	O	16	GLY	C-N	7.44	1.43	1.33
3	O	7	THR	C-O	7.43	1.33	1.24
3	G	30	LYS	C-N	7.41	1.44	1.33
3	G	167	VAL	C-O	7.41	1.32	1.24
3	O	199	GLY	N-CA	7.41	1.56	1.45
3	O	26	ASP	C-O	7.41	1.32	1.24
4	P	29	ALA	N-CA	-7.40	1.37	1.46
3	G	49	ALA	C-O	7.39	1.32	1.24
2	M	80	ALA	CA-C	7.38	1.63	1.53
4	H	76	GLY	N-CA	7.38	1.53	1.45
3	O	52	ALA	CA-C	7.37	1.62	1.52
3	O	36	VAL	C-O	7.37	1.32	1.24
3	G	162	ASN	CA-CB	-7.36	1.41	1.53
3	G	37	ALA	CA-CB	-7.36	1.40	1.53
3	O	28	LEU	C-O	7.33	1.33	1.24
3	G	162	ASN	C-O	7.33	1.33	1.24
3	O	29	LYS	CA-C	7.32	1.61	1.52
1	J	352	PRO	CA-CB	-7.31	1.43	1.53
3	G	48	GLU	C-N	7.30	1.43	1.33
3	G	170	PRO	C-O	7.30	1.33	1.24
3	O	38	GLU	C-O	7.30	1.32	1.24
3	O	133	TYR	CA-C	7.28	1.62	1.52
3	G	16	GLY	C-N	7.28	1.43	1.33
3	O	162	ASN	CA-CB	-7.27	1.41	1.53
3	O	22	GLN	N-CA	7.23	1.55	1.46
3	G	189	GLU	C-O	7.23	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	167	VAL	C-O	7.22	1.32	1.24
3	G	192	PHE	C-N	7.22	1.43	1.34
1	B	352	PRO	CA-CB	-7.22	1.43	1.53
3	G	165	GLU	C-O	7.22	1.33	1.24
3	G	38	GLU	C-O	7.22	1.32	1.24
3	O	162	ASN	C-O	7.22	1.33	1.24
1	K	352	PRO	CA-CB	-7.21	1.43	1.53
3	G	133	TYR	CA-C	7.20	1.62	1.52
4	H	36	LEU	C-N	7.20	1.43	1.33
3	O	49	ALA	C-O	7.20	1.32	1.24
3	O	170	PRO	C-O	7.20	1.32	1.24
3	O	165	GLU	C-O	7.20	1.33	1.24
3	O	37	ALA	CA-CB	-7.18	1.40	1.53
3	G	28	LEU	C-O	7.18	1.33	1.24
3	O	192	PHE	C-N	7.15	1.43	1.34
3	G	22	GLN	N-CA	7.15	1.55	1.46
3	O	189	GLU	C-O	7.14	1.32	1.24
3	O	30	LYS	C-N	7.12	1.43	1.33
4	H	76	GLY	CA-C	7.11	1.59	1.51
3	G	144	GLU	N-CA	-7.09	1.37	1.46
2	L	275	GLU	CA-CB	-7.07	1.41	1.53
3	G	37	ALA	C-O	7.06	1.33	1.24
4	P	36	LEU	C-N	7.06	1.42	1.33
3	O	48	GLU	C-N	7.06	1.43	1.33
2	N	275	GLU	CA-CB	-7.05	1.41	1.53
3	G	29	LYS	CA-C	7.05	1.61	1.52
3	G	25	VAL	CA-CB	7.04	1.64	1.54
4	P	75	ALA	C-N	7.03	1.45	1.33
3	O	144	GLU	N-CA	-7.00	1.37	1.46
2	M	275	GLU	CA-CB	-6.99	1.41	1.53
2	F	275	GLU	CA-CB	-6.97	1.41	1.53
3	O	20	LEU	C-O	6.97	1.32	1.24
2	E	275	GLU	CA-CB	-6.95	1.41	1.53
3	G	139	ARG	CA-CB	6.95	1.65	1.53
3	O	160	ARG	C-O	6.95	1.32	1.24
1	C	352	PRO	CA-CB	-6.94	1.43	1.53
3	O	172	ILE	CA-C	-6.93	1.44	1.52
3	O	37	ALA	C-O	6.89	1.32	1.24
3	G	20	LEU	C-O	6.88	1.32	1.24
3	G	203	ALA	CA-CB	-6.85	1.42	1.53
3	O	184	GLU	C-O	6.85	1.31	1.24
2	D	275	GLU	CA-CB	-6.84	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	154	ILE	C-N	6.83	1.43	1.33
2	L	81	ARG	N-CA	6.83	1.53	1.46
3	G	160	ARG	C-O	6.82	1.32	1.24
3	O	203	ALA	CA-CB	-6.79	1.42	1.53
3	O	154	ILE	C-N	6.78	1.43	1.33
3	O	25	VAL	CA-CB	6.77	1.63	1.54
3	G	155	LYS	CA-CB	6.77	1.65	1.53
3	O	139	ARG	CA-CB	6.76	1.64	1.53
3	O	188	ARG	C-O	6.75	1.32	1.24
3	G	184	GLU	C-O	6.72	1.31	1.24
1	J	19	MET	CA-CB	-6.72	1.42	1.53
1	K	19	MET	CA-CB	-6.69	1.42	1.53
1	I	19	MET	CA-CB	-6.68	1.42	1.53
1	C	19	MET	CA-CB	-6.66	1.42	1.53
4	H	58	ALA	CA-CB	-6.64	1.42	1.53
3	G	150	ILE	N-CA	6.62	1.54	1.46
1	A	19	MET	CA-CB	-6.62	1.42	1.53
1	B	19	MET	CA-CB	-6.61	1.42	1.53
3	G	172	ILE	CA-C	-6.59	1.44	1.52
3	G	190	ASP	C-O	6.58	1.31	1.24
3	O	155	LYS	CA-CB	6.58	1.64	1.53
3	O	181	GLN	C-O	6.58	1.32	1.24
3	G	188	ARG	C-O	6.55	1.31	1.24
3	O	133	TYR	C-N	6.54	1.42	1.33
3	O	35	LEU	C-O	6.53	1.32	1.24
2	L	80	ALA	CA-C	6.50	1.61	1.53
4	P	58	ALA	CA-CB	-6.49	1.43	1.53
3	G	178	PHE	C-O	6.48	1.31	1.24
3	O	150	ILE	N-CA	6.48	1.54	1.46
3	G	141	ALA	N-CA	6.47	1.54	1.46
3	G	133	TYR	C-N	6.44	1.42	1.33
3	O	178	PHE	C-O	6.41	1.31	1.24
3	O	141	ALA	N-CA	6.39	1.54	1.46
3	O	190	ASP	C-O	6.38	1.31	1.24
3	G	35	LEU	C-O	6.37	1.32	1.24
3	G	181	GLN	CA-C	6.37	1.61	1.52
3	G	142	ASN	C-O	6.36	1.31	1.24
3	O	171	GLY	C-O	6.35	1.32	1.23
3	G	149	LYS	N-CA	-6.34	1.38	1.46
3	O	161	VAL	C-O	6.33	1.31	1.24
3	G	202	GLU	N-CA	6.32	1.53	1.46
3	G	181	GLN	C-O	6.32	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	202	GLU	N-CA	6.31	1.53	1.46
3	O	181	GLN	CA-C	6.30	1.61	1.52
3	G	171	GLY	C-O	6.29	1.32	1.23
2	D	81	ARG	C-N	6.28	1.42	1.33
3	G	135	GLU	CA-CB	6.26	1.63	1.53
3	O	141	ALA	CA-CB	6.26	1.64	1.53
2	M	80	ALA	N-CA	6.26	1.53	1.45
3	O	183	LEU	N-CA	6.26	1.54	1.46
3	G	133	TYR	C-O	6.24	1.32	1.24
3	G	186	ARG	C-O	6.21	1.31	1.24
4	H	28	GLU	CA-C	6.21	1.61	1.52
3	G	188	ARG	C-N	6.21	1.42	1.33
3	O	149	LYS	N-CA	-6.17	1.38	1.46
3	O	13	GLN	C-N	6.17	1.41	1.33
4	P	28	GLU	CA-C	6.17	1.60	1.52
3	O	188	ARG	C-N	6.15	1.42	1.33
3	O	133	TYR	C-O	6.13	1.31	1.24
3	G	183	LEU	N-CA	6.13	1.54	1.46
3	G	190	ASP	CA-C	6.13	1.60	1.52
3	G	31	LYS	CA-CB	6.12	1.63	1.53
4	H	40	GLY	C-N	6.12	1.44	1.33
3	O	38	GLU	CA-C	6.12	1.60	1.52
3	G	42	LEU	C-O	6.09	1.31	1.24
3	O	142	ASN	C-O	6.09	1.31	1.24
3	G	141	ALA	CA-CB	6.08	1.64	1.53
3	G	38	GLU	CA-C	6.06	1.60	1.52
3	O	31	LYS	CA-CB	6.06	1.63	1.53
3	O	159	ARG	C-O	6.05	1.31	1.24
2	L	81	ARG	CA-C	6.05	1.59	1.52
4	P	40	GLY	C-N	6.04	1.44	1.33
3	O	190	ASP	CA-C	6.04	1.60	1.52
2	N	250	ASP	C-O	-6.01	1.15	1.23
3	G	161	VAL	C-O	6.01	1.31	1.24
2	D	250	ASP	C-O	-6.00	1.15	1.23
4	P	45	VAL	CA-C	-6.00	1.45	1.52
2	L	250	ASP	C-O	-5.99	1.15	1.23
2	E	250	ASP	C-O	-5.98	1.15	1.23
2	D	80	ALA	C-N	5.97	1.41	1.33
2	M	250	ASP	C-O	-5.96	1.15	1.23
3	G	13	GLN	C-N	5.95	1.41	1.33
3	O	42	LEU	C-O	5.95	1.31	1.24
4	H	31	SER	N-CA	-5.94	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	5	SER	CA-CB	5.94	1.62	1.53
3	O	139	ARG	CA-C	5.92	1.60	1.52
3	O	135	GLU	CA-CB	5.90	1.62	1.53
3	O	200	LYS	CA-CB	5.90	1.63	1.53
3	O	29	LYS	C-O	5.89	1.30	1.24
2	F	250	ASP	C-O	-5.88	1.15	1.23
4	P	31	SER	N-CA	-5.88	1.39	1.46
3	G	200	LYS	CA-CB	5.87	1.63	1.53
3	G	139	ARG	CA-C	5.86	1.60	1.52
3	G	159	ARG	N-CA	5.83	1.53	1.46
4	H	45	VAL	CA-C	-5.83	1.45	1.52
2	E	26	ASP	CA-CB	-5.80	1.43	1.53
3	G	159	ARG	C-O	5.80	1.30	1.24
3	O	186	ARG	C-O	5.78	1.31	1.24
4	P	35	THR	CA-C	5.78	1.60	1.52
4	H	35	THR	CA-C	5.75	1.60	1.52
3	O	5	SER	CA-CB	5.75	1.62	1.53
2	D	249	HIS	C-O	-5.74	1.16	1.24
3	O	142	ASN	C-N	5.74	1.41	1.33
2	L	26	ASP	CA-CB	-5.74	1.43	1.53
3	G	30	LYS	N-CA	5.73	1.53	1.46
3	O	41	GLY	C-O	5.73	1.31	1.23
2	N	26	ASP	CA-CB	-5.72	1.43	1.53
3	G	43	VAL	N-CA	5.70	1.53	1.46
3	G	135	GLU	CA-C	5.70	1.60	1.52
2	M	26	ASP	CA-CB	-5.68	1.43	1.53
3	G	166	GLN	C-O	5.67	1.30	1.24
2	E	79	VAL	C-N	5.67	1.41	1.33
3	O	166	GLN	C-O	5.67	1.30	1.24
3	G	166	GLN	N-CA	-5.65	1.39	1.46
3	G	182	VAL	C-O	5.65	1.30	1.24
3	O	177	ARG	N-CA	5.65	1.53	1.46
3	O	30	LYS	N-CA	5.65	1.53	1.46
3	O	43	VAL	N-CA	5.64	1.53	1.46
3	O	182	VAL	C-O	5.64	1.30	1.24
3	O	159	ARG	N-CA	5.63	1.53	1.46
2	E	249	HIS	C-O	-5.62	1.16	1.24
2	D	26	ASP	CA-CB	-5.62	1.44	1.53
3	G	205	GLU	C-O	5.61	1.34	1.23
2	F	249	HIS	C-O	-5.59	1.16	1.24
3	O	43	VAL	C-O	5.59	1.30	1.24
3	O	11	LEU	C-N	5.58	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	205	GLU	C-O	5.58	1.34	1.23
3	G	177	ARG	N-CA	5.58	1.53	1.46
2	M	249	HIS	C-O	-5.58	1.16	1.24
2	F	26	ASP	CA-CB	-5.56	1.44	1.53
3	G	43	VAL	CA-CB	5.56	1.62	1.54
3	G	15	ARG	N-CA	5.55	1.52	1.46
3	G	41	GLY	C-O	5.54	1.31	1.23
2	L	249	HIS	C-O	-5.54	1.16	1.24
3	G	29	LYS	C-O	5.53	1.30	1.24
3	O	43	VAL	CA-CB	5.53	1.61	1.54
3	G	24	GLY	N-CA	5.53	1.52	1.45
3	O	190	ASP	CA-CB	-5.52	1.44	1.53
2	N	249	HIS	C-O	-5.52	1.16	1.24
3	G	133	TYR	N-CA	-5.52	1.39	1.46
3	G	8	ARG	CA-C	5.51	1.60	1.52
3	O	181	GLN	C-N	5.51	1.40	1.33
3	O	158	THR	N-CA	5.50	1.53	1.46
3	O	15	ARG	N-CA	5.50	1.52	1.46
3	G	158	THR	N-CA	5.49	1.53	1.46
2	N	81	ARG	CA-C	5.49	1.59	1.52
3	O	37	ALA	C-N	5.46	1.40	1.33
3	G	11	LEU	C-N	5.45	1.40	1.33
3	G	190	ASP	CA-CB	-5.45	1.45	1.53
3	G	177	ARG	C-O	5.45	1.30	1.24
3	O	156	LYS	CA-CB	5.45	1.62	1.54
4	P	91	ARG	C-O	5.45	1.30	1.24
1	K	70	PRO	C-N	5.44	1.41	1.33
3	O	8	ARG	CA-C	5.41	1.60	1.52
3	O	133	TYR	N-CA	-5.41	1.39	1.46
3	O	198	LYS	C-N	5.41	1.41	1.33
3	O	204	ARG	C-O	5.40	1.30	1.24
3	G	204	ARG	C-O	5.38	1.30	1.24
4	H	91	ARG	C-O	5.38	1.30	1.24
2	M	63	THR	CA-CB	-5.38	1.44	1.53
2	F	291	LEU	C-O	-5.37	1.17	1.24
3	G	182	VAL	C-N	5.37	1.41	1.33
3	O	186	ARG	CA-CB	5.35	1.62	1.53
3	O	24	GLY	N-CA	5.35	1.52	1.45
3	O	166	GLN	N-CA	-5.34	1.39	1.46
3	G	198	LYS	C-N	5.33	1.41	1.33
2	N	63	THR	CA-CB	-5.33	1.44	1.53
3	G	186	ARG	CA-CB	5.33	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	37	ALA	C-N	5.33	1.40	1.33
3	O	135	GLU	CA-C	5.33	1.59	1.52
2	L	63	THR	CA-CB	-5.33	1.44	1.53
3	G	149	LYS	CA-CB	-5.31	1.44	1.53
3	O	44	ARG	CA-CB	-5.31	1.43	1.53
3	G	181	GLN	C-N	5.30	1.40	1.33
3	G	22	GLN	CA-CB	5.30	1.62	1.53
2	F	63	THR	CA-CB	-5.29	1.44	1.53
3	O	177	ARG	C-O	5.29	1.30	1.24
4	P	76	GLY	C-N	5.29	1.40	1.33
3	O	135	GLU	N-CA	5.28	1.52	1.46
3	G	179	ILE	CA-C	5.28	1.59	1.52
3	G	21	ALA	N-CA	5.27	1.52	1.46
3	O	21	ALA	C-N	5.27	1.41	1.33
4	P	20	GLY	C-O	-5.26	1.16	1.23
3	G	142	ASN	C-N	5.26	1.40	1.33
2	M	291	LEU	C-O	-5.26	1.17	1.24
3	G	140	VAL	N-CA	5.25	1.52	1.46
3	G	157	THR	CA-CB	-5.25	1.44	1.53
3	O	179	ILE	CA-C	5.25	1.59	1.52
3	O	194	LEU	N-CA	5.25	1.52	1.46
3	O	149	LYS	CA-CB	-5.24	1.44	1.53
2	E	63	THR	CA-CB	-5.24	1.44	1.53
3	G	27	LEU	C-O	5.24	1.30	1.24
3	G	134	ALA	CA-C	5.23	1.59	1.52
3	G	38	GLU	CA-CB	5.23	1.61	1.53
3	G	44	ARG	CA-CB	-5.22	1.43	1.53
3	O	11	LEU	CA-C	5.22	1.59	1.52
3	O	38	GLU	CA-CB	5.22	1.61	1.53
3	O	134	ALA	CA-C	5.22	1.59	1.52
3	O	145	THR	C-O	5.21	1.30	1.24
3	G	21	ALA	C-N	5.21	1.41	1.33
3	G	43	VAL	C-O	5.20	1.30	1.24
2	N	291	LEU	C-O	-5.19	1.17	1.24
3	G	11	LEU	CA-C	5.19	1.59	1.52
3	O	182	VAL	C-N	5.18	1.41	1.33
3	O	42	LEU	CA-C	5.16	1.59	1.52
3	O	22	GLN	CA-CB	5.16	1.62	1.53
2	D	63	THR	CA-CB	-5.16	1.44	1.53
4	H	20	GLY	C-O	-5.14	1.16	1.23
3	O	199	GLY	CA-C	-5.12	1.44	1.51
3	G	156	LYS	CA-CB	5.10	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	53	LEU	CA-CB	5.09	1.62	1.53
3	G	194	LEU	N-CA	5.09	1.52	1.46
4	H	72	LEU	N-CA	-5.08	1.41	1.46
3	G	144	GLU	CA-C	5.07	1.59	1.52
3	G	174	ALA	CA-C	5.07	1.59	1.52
3	O	47	MET	CA-C	5.06	1.59	1.52
3	G	54	ASP	N-CA	5.06	1.52	1.46
3	G	42	LEU	CA-C	5.05	1.59	1.52
3	O	21	ALA	N-CA	5.05	1.52	1.46
4	P	72	LEU	N-CA	-5.04	1.41	1.46
3	O	157	THR	CA-CB	-5.04	1.44	1.53
2	L	291	LEU	C-O	-5.04	1.17	1.24
3	O	139	ARG	C-O	5.04	1.30	1.24
3	G	139	ARG	C-O	5.03	1.30	1.24
3	G	51	LYS	N-CA	5.03	1.52	1.46
2	E	291	LEU	C-O	-5.03	1.17	1.24
3	G	51	LYS	C-N	5.03	1.40	1.33
3	G	47	MET	CA-C	5.02	1.59	1.52
3	G	30	LYS	CA-C	5.02	1.59	1.52
2	D	249	HIS	C-N	5.02	1.41	1.33
3	O	14	ARG	CA-C	5.02	1.59	1.52

All (660) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	325	ASP	O-C-N	-47.92	58.86	122.59
1	J	325	ASP	O-C-N	-47.91	58.87	122.59
1	C	325	ASP	O-C-N	-47.91	58.87	122.59
1	A	325	ASP	O-C-N	-47.90	58.89	122.59
1	K	325	ASP	O-C-N	-47.86	58.94	122.59
1	B	325	ASP	O-C-N	-47.85	58.95	122.59
4	P	76	GLY	N-CA-C	44.09	179.98	112.51
1	K	70	PRO	CA-C-N	-35.85	53.06	121.54
1	K	70	PRO	C-N-CA	-35.85	53.06	121.54
1	I	429	SER	CA-C-N	-33.69	68.49	122.73
1	I	429	SER	C-N-CA	-33.69	68.49	122.73
1	I	429	SER	O-C-N	33.48	163.84	123.33
4	P	74	ILE	O-C-N	-28.64	92.46	123.10
1	C	325	ASP	CA-C-N	-28.00	75.94	121.87
1	C	325	ASP	C-N-CA	-28.00	75.94	121.87
1	A	325	ASP	CA-C-N	-27.95	76.03	121.87
1	A	325	ASP	C-N-CA	-27.95	76.03	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	325	ASP	CA-C-N	-27.91	76.09	121.87
1	K	325	ASP	C-N-CA	-27.91	76.09	121.87
1	B	325	ASP	CA-C-N	-27.88	76.15	121.87
1	B	325	ASP	C-N-CA	-27.88	76.15	121.87
1	J	325	ASP	CA-C-N	-27.87	76.16	121.87
1	J	325	ASP	C-N-CA	-27.87	76.16	121.87
1	I	325	ASP	CA-C-N	-27.81	76.27	121.87
1	I	325	ASP	C-N-CA	-27.81	76.27	121.87
2	D	316	MET	O-C-N	-26.10	91.31	121.32
2	L	316	MET	O-C-N	-26.00	91.42	121.32
2	E	316	MET	O-C-N	-26.00	91.42	121.32
2	F	316	MET	O-C-N	-25.96	91.47	121.32
2	N	316	MET	O-C-N	-25.89	91.55	121.32
2	M	316	MET	O-C-N	-25.88	91.56	121.32
4	P	75	ALA	N-CA-C	23.74	143.98	110.50
4	H	77	LEU	CA-C-N	-18.84	88.66	120.68
4	H	77	LEU	C-N-CA	-18.84	88.66	120.68
2	E	81	ARG	N-CA-C	18.31	133.09	108.38
4	P	77	LEU	CA-C-N	-16.84	92.06	120.68
4	P	77	LEU	C-N-CA	-16.84	92.06	120.68
3	O	133	TYR	N-CA-C	-16.83	91.85	112.38
3	O	157	THR	N-CA-C	-16.78	92.07	112.54
3	G	133	TYR	N-CA-C	-16.75	91.95	112.38
3	G	157	THR	N-CA-C	-16.74	92.12	112.54
3	G	12	LEU	N-CA-C	-16.56	92.92	110.97
3	O	12	LEU	N-CA-C	-16.47	93.02	110.97
1	K	70	PRO	O-C-N	15.92	144.13	122.64
4	P	76	GLY	CA-C-O	-15.52	99.96	122.62
3	O	203	ALA	N-CA-C	-15.37	89.91	112.04
3	G	203	ALA	N-CA-C	-15.33	89.96	112.04
4	P	63	MET	N-CA-C	15.27	130.90	108.60
4	H	75	ALA	N-CA-C	14.96	131.93	110.23
2	L	360	ARG	N-CA-C	-14.77	94.36	112.38
4	P	75	ALA	CA-C-N	14.39	141.44	121.01
4	P	75	ALA	C-N-CA	14.39	141.44	121.01
3	G	142	ASN	N-CA-C	-14.35	95.71	111.36
3	O	142	ASN	N-CA-C	-14.15	95.94	111.36
2	D	81	ARG	N-CA-C	14.06	128.15	108.74
4	P	76	GLY	CA-C-N	14.04	146.97	121.70
4	P	76	GLY	C-N-CA	14.04	146.97	121.70
3	G	153	GLU	N-CA-C	13.91	130.14	112.89
3	O	6	PRO	CA-C-N	-13.84	97.15	120.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	6	PRO	C-N-CA	-13.84	97.15	120.68
3	O	187	GLU	N-CA-C	13.80	133.58	113.02
3	O	153	GLU	N-CA-C	13.73	129.91	112.89
3	G	6	PRO	CA-C-N	-13.70	97.38	120.68
3	G	6	PRO	C-N-CA	-13.70	97.38	120.68
3	O	47	MET	N-CA-C	13.60	139.78	110.80
3	G	47	MET	N-CA-C	13.57	139.70	110.80
1	A	69	LEU	CA-C-N	13.52	134.06	119.05
1	A	69	LEU	C-N-CA	13.52	134.06	119.05
1	K	430	LEU	N-CA-C	-13.39	97.00	113.20
2	E	80	ALA	N-CA-C	13.31	130.17	109.81
3	O	139	ARG	N-CA-C	-13.18	82.73	110.80
3	G	139	ARG	N-CA-C	-13.15	82.78	110.80
2	D	360	ARG	N-CA-C	-13.04	96.47	112.38
3	G	194	LEU	N-CA-C	12.88	127.12	111.40
3	O	194	LEU	N-CA-C	12.80	127.02	111.40
4	H	74	ILE	O-C-N	-12.66	109.53	123.20
3	G	187	GLU	N-CA-C	12.58	133.77	113.89
3	O	186	ARG	CA-C-N	-12.58	102.08	122.08
3	O	186	ARG	C-N-CA	-12.58	102.08	122.08
3	G	186	ARG	CA-C-N	-12.45	102.56	121.99
3	G	186	ARG	C-N-CA	-12.45	102.56	121.99
2	E	79	VAL	O-C-N	-11.98	107.59	122.57
1	J	429	SER	O-C-N	-11.96	107.84	123.14
3	G	188	ARG	N-CA-C	-11.95	98.26	111.28
3	O	9	MET	CA-C-N	-11.84	98.27	121.94
3	O	9	MET	C-N-CA	-11.84	98.27	121.94
3	O	188	ARG	N-CA-C	-11.82	98.40	111.28
3	G	9	MET	CA-C-N	-11.82	98.31	121.94
3	G	9	MET	C-N-CA	-11.82	98.31	121.94
1	C	70	PRO	N-CA-C	-11.70	97.26	113.53
3	O	49	ALA	CA-C-N	-11.55	98.84	121.94
3	O	49	ALA	C-N-CA	-11.55	98.84	121.94
3	G	49	ALA	CA-C-N	-11.51	98.92	121.94
3	G	49	ALA	C-N-CA	-11.51	98.92	121.94
3	G	7	THR	CA-C-N	-11.42	103.71	120.38
3	G	7	THR	C-N-CA	-11.42	103.71	120.38
3	G	167	VAL	O-C-N	-11.41	110.72	121.91
3	O	167	VAL	O-C-N	-11.40	110.74	121.91
2	N	351	PRO	N-CA-CB	11.33	110.40	102.81
3	O	7	THR	CA-C-N	-11.32	103.85	120.38
3	O	7	THR	C-N-CA	-11.32	103.85	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	351	PRO	N-CA-CB	11.28	110.36	102.81
2	D	351	PRO	N-CA-CB	11.20	110.31	102.81
3	G	47	MET	CA-C-N	-11.13	100.27	121.54
3	G	47	MET	C-N-CA	-11.13	100.27	121.54
4	H	76	GLY	CA-C-N	11.13	141.74	121.70
4	H	76	GLY	C-N-CA	11.13	141.74	121.70
3	G	6	PRO	N-CA-CB	11.13	114.94	103.25
1	I	63	PRO	N-CA-CB	11.13	113.76	103.19
3	O	47	MET	CA-C-N	-11.13	100.28	121.54
3	O	47	MET	C-N-CA	-11.13	100.28	121.54
1	C	63	PRO	N-CA-CB	11.08	113.71	103.19
2	L	351	PRO	N-CA-CB	11.07	110.22	102.81
1	K	63	PRO	N-CA-CB	11.03	113.67	103.19
2	M	81	ARG	N-CA-C	11.02	124.69	108.60
2	F	351	PRO	N-CA-CB	10.99	110.18	102.81
2	E	351	PRO	N-CA-CB	10.98	110.17	102.81
1	B	63	PRO	N-CA-CB	10.98	113.62	103.19
1	A	63	PRO	N-CA-CB	10.92	113.56	103.19
1	J	63	PRO	N-CA-CB	10.92	113.56	103.19
1	I	70	PRO	N-CA-C	-10.91	98.37	113.53
3	O	6	PRO	N-CA-CB	10.84	114.64	103.25
3	O	38	GLU	N-CA-C	10.47	122.39	110.97
3	G	38	GLU	N-CA-C	10.35	122.26	110.97
3	G	163	ALA	N-CA-C	10.30	123.77	111.82
3	O	163	ALA	N-CA-C	10.28	123.74	111.82
3	G	167	VAL	CA-C-N	-10.24	103.53	121.97
3	G	167	VAL	C-N-CA	-10.24	103.53	121.97
3	O	167	VAL	CA-C-N	-10.24	103.53	121.97
3	O	167	VAL	C-N-CA	-10.24	103.53	121.97
3	G	183	LEU	CA-C-N	10.11	134.19	120.54
3	G	183	LEU	C-N-CA	10.11	134.19	120.54
3	O	183	LEU	CA-C-N	10.07	134.14	120.54
3	O	183	LEU	C-N-CA	10.07	134.14	120.54
3	O	156	LYS	N-CA-C	9.96	129.63	113.89
3	G	156	LYS	N-CA-C	9.93	129.58	113.89
3	G	19	ARG	N-CA-C	9.90	123.10	111.71
3	O	19	ARG	N-CA-C	9.88	123.07	111.71
1	B	429	SER	O-C-N	9.84	135.93	123.14
4	P	68	LEU	CA-C-N	9.64	130.25	119.93
4	P	68	LEU	C-N-CA	9.64	130.25	119.93
4	H	68	LEU	CA-C-N	9.59	130.19	119.93
4	H	68	LEU	C-N-CA	9.59	130.19	119.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	LEU	N-CA-C	-9.54	98.22	110.53
2	D	80	ALA	N-CA-C	9.54	124.92	109.85
1	I	69	LEU	CA-C-N	9.52	129.62	119.05
1	I	69	LEU	C-N-CA	9.52	129.62	119.05
3	G	204	ARG	N-CA-C	9.43	122.76	111.82
3	G	178	PHE	N-CA-C	-9.41	99.94	111.33
4	P	86	VAL	N-CA-C	9.38	120.19	110.62
3	O	30	LYS	CA-C-N	9.37	139.44	121.54
3	O	30	LYS	C-N-CA	9.37	139.44	121.54
3	G	30	LYS	CA-C-N	9.36	139.41	121.54
3	G	30	LYS	C-N-CA	9.36	139.41	121.54
4	H	76	GLY	CA-C-O	-9.27	110.83	121.68
3	O	204	ARG	N-CA-C	9.25	122.55	111.82
3	O	178	PHE	N-CA-C	-9.24	100.15	111.33
3	G	49	ALA	CA-C-O	9.18	130.15	120.70
4	P	76	GLY	O-C-N	-9.15	109.81	122.61
3	O	11	LEU	N-CA-C	-9.12	101.58	112.89
3	O	14	ARG	N-CA-C	9.12	120.83	111.07
3	G	11	LEU	N-CA-C	-9.11	101.60	112.89
3	G	156	LYS	CA-C-N	-9.09	105.54	120.72
3	G	156	LYS	C-N-CA	-9.09	105.54	120.72
3	O	156	LYS	CA-C-N	-9.07	105.58	120.72
3	O	156	LYS	C-N-CA	-9.07	105.58	120.72
3	G	14	ARG	N-CA-C	9.04	120.74	111.07
3	O	49	ALA	CA-C-O	9.03	130.00	120.70
3	O	181	GLN	N-CA-C	9.03	123.85	113.01
3	G	181	GLN	N-CA-C	8.97	123.77	113.01
3	G	174	ALA	CA-C-N	-8.93	108.14	120.38
3	G	174	ALA	C-N-CA	-8.93	108.14	120.38
3	G	192	PHE	N-CA-C	8.93	123.49	112.23
3	G	37	ALA	CA-C-N	8.89	132.38	120.65
3	G	37	ALA	C-N-CA	8.89	132.38	120.65
3	G	31	LYS	O-C-N	8.88	134.40	122.59
3	O	31	LYS	O-C-N	8.86	134.37	122.59
3	O	174	ALA	CA-C-N	-8.84	108.27	120.38
3	O	174	ALA	C-N-CA	-8.84	108.27	120.38
2	L	359	SER	N-CA-C	-8.81	96.40	109.62
3	O	192	PHE	N-CA-C	8.81	123.33	112.23
3	O	155	LYS	CA-C-N	-8.79	108.27	121.99
3	O	155	LYS	C-N-CA	-8.79	108.27	121.99
3	O	37	ALA	CA-C-N	8.76	132.21	120.65
3	O	37	ALA	C-N-CA	8.76	132.21	120.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	155	LYS	CA-C-N	-8.74	108.36	121.99
3	G	155	LYS	C-N-CA	-8.74	108.36	121.99
4	P	35	THR	CB-CA-C	-8.62	97.01	110.81
4	H	35	THR	CB-CA-C	-8.62	97.03	110.81
2	N	81	ARG	N-CA-C	8.48	121.59	108.96
1	C	244	TRP	N-CA-C	8.40	126.21	113.61
1	K	244	TRP	N-CA-C	8.39	126.19	113.61
1	J	244	TRP	N-CA-C	8.38	126.17	113.61
2	L	289	THR	O-C-N	-8.37	111.11	122.33
1	I	244	TRP	N-CA-C	8.36	126.15	113.61
1	A	244	TRP	N-CA-C	8.35	126.13	113.61
1	B	244	TRP	N-CA-C	8.34	126.12	113.61
2	D	289	THR	O-C-N	-8.30	111.21	122.33
2	E	289	THR	O-C-N	-8.29	111.22	122.33
2	M	289	THR	O-C-N	-8.26	111.27	122.33
2	N	289	THR	O-C-N	-8.25	111.27	122.33
3	O	170	PRO	N-CA-CB	8.20	111.82	102.88
2	F	289	THR	O-C-N	-8.19	111.35	122.33
2	D	359	SER	N-CA-C	-8.18	97.35	109.62
2	L	284	PRO	N-CA-CB	8.13	110.40	103.25
2	D	284	PRO	N-CA-CB	8.11	110.38	103.25
2	N	284	PRO	N-CA-CB	8.10	110.38	103.25
3	G	170	PRO	N-CA-CB	8.08	111.69	102.88
3	G	158	THR	N-CA-C	8.07	122.39	112.23
2	E	284	PRO	N-CA-CB	8.06	110.34	103.25
3	G	12	LEU	O-C-N	8.03	130.38	122.03
2	M	284	PRO	N-CA-CB	8.00	110.29	103.25
3	O	13	GLN	CA-C-N	7.99	130.82	120.44
3	O	13	GLN	C-N-CA	7.99	130.82	120.44
3	O	12	LEU	O-C-N	7.94	130.29	122.03
2	F	284	PRO	N-CA-CB	7.93	110.23	103.25
3	G	13	GLN	CA-C-N	7.88	130.69	120.44
3	G	13	GLN	C-N-CA	7.88	130.69	120.44
3	O	158	THR	N-CA-C	7.88	122.66	112.89
3	O	182	VAL	O-C-N	7.87	133.85	122.04
1	I	351	PRO	N-CA-CB	7.87	107.59	103.19
1	K	351	PRO	N-CA-CB	7.84	107.58	103.19
1	A	351	PRO	N-CA-CB	7.78	107.55	103.19
3	O	140	VAL	N-CA-C	7.77	125.49	109.34
3	G	163	ALA	CA-C-N	7.76	131.46	120.28
3	G	163	ALA	C-N-CA	7.76	131.46	120.28
1	C	12	PRO	N-CA-CB	7.76	111.39	103.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	160	ARG	N-CA-C	-7.75	102.93	112.38
3	O	163	ALA	CA-C-N	7.73	131.42	120.28
3	O	163	ALA	C-N-CA	7.73	131.42	120.28
3	G	47	MET	CA-C-O	7.72	131.55	120.51
2	M	80	ALA	N-CA-C	7.72	120.49	110.53
3	G	140	VAL	N-CA-C	7.71	125.38	109.34
3	G	165	GLU	CA-C-N	-7.70	109.83	120.38
3	G	165	GLU	C-N-CA	-7.70	109.83	120.38
3	G	160	ARG	N-CA-C	-7.69	102.99	112.38
2	D	17	PRO	N-CA-CB	7.69	110.50	103.20
3	G	182	VAL	O-C-N	7.68	133.56	122.04
2	F	17	PRO	N-CA-CB	7.67	110.49	103.20
1	K	12	PRO	N-CA-CB	7.67	111.30	103.25
2	E	17	PRO	N-CA-CB	7.67	110.49	103.20
3	O	165	GLU	CA-C-N	-7.65	109.90	120.38
3	O	165	GLU	C-N-CA	-7.65	109.90	120.38
1	C	351	PRO	N-CA-CB	7.61	107.45	103.19
3	G	154	ILE	N-CA-C	-7.61	93.52	109.34
1	A	12	PRO	N-CA-CB	7.59	111.22	103.25
3	O	47	MET	CA-C-O	7.59	131.36	120.51
1	J	12	PRO	N-CA-CB	7.58	111.21	103.25
1	B	12	PRO	N-CA-CB	7.58	111.21	103.25
3	O	154	ILE	N-CA-C	-7.57	93.61	109.34
2	L	17	PRO	N-CA-CB	7.56	110.39	103.20
2	N	17	PRO	N-CA-CB	7.55	110.37	103.20
1	B	351	PRO	N-CA-CB	7.54	107.41	103.19
1	I	12	PRO	N-CA-CB	7.53	111.16	103.25
1	J	351	PRO	N-CA-CB	7.53	107.41	103.19
2	M	17	PRO	N-CA-CB	7.50	110.33	103.20
3	G	188	ARG	N-CA-CB	7.49	121.13	110.12
3	O	21	ALA	O-C-N	7.47	132.53	122.59
3	G	166	GLN	CA-C-N	-7.46	111.16	120.56
3	G	166	GLN	C-N-CA	-7.46	111.16	120.56
3	O	196	ARG	N-CA-CB	-7.46	99.08	110.20
3	G	196	ARG	N-CA-CB	-7.45	99.10	110.20
3	G	202	GLU	CA-C-O	7.44	128.41	119.78
3	O	149	LYS	N-CA-C	-7.43	94.98	110.80
4	P	62	LEU	CA-C-N	-7.39	109.16	121.80
4	P	62	LEU	C-N-CA	-7.39	109.16	121.80
3	O	32	ARG	CA-C-O	-7.38	112.73	120.55
3	O	166	GLN	CA-C-N	-7.38	111.26	120.56
3	O	166	GLN	C-N-CA	-7.38	111.26	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	21	ALA	O-C-N	7.38	132.40	122.59
1	B	429	SER	CA-C-N	-7.36	107.60	122.55
1	B	429	SER	C-N-CA	-7.36	107.60	122.55
3	O	188	ARG	N-CA-CB	7.36	120.93	110.12
3	G	149	LYS	N-CA-C	-7.35	95.15	110.80
3	G	193	ARG	N-CA-C	-7.31	103.31	111.71
3	G	151	GLY	N-CA-C	-7.30	95.88	113.18
3	G	32	ARG	CA-C-O	-7.27	112.85	120.55
2	F	81	ARG	N-CA-C	7.26	120.20	109.24
3	O	151	GLY	N-CA-C	-7.24	96.02	113.18
3	G	5	SER	O-C-N	7.23	129.64	121.32
3	O	202	GLU	CA-C-O	7.21	128.15	119.78
3	O	136	ALA	N-CA-C	-7.21	95.45	110.80
3	O	51	LYS	CA-C-N	7.18	130.24	120.54
3	O	51	LYS	C-N-CA	7.18	130.24	120.54
2	L	81	ARG	CA-C-N	-7.16	112.84	122.72
2	L	81	ARG	C-N-CA	-7.16	112.84	122.72
3	O	5	SER	O-C-N	7.14	129.53	121.32
3	O	51	LYS	N-CA-C	-7.12	103.52	111.71
4	P	77	LEU	O-C-N	-7.12	111.61	123.00
3	G	137	LEU	CA-C-N	-7.09	109.91	121.19
3	G	137	LEU	C-N-CA	-7.09	109.91	121.19
3	G	51	LYS	N-CA-C	-7.09	103.56	111.71
3	G	51	LYS	CA-C-N	7.08	130.09	120.54
3	G	51	LYS	C-N-CA	7.08	130.09	120.54
3	G	136	ALA	N-CA-C	-7.05	95.77	110.80
3	O	137	LEU	CA-C-N	-7.03	110.02	121.19
3	O	137	LEU	C-N-CA	-7.03	110.02	121.19
2	D	79	VAL	O-C-N	-7.02	113.79	122.57
3	O	193	ARG	N-CA-C	-6.98	103.68	111.71
3	G	31	LYS	CA-C-N	6.97	129.62	120.28
3	G	31	LYS	C-N-CA	6.97	129.62	120.28
3	G	195	LYS	CA-C-O	6.96	127.97	120.10
3	O	195	LYS	CA-C-O	6.96	127.96	120.10
3	G	15	ARG	N-CA-C	-6.95	103.31	111.03
3	O	31	LYS	CA-C-N	6.93	129.57	120.28
3	O	31	LYS	C-N-CA	6.93	129.57	120.28
1	J	557	GLU	O-C-N	-6.88	113.45	122.39
3	G	196	ARG	CB-CA-C	6.87	123.27	110.70
1	C	557	GLU	O-C-N	-6.85	113.49	122.39
4	P	40	GLY	N-CA-C	6.83	120.89	113.58
3	O	15	ARG	N-CA-C	-6.82	103.46	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	196	ARG	CB-CA-C	6.81	123.17	110.70
1	B	557	GLU	O-C-N	-6.81	113.54	122.39
1	A	557	GLU	O-C-N	-6.81	113.54	122.39
4	H	40	GLY	O-C-N	6.80	128.15	122.71
1	I	557	GLU	O-C-N	-6.79	113.56	122.39
4	H	81	PHE	N-CA-C	-6.78	104.65	113.12
1	K	557	GLU	O-C-N	-6.76	113.60	122.39
4	H	40	GLY	N-CA-C	6.76	120.81	113.58
3	O	187	GLU	CA-C-O	-6.72	112.02	119.34
4	P	40	GLY	O-C-N	6.71	128.08	122.71
3	G	32	ARG	CA-C-N	6.70	129.55	120.44
3	G	32	ARG	C-N-CA	6.70	129.55	120.44
4	P	81	PHE	N-CA-C	-6.69	104.76	113.12
3	G	199	GLY	N-CA-C	-6.65	97.42	113.18
3	O	179	ILE	CA-C-N	-6.63	111.29	120.38
3	O	179	ILE	C-N-CA	-6.63	111.29	120.38
3	O	199	GLY	N-CA-C	-6.63	97.47	113.18
2	M	66	LEU	N-CA-CB	-6.57	107.53	114.10
3	G	179	ILE	CA-C-N	-6.55	111.40	120.38
3	G	179	ILE	C-N-CA	-6.55	111.40	120.38
3	O	32	ARG	CA-C-N	6.55	129.35	120.44
3	O	32	ARG	C-N-CA	6.55	129.35	120.44
2	N	66	LEU	N-CA-CB	-6.54	107.56	114.10
2	E	66	LEU	N-CA-CB	-6.54	107.56	114.10
2	F	66	LEU	N-CA-CB	-6.53	107.57	114.10
2	D	66	LEU	N-CA-CB	-6.51	107.59	114.10
2	L	66	LEU	N-CA-CB	-6.50	107.60	114.10
4	P	62	LEU	O-C-N	-6.48	115.35	122.09
1	A	142	GLY	CA-C-N	6.45	133.31	121.70
1	A	142	GLY	C-N-CA	6.45	133.31	121.70
3	G	161	VAL	O-C-N	6.44	130.62	122.57
3	O	161	VAL	O-C-N	6.44	130.62	122.57
4	P	95	ARG	N-CA-C	-6.37	104.25	111.07
4	H	95	ARG	N-CA-C	-6.37	104.26	111.07
1	B	39	ILE	CB-CA-C	-6.37	104.41	111.35
3	G	145	THR	N-CA-C	6.34	118.19	111.28
2	E	81	ARG	CA-C-O	-6.33	114.53	121.31
4	P	34	GLU	CA-C-O	-6.32	114.18	120.82
3	G	182	VAL	CB-CA-C	-6.32	102.74	111.65
1	K	142	GLY	CA-C-N	6.31	133.06	121.70
1	K	142	GLY	C-N-CA	6.31	133.06	121.70
1	J	226	ILE	N-CA-CB	6.31	119.79	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	142	GLY	CA-C-N	6.30	133.05	121.70
1	I	142	GLY	C-N-CA	6.30	133.05	121.70
1	C	142	GLY	CA-C-N	6.30	133.04	121.70
1	C	142	GLY	C-N-CA	6.30	133.04	121.70
1	K	39	ILE	CB-CA-C	-6.30	104.48	111.35
3	G	10	ASN	CA-C-N	-6.30	110.12	121.14
3	G	10	ASN	C-N-CA	-6.30	110.12	121.14
1	A	39	ILE	CB-CA-C	-6.29	104.49	111.35
1	C	226	ILE	N-CA-CB	6.29	119.77	111.40
1	J	39	ILE	CB-CA-C	-6.28	104.51	111.35
3	O	10	ASN	CA-C-N	-6.27	110.16	121.14
3	O	10	ASN	C-N-CA	-6.27	110.16	121.14
4	H	34	GLU	CA-C-O	-6.27	114.24	120.82
1	B	142	GLY	CA-C-N	6.26	132.97	121.70
1	B	142	GLY	C-N-CA	6.26	132.97	121.70
1	I	39	ILE	CB-CA-C	-6.26	104.53	111.35
3	O	167	VAL	CB-CA-C	6.26	119.98	111.97
2	D	81	ARG	CA-C-O	-6.25	114.73	121.36
1	J	142	GLY	CA-C-N	6.25	132.96	121.70
1	J	142	GLY	C-N-CA	6.25	132.96	121.70
3	O	145	THR	N-CA-C	6.25	118.10	111.28
4	P	64	ARG	N-CA-C	-6.25	105.24	112.92
3	G	169	ILE	N-CA-C	6.24	122.35	108.88
1	I	226	ILE	N-CA-CB	6.23	119.68	111.40
3	O	182	VAL	CB-CA-C	-6.23	102.87	111.65
1	C	39	ILE	CB-CA-C	-6.22	104.56	111.35
1	I	143	PHE	N-CA-C	6.21	128.38	111.00
1	C	229	PRO	N-CA-CB	6.21	110.96	103.45
3	G	138	ILE	N-CA-C	6.21	121.07	113.00
3	G	167	VAL	CB-CA-C	6.21	119.91	111.97
1	A	70	PRO	N-CA-C	-6.19	104.93	113.53
3	G	172	ILE	O-C-N	6.18	130.30	122.57
3	O	169	ILE	N-CA-C	6.18	122.23	108.88
3	G	159	ARG	O-C-N	6.18	128.70	122.03
1	K	226	ILE	N-CA-CB	6.17	119.61	111.40
1	A	226	ILE	N-CA-CB	6.16	119.59	111.40
1	C	143	PHE	N-CA-C	6.16	128.25	111.00
1	B	354	LEU	N-CA-C	6.16	117.99	111.28
1	J	143	PHE	N-CA-C	6.16	128.24	111.00
3	O	138	ILE	N-CA-C	6.15	121.00	113.00
1	K	143	PHE	N-CA-C	6.15	128.21	111.00
1	B	143	PHE	N-CA-C	6.14	128.20	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ILE	N-CA-CB	6.14	119.56	111.40
3	O	172	ILE	O-C-N	6.13	130.24	122.57
1	A	210	ARG	CA-C-O	-6.13	114.38	120.82
1	I	229	PRO	N-CA-CB	6.13	110.87	103.45
1	I	354	LEU	N-CA-C	6.12	117.95	111.28
1	K	354	LEU	N-CA-C	6.12	117.95	111.28
3	O	203	ALA	CA-C-N	6.11	129.60	120.31
3	O	203	ALA	C-N-CA	6.11	129.60	120.31
1	B	229	PRO	N-CA-CB	6.11	110.84	103.45
3	O	137	LEU	O-C-N	-6.09	114.48	122.59
1	J	229	PRO	N-CA-CB	6.09	110.82	103.45
2	L	81	ARG	N-CA-C	6.08	117.48	108.60
1	C	354	LEU	N-CA-C	6.07	117.90	111.28
1	I	350	TYR	CA-C-N	6.07	124.09	119.66
1	I	350	TYR	C-N-CA	6.07	124.09	119.66
1	C	559	PHE	CA-C-N	6.07	125.75	119.56
1	C	559	PHE	C-N-CA	6.07	125.75	119.56
1	I	559	PHE	CA-C-N	6.07	125.75	119.56
1	I	559	PHE	C-N-CA	6.07	125.75	119.56
1	J	354	LEU	N-CA-C	6.06	117.89	111.28
1	A	143	PHE	N-CA-C	6.06	127.97	111.00
3	O	29	LYS	N-CA-C	-6.05	104.37	110.97
1	K	229	PRO	N-CA-CB	6.05	110.77	103.45
1	B	559	PHE	CA-C-N	6.04	125.72	119.56
1	B	559	PHE	C-N-CA	6.04	125.72	119.56
3	O	164	LEU	CA-C-O	6.04	126.93	120.10
3	G	164	LEU	CA-C-O	6.04	126.92	120.10
1	K	559	PHE	CA-C-N	6.02	125.70	119.56
1	K	559	PHE	C-N-CA	6.02	125.70	119.56
2	F	94	ASN	CA-C-N	6.01	127.71	120.13
2	F	94	ASN	C-N-CA	6.01	127.71	120.13
1	K	210	ARG	CA-C-O	-6.00	114.52	120.82
1	A	354	LEU	N-CA-C	5.99	117.81	111.28
3	G	47	MET	N-CA-CB	-5.99	100.36	110.49
3	G	187	GLU	CA-C-O	-5.99	112.26	119.03
3	O	47	MET	N-CA-CB	-5.97	100.40	110.49
1	A	559	PHE	CA-C-N	5.97	125.65	119.56
1	A	559	PHE	C-N-CA	5.97	125.65	119.56
1	J	199	LEU	N-CA-C	5.95	118.20	110.53
1	J	559	PHE	CA-C-N	5.93	125.61	119.56
1	J	559	PHE	C-N-CA	5.93	125.61	119.56
3	G	27	LEU	N-CA-C	5.92	119.77	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	203	ALA	CA-C-N	5.92	129.31	120.31
3	G	203	ALA	C-N-CA	5.92	129.31	120.31
1	B	210	ARG	CA-C-O	-5.92	114.60	120.82
1	A	229	PRO	N-CA-CB	5.92	110.61	103.45
3	O	47	MET	O-C-N	-5.91	114.72	122.59
3	O	193	ARG	O-C-N	5.90	129.13	122.22
3	G	137	LEU	O-C-N	-5.90	114.74	122.59
1	J	210	ARG	CA-C-O	-5.90	114.63	120.82
3	G	29	LYS	N-CA-C	-5.89	104.55	110.97
2	N	94	ASN	CA-C-N	5.89	127.56	120.13
2	N	94	ASN	C-N-CA	5.89	127.56	120.13
2	E	94	ASN	CA-C-N	5.88	127.54	120.13
2	E	94	ASN	C-N-CA	5.88	127.54	120.13
3	G	47	MET	O-C-N	-5.88	114.78	122.59
3	O	201	ILE	CA-C-O	5.87	127.07	120.85
1	I	210	ARG	CA-C-O	-5.85	114.67	120.82
1	C	210	ARG	CA-C-O	-5.85	114.68	120.82
3	G	201	ILE	CA-C-O	5.85	127.05	120.85
3	O	27	LEU	N-CA-C	5.84	119.67	112.54
1	B	168	VAL	N-CA-CB	-5.82	104.05	110.51
2	M	94	ASN	CA-C-N	5.82	127.46	120.13
2	M	94	ASN	C-N-CA	5.82	127.46	120.13
3	G	7	THR	N-CA-C	5.82	119.56	112.23
2	L	94	ASN	CA-C-N	5.82	127.46	120.13
2	L	94	ASN	C-N-CA	5.82	127.46	120.13
3	O	143	THR	CA-C-O	5.81	127.59	120.56
3	G	193	ARG	O-C-N	5.81	129.01	122.22
1	B	41	ARG	CA-C-O	-5.79	114.17	120.36
2	E	80	ALA	CA-C-N	5.78	131.70	122.10
2	E	80	ALA	C-N-CA	5.78	131.70	122.10
3	G	143	THR	CA-C-O	5.78	127.55	120.56
2	D	94	ASN	CA-C-N	5.78	127.41	120.13
2	D	94	ASN	C-N-CA	5.78	127.41	120.13
1	K	168	VAL	N-CA-CB	-5.77	104.10	110.51
3	G	158	THR	CA-C-N	5.76	128.47	120.63
3	G	158	THR	C-N-CA	5.76	128.47	120.63
1	I	168	VAL	N-CA-CB	-5.75	104.12	110.51
3	O	196	ARG	N-CA-C	5.75	118.76	111.69
3	O	7	THR	N-CA-C	5.75	119.47	112.23
1	A	143	PHE	CA-C-O	5.75	130.57	120.80
1	C	143	PHE	CA-C-O	5.74	130.55	120.80
1	K	143	PHE	CA-C-O	5.71	130.51	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	201	ILE	N-CA-C	5.71	116.48	110.72
2	D	289	THR	CA-C-N	5.70	127.85	120.44
2	D	289	THR	C-N-CA	5.70	127.85	120.44
1	I	41	ARG	CA-C-O	-5.70	114.26	120.36
2	L	289	THR	CA-C-N	5.69	127.84	120.44
2	L	289	THR	C-N-CA	5.69	127.84	120.44
1	A	41	ARG	CA-C-O	-5.69	114.28	120.36
3	G	140	VAL	CA-C-N	5.67	131.90	122.54
3	G	140	VAL	C-N-CA	5.67	131.90	122.54
3	O	7	THR	O-C-N	-5.67	114.73	122.33
3	G	165	GLU	N-CA-C	5.67	122.88	110.80
1	C	41	ARG	CA-C-O	-5.67	114.30	120.36
2	N	289	THR	CA-C-N	5.67	127.81	120.44
2	N	289	THR	C-N-CA	5.67	127.81	120.44
3	O	165	GLU	N-CA-C	5.66	122.86	110.80
3	G	201	ILE	N-CA-C	5.66	116.44	110.72
1	J	143	PHE	CA-C-O	5.66	130.42	120.80
1	B	143	PHE	CA-C-O	5.66	130.42	120.80
1	C	168	VAL	N-CA-CB	-5.66	104.23	110.51
3	G	7	THR	O-C-N	-5.66	114.75	122.33
4	H	76	GLY	O-C-N	-5.65	117.01	123.51
1	A	350	TYR	CA-C-N	5.65	123.78	119.66
1	A	350	TYR	C-N-CA	5.65	123.78	119.66
1	A	168	VAL	N-CA-CB	-5.64	104.25	110.51
1	I	143	PHE	CA-C-O	5.63	130.38	120.80
3	G	39	PHE	N-CA-C	5.63	117.50	111.36
1	K	350	TYR	CA-C-N	5.63	123.77	119.66
1	K	350	TYR	C-N-CA	5.63	123.77	119.66
1	K	41	ARG	CA-C-O	-5.62	114.35	120.36
2	F	289	THR	CA-C-N	5.62	127.74	120.44
2	F	289	THR	C-N-CA	5.62	127.74	120.44
1	J	168	VAL	N-CA-CB	-5.61	104.28	110.51
2	E	289	THR	CA-C-N	5.61	127.73	120.44
2	E	289	THR	C-N-CA	5.61	127.73	120.44
3	G	46	ALA	N-CA-C	-5.60	98.86	110.80
1	C	350	TYR	CA-C-N	5.60	123.75	119.66
1	C	350	TYR	C-N-CA	5.60	123.75	119.66
3	O	140	VAL	CA-C-N	5.60	131.78	122.54
3	O	140	VAL	C-N-CA	5.60	131.78	122.54
3	O	163	ALA	CA-C-O	-5.60	113.53	119.97
2	M	289	THR	CA-C-N	5.59	127.71	120.44
2	M	289	THR	C-N-CA	5.59	127.71	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	163	ALA	CA-C-O	-5.59	113.55	119.97
4	P	38	GLU	N-CA-C	-5.58	105.34	111.82
3	G	182	VAL	CA-C-N	5.58	132.20	121.54
3	G	182	VAL	C-N-CA	5.58	132.20	121.54
1	J	350	TYR	CA-C-N	5.58	123.73	119.66
1	J	350	TYR	C-N-CA	5.58	123.73	119.66
1	J	41	ARG	CA-C-O	-5.57	114.40	120.36
3	O	39	PHE	N-CA-C	5.57	117.43	111.36
3	G	157	THR	N-CA-CB	5.57	119.63	110.39
3	G	196	ARG	N-CA-C	5.55	118.52	111.69
4	H	38	GLU	N-CA-C	-5.55	105.38	111.82
3	O	159	ARG	O-C-N	5.55	128.55	122.11
2	E	80	ALA	CA-C-O	-5.55	115.14	121.68
3	O	171	GLY	N-CA-C	-5.54	100.04	113.18
3	O	182	VAL	CA-C-N	5.54	132.13	121.54
3	O	182	VAL	C-N-CA	5.54	132.13	121.54
3	G	15	ARG	CA-C-O	-5.54	115.20	120.90
3	G	132	ARG	CA-C-N	-5.53	111.75	120.60
3	G	132	ARG	C-N-CA	-5.53	111.75	120.60
1	I	222	GLY	CA-C-N	-5.53	115.30	123.05
1	I	222	GLY	C-N-CA	-5.53	115.30	123.05
1	A	222	GLY	CA-C-N	-5.53	115.31	123.05
1	A	222	GLY	C-N-CA	-5.53	115.31	123.05
3	O	31	LYS	N-CA-C	5.53	122.57	110.80
3	O	202	GLU	O-C-N	5.52	129.82	122.26
1	C	222	GLY	CA-C-N	-5.49	115.36	123.05
1	C	222	GLY	C-N-CA	-5.49	115.36	123.05
3	G	31	LYS	N-CA-C	5.49	122.50	110.80
3	O	46	ALA	N-CA-C	-5.49	99.12	110.80
3	O	157	THR	N-CA-CB	5.48	119.49	110.39
1	B	222	GLY	CA-C-N	-5.48	115.38	123.05
1	B	222	GLY	C-N-CA	-5.48	115.38	123.05
3	G	23	LYS	N-CA-C	-5.47	105.47	111.82
3	O	15	ARG	CA-C-O	-5.46	115.27	120.90
3	G	171	GLY	N-CA-C	-5.46	100.25	113.18
3	G	202	GLU	O-C-N	5.44	129.72	122.26
3	O	23	LYS	N-CA-C	-5.43	105.52	111.82
2	D	356	PRO	N-CA-CB	5.43	108.95	103.25
4	H	77	LEU	CA-C-O	-5.43	111.57	120.80
1	K	222	GLY	CA-C-N	-5.42	115.46	123.05
1	K	222	GLY	C-N-CA	-5.42	115.46	123.05
1	B	350	TYR	CA-C-N	5.42	123.62	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	TYR	C-N-CA	5.42	123.62	119.66
3	G	172	ILE	CB-CA-C	-5.40	102.43	111.29
3	G	178	PHE	O-C-N	5.39	127.83	122.12
1	J	222	GLY	CA-C-N	-5.38	115.52	123.05
1	J	222	GLY	C-N-CA	-5.38	115.52	123.05
1	B	67	THR	N-CA-CB	5.38	118.14	110.67
3	O	30	LYS	O-C-N	5.37	127.82	122.12
3	O	132	ARG	CA-C-N	-5.36	112.03	120.60
3	O	132	ARG	C-N-CA	-5.36	112.03	120.60
3	G	165	GLU	CA-C-O	5.35	128.16	120.51
1	J	294	MET	CA-C-N	5.34	125.28	119.78
1	J	294	MET	C-N-CA	5.34	125.28	119.78
1	K	294	MET	CA-C-N	5.33	125.27	119.78
1	K	294	MET	C-N-CA	5.33	125.27	119.78
1	B	294	MET	CA-C-N	5.33	125.27	119.78
1	B	294	MET	C-N-CA	5.33	125.27	119.78
2	L	419	GLU	CA-C-O	5.30	126.04	120.42
3	O	178	PHE	O-C-N	5.30	127.74	122.12
3	O	172	ILE	CB-CA-C	-5.30	102.60	111.29
1	C	67	THR	N-CA-CB	5.30	118.03	110.67
1	C	294	MET	CA-C-N	5.29	125.23	119.78
1	C	294	MET	C-N-CA	5.29	125.23	119.78
3	G	30	LYS	O-C-N	5.29	127.72	122.12
3	G	43	VAL	CA-C-N	-5.29	112.12	120.63
3	G	43	VAL	C-N-CA	-5.29	112.12	120.63
3	G	194	LEU	CA-C-O	-5.29	114.89	120.55
3	O	165	GLU	CA-C-O	5.28	128.06	120.51
2	E	356	PRO	N-CA-CB	5.27	108.78	103.25
2	L	356	PRO	N-CA-CB	5.26	108.77	103.25
1	I	67	THR	N-CA-CB	5.25	117.96	110.67
4	P	77	LEU	CA-C-O	-5.25	111.88	120.80
2	M	419	GLU	CA-C-O	5.24	125.97	120.42
3	O	203	ALA	CA-C-O	-5.24	113.76	120.31
1	A	294	MET	CA-C-N	5.24	125.17	119.78
1	A	294	MET	C-N-CA	5.24	125.17	119.78
3	G	31	LYS	CB-CA-C	-5.24	100.00	110.42
2	M	356	PRO	N-CA-CB	5.23	108.74	103.25
3	G	144	GLU	CA-C-N	5.22	127.28	120.28
3	G	144	GLU	C-N-CA	5.22	127.28	120.28
1	K	67	THR	N-CA-CB	5.22	117.93	110.67
3	O	31	LYS	CB-CA-C	-5.22	100.03	110.42
1	K	347	GLU	CA-C-O	-5.22	115.27	120.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	67	THR	N-CA-CB	5.21	117.91	110.67
2	F	419	GLU	CA-C-O	5.20	125.94	120.42
2	N	356	PRO	N-CA-CB	5.20	108.71	103.25
3	O	156	LYS	O-C-N	-5.20	116.56	122.23
3	O	194	LEU	CA-C-O	-5.20	114.99	120.55
3	O	136	ALA	O-C-N	5.19	129.50	122.59
1	A	347	GLU	CA-C-O	-5.18	115.31	120.96
2	E	419	GLU	CA-C-O	5.18	125.92	120.42
1	I	294	MET	CA-C-N	5.18	125.12	119.78
1	I	294	MET	C-N-CA	5.18	125.12	119.78
3	G	203	ALA	CA-C-O	-5.18	113.83	120.31
2	M	79	VAL	O-C-N	-5.18	116.10	122.57
1	A	67	THR	N-CA-CB	5.18	117.87	110.67
3	O	189	GLU	CB-CA-C	5.17	119.48	110.79
3	O	25	VAL	CA-C-O	5.17	125.83	120.25
1	C	13	ALA	CA-C-N	-5.16	116.43	122.93
1	C	13	ALA	C-N-CA	-5.16	116.43	122.93
3	G	54	ASP	CA-C-N	-5.16	112.42	121.70
3	G	54	ASP	C-N-CA	-5.16	112.42	121.70
4	H	69	PRO	CA-C-O	-5.15	115.70	121.32
3	G	189	GLU	CB-CA-C	5.15	119.44	110.79
2	D	419	GLU	CA-C-O	5.15	125.88	120.42
2	E	81	ARG	O-C-N	-5.14	117.49	122.99
3	O	54	ASP	CA-C-N	-5.14	112.44	121.70
3	O	54	ASP	C-N-CA	-5.14	112.44	121.70
3	G	174	ALA	N-CA-C	5.14	121.75	110.80
3	O	170	PRO	CA-C-O	5.14	125.25	118.98
1	C	347	GLU	CA-C-O	-5.14	115.36	120.96
3	G	136	ALA	O-C-N	5.13	129.41	122.59
3	O	174	ALA	N-CA-C	5.13	121.72	110.80
1	J	347	GLU	CA-C-O	-5.13	115.37	120.96
4	H	77	LEU	O-C-N	-5.12	114.80	123.00
3	O	49	ALA	CB-CA-C	-5.12	102.81	110.90
3	G	156	LYS	O-C-N	-5.10	116.67	122.23
3	G	26	ASP	O-C-N	5.10	127.53	122.08
3	G	49	ALA	CB-CA-C	-5.09	102.85	110.90
2	F	356	PRO	N-CA-CB	5.09	108.59	103.25
3	O	43	VAL	CA-C-N	-5.09	112.43	120.63
3	O	43	VAL	C-N-CA	-5.09	112.43	120.63
3	O	144	GLU	CA-C-N	5.09	127.10	120.28
3	O	144	GLU	C-N-CA	5.09	127.10	120.28
3	O	23	LYS	CA-C-N	5.07	125.72	119.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	23	LYS	C-N-CA	5.07	125.72	119.99
2	N	419	GLU	CA-C-O	5.06	125.79	120.42
3	O	47	MET	CB-CA-C	-5.06	100.35	110.42
3	G	170	PRO	CA-C-O	5.06	125.16	118.98
3	G	4	VAL	N-CA-C	5.06	119.86	109.34
1	K	429	SER	N-CA-C	-5.05	100.06	108.34
3	O	4	VAL	N-CA-C	5.05	119.84	109.34
3	O	185	GLN	N-CA-C	-5.05	100.05	110.80
3	O	26	ASP	O-C-N	5.04	127.47	122.08
1	I	13	ALA	CA-C-N	-5.03	116.59	122.93
1	I	13	ALA	C-N-CA	-5.03	116.59	122.93
3	G	47	MET	CB-CA-C	-5.03	100.42	110.42
3	G	204	ARG	O-C-N	5.01	128.43	122.27

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	557	GLU	Mainchain
1	A	69	LEU	Peptide
1	B	178	GLY	Peptide
1	B	210	ARG	Mainchain
1	B	297	ALA	Mainchain
1	B	325	ASP	Mainchain
1	B	557	GLU	Mainchain
1	C	178	GLY	Peptide
1	C	210	ARG	Mainchain
1	C	297	ALA	Mainchain
1	C	325	ASP	Mainchain
1	C	557	GLU	Mainchain
2	D	316	MET	Mainchain
2	D	427	GLN	Peptide
2	D	79	VAL	Peptide,Mainchain
2	E	316	MET	Mainchain
2	E	427	GLN	Peptide
2	E	79	VAL	Peptide,Mainchain
2	F	316	MET	Mainchain
2	F	427	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	F	79	VAL	Mainchain
4	H	39	ARG	Peptide
4	H	76	GLY	Peptide
4	H	82	GLN	Peptide
1	I	178	GLY	Peptide
1	I	210	ARG	Mainchain
1	I	297	ALA	Mainchain
1	I	325	ASP	Mainchain
1	I	557	GLU	Mainchain
1	I	69	LEU	Peptide
1	J	178	GLY	Peptide
1	J	210	ARG	Mainchain
1	J	297	ALA	Mainchain
1	J	325	ASP	Mainchain
1	J	429	SER	Mainchain
1	J	557	GLU	Mainchain
1	K	178	GLY	Peptide
1	K	210	ARG	Mainchain
1	K	297	ALA	Mainchain
1	K	325	ASP	Mainchain
1	K	557	GLU	Mainchain
1	K	70	PRO	Mainchain
2	L	316	MET	Mainchain
2	L	427	GLN	Peptide
2	L	79	VAL	Peptide,Mainchain
2	M	316	MET	Mainchain
2	M	427	GLN	Peptide
2	M	79	VAL	Mainchain
2	N	316	MET	Mainchain
2	N	427	GLN	Peptide
2	N	79	VAL	Mainchain
4	P	39	ARG	Peptide
4	P	82	GLN	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	2752	0	1302	96	0
1	B	2752	0	1303	67	0
1	C	2752	0	1303	103	0
1	I	2752	0	1300	125	0
1	J	2752	0	1303	63	2
1	K	2752	0	1302	98	0
2	D	2212	0	1009	67	0
2	E	2212	0	1008	80	0
2	F	2212	0	1009	97	0
2	L	2212	0	1009	83	0
2	M	2212	0	1009	60	2
2	N	2212	0	1009	76	0
3	G	639	0	299	140	0
3	O	639	0	299	145	0
4	H	509	0	255	15	0
4	P	509	0	255	27	0
5	A	27	0	12	2	0
5	C	27	0	12	1	0
5	I	27	0	12	0	0
5	K	27	0	12	5	0
All	All	32188	0	15022	1069	2

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 23.

All (1069) 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)
3:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.65
3:O:189:GLU:CB	3:O:189:GLU:CA	1.76	1.64
3:G:205:GLU:CB	3:G:205:GLU:CA	1.78	1.62
3:G:163:ALA:C	3:G:163:ALA:CA	1.74	1.59
3:O:163:ALA:C	3:O:163:ALA:CA	1.74	1.59
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
3:G:189:GLU:CA	3:G:189:GLU:CB	1.76	1.58
1:C:352:PRO:CB	2:F:269:GLU:CA	1.80	1.58
3:O:205:GLU:CA	3:O:205:GLU:CB	1.78	1.58
1:J:475:ALA:HB1	4:P:100:PHE:CB	1.33	1.57
3:G:52:ALA:CB	3:G:52:ALA:CA	1.75	1.57
1:I:71:LEU:CB	1:I:188:PRO:HA	1.09	1.56
3:G:194:LEU:C	3:G:194:LEU:CA	1.75	1.56
2:E:80:ALA:C	2:E:80:ALA:CA	1.78	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:4:VAL:C	3:O:4:VAL:CA	1.78	1.55
3:G:4:VAL:C	3:G:4:VAL:CA	1.78	1.54
2:E:81:ARG:CA	2:E:81:ARG:N	1.67	1.54
2:E:81:ARG:CA	2:E:81:ARG:C	1.77	1.54
3:O:194:LEU:C	3:O:194:LEU:CA	1.75	1.54
3:G:7:THR:CB	3:G:7:THR:CA	1.86	1.54
3:G:142:ASN:CB	3:G:142:ASN:CA	1.75	1.54
1:K:52:TYR:HA	1:K:295:PRO:CB	1.08	1.54
3:O:31:LYS:N	3:O:31:LYS:CA	1.71	1.53
3:O:167:VAL:C	3:O:167:VAL:CA	1.81	1.53
4:P:75:ALA:C	4:P:75:ALA:CA	1.81	1.53
1:I:24:MET:HA	2:L:66:LEU:CA	1.38	1.53
3:G:167:VAL:C	3:G:167:VAL:CA	1.81	1.51
1:K:52:TYR:CA	1:K:295:PRO:CB	1.85	1.51
2:N:140:VAL:CB	2:N:435:SER:CB	1.84	1.51
3:O:7:THR:CA	3:O:7:THR:CB	1.86	1.51
3:O:27:LEU:CB	3:O:27:LEU:CA	1.87	1.51
3:G:27:LEU:CA	3:G:27:LEU:CB	1.87	1.50
3:G:31:LYS:N	3:G:31:LYS:CA	1.70	1.50
3:O:196:ARG:CA	3:O:196:ARG:C	1.84	1.50
1:I:267:VAL:N	2:N:124:ARG:CB	1.70	1.49
1:C:344:MET:CB	2:F:272:ALA:HB1	1.42	1.49
4:P:75:ALA:CA	4:P:75:ALA:N	1.73	1.47
1:C:352:PRO:CB	2:F:269:GLU:HA	1.00	1.46
3:G:196:ARG:C	3:G:196:ARG:CA	1.84	1.46
1:C:25:TYR:CB	2:F:65:GLY:HA2	1.42	1.46
1:I:25:TYR:N	2:L:66:LEU:H	0.97	1.44
1:B:471:VAL:CB	4:H:98:ILE:CB	1.95	1.43
1:I:24:MET:CA	2:L:66:LEU:HA	1.48	1.42
1:I:266:LEU:C	2:N:124:ARG:CB	1.93	1.41
1:I:25:TYR:H	2:L:66:LEU:N	1.16	1.40
2:E:359:SER:CB	2:E:362:MET:CB	1.99	1.40
1:J:475:ALA:CB	4:P:100:PHE:CB	1.99	1.38
1:I:11:GLY:CA	2:N:50:VAL:H	1.36	1.36
3:G:44:ARG:O	3:G:47:MET:CB	1.71	1.36
4:P:75:ALA:HB3	4:P:85:ASP:CB	1.53	1.35
1:C:11:GLY:HA3	2:E:50:VAL:N	1.38	1.34
3:O:44:ARG:O	3:O:47:MET:CB	1.72	1.34
1:J:9:ILE:CB	2:L:50:VAL:O	1.75	1.34
1:I:71:LEU:CB	1:I:188:PRO:CA	2.05	1.33
1:I:259:GLY:O	2:N:296:GLU:C	1.73	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:CB	2:F:124:ARG:CB	2.08	1.31
1:K:259:GLY:N	2:M:296:GLU:CA	1.83	1.31
1:B:25:TYR:O	2:E:65:GLY:HA2	1.15	1.29
1:K:69:LEU:CB	1:K:72:ALA:HB3	1.61	1.29
1:I:11:GLY:HA3	2:N:50:VAL:C	1.58	1.28
1:C:11:GLY:CA	2:E:50:VAL:H	1.45	1.28
1:C:344:MET:CB	2:F:272:ALA:CB	2.11	1.27
1:C:25:TYR:N	2:F:66:LEU:H	1.33	1.27
1:K:44:GLY:HA2	2:N:69:ALA:CB	1.64	1.27
2:F:427:GLN:CB	1:K:126:GLY:HA3	1.66	1.26
1:I:11:GLY:HA3	2:N:50:VAL:CA	1.63	1.26
1:I:224:ALA:CB	1:I:405:ALA:HB3	1.65	1.25
1:C:224:ALA:CB	1:C:405:ALA:HB3	1.65	1.25
4:H:84:HIS:O	4:H:86:VAL:N	1.67	1.25
1:J:224:ALA:CB	1:J:405:ALA:HB3	1.65	1.25
1:J:419:PHE:O	1:J:496:GLN:HA	1.25	1.25
1:B:224:ALA:CB	1:B:405:ALA:HB3	1.65	1.24
2:N:360:ARG:O	2:N:362:MET:N	1.70	1.24
1:C:25:TYR:H	2:F:66:LEU:N	1.30	1.24
1:A:224:ALA:CB	1:A:405:ALA:HB3	1.65	1.24
1:K:224:ALA:CB	1:K:405:ALA:HB3	1.66	1.23
1:B:25:TYR:O	2:E:65:GLY:CA	1.87	1.22
1:B:419:PHE:O	1:B:496:GLN:HA	1.37	1.22
1:I:11:GLY:CA	2:N:50:VAL:N	2.00	1.22
4:P:74:ILE:O	4:P:75:ALA:HA	1.35	1.21
1:C:44:GLY:HA2	2:F:69:ALA:CB	1.69	1.21
4:P:75:ALA:CB	4:P:85:ASP:CB	2.18	1.20
1:A:11:GLY:CA	2:F:50:VAL:H	1.56	1.19
2:N:61:GLU:O	2:N:227:PRO:CB	1.90	1.18
1:J:263:THR:CB	2:L:125:ARG:C	2.15	1.17
1:A:11:GLY:HA3	2:F:50:VAL:O	1.42	1.17
1:I:259:GLY:C	2:N:296:GLU:C	2.05	1.17
1:I:11:GLY:HA3	2:N:50:VAL:N	1.60	1.16
1:A:11:GLY:HA3	2:F:50:VAL:C	1.72	1.15
1:I:24:MET:C	2:L:66:LEU:H	1.53	1.15
1:I:11:GLY:HA3	2:N:50:VAL:O	1.47	1.15
1:K:44:GLY:HA2	2:N:69:ALA:HB3	1.15	1.15
1:C:208:GLY:HA2	1:C:507:CYS:O	1.46	1.14
1:I:25:TYR:N	2:L:66:LEU:N	1.76	1.13
4:P:84:HIS:O	4:P:86:VAL:N	1.81	1.13
1:A:11:GLY:HA2	2:F:50:VAL:H	1.02	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:266:LEU:CB	2:M:124:ARG:CB	2.26	1.12
1:B:10:ALA:H	2:D:50:VAL:CB	1.62	1.11
1:K:69:LEU:CB	1:K:72:ALA:CB	2.27	1.11
1:J:419:PHE:O	1:J:496:GLN:CA	1.99	1.09
1:I:266:LEU:CB	2:N:124:ARG:CB	2.30	1.09
1:J:24:MET:HA	2:M:67:ASP:O	1.52	1.09
1:K:259:GLY:O	2:M:296:GLU:C	1.96	1.08
2:L:334:GLU:O	2:L:361:LEU:N	1.86	1.08
2:D:149:LYS:O	2:D:334:GLU:N	1.87	1.07
1:A:259:GLY:N	2:F:296:GLU:HA	1.59	1.07
1:C:24:MET:HA	2:F:66:LEU:HA	1.32	1.07
1:K:10:ALA:O	2:M:50:VAL:CB	2.03	1.07
2:F:149:LYS:O	2:F:334:GLU:N	1.87	1.06
3:O:176:ILE:O	3:O:179:ILE:CB	2.03	1.06
3:G:176:ILE:O	3:G:179:ILE:CB	2.03	1.06
2:L:149:LYS:O	2:L:334:GLU:N	1.87	1.06
2:N:149:LYS:O	2:N:334:GLU:N	1.87	1.06
1:C:344:MET:CB	2:F:272:ALA:CA	2.32	1.06
2:E:149:LYS:O	2:E:334:GLU:N	1.87	1.06
1:I:24:MET:CA	2:L:66:LEU:CA	2.18	1.06
1:B:10:ALA:O	2:D:50:VAL:N	1.89	1.06
1:K:52:TYR:CB	1:K:295:PRO:CB	2.34	1.06
1:B:9:ILE:CB	2:D:50:VAL:O	2.04	1.05
2:M:149:LYS:O	2:M:334:GLU:N	1.87	1.05
1:C:208:GLY:O	1:C:507:CYS:CB	2.04	1.04
3:O:7:THR:O	3:O:8:ARG:C	1.98	1.04
2:F:61:GLU:O	2:F:227:PRO:CB	2.06	1.03
1:K:259:GLY:O	2:M:296:GLU:O	1.74	1.03
1:A:259:GLY:N	2:F:296:GLU:CA	2.17	1.03
1:I:11:GLY:HA2	2:N:50:VAL:N	1.67	1.03
2:N:360:ARG:C	2:N:362:MET:H	1.67	1.02
1:C:12:PRO:N	2:E:49:GLU:CB	2.22	1.02
1:C:224:ALA:HB1	1:C:405:ALA:HB3	1.41	1.02
3:G:7:THR:O	3:G:8:ARG:C	1.98	1.02
1:A:224:ALA:HB1	1:A:405:ALA:HB3	1.41	1.01
1:C:52:TYR:CB	1:C:295:PRO:CB	2.38	1.01
1:I:224:ALA:HB1	1:I:405:ALA:HB3	1.41	1.01
1:A:11:GLY:CA	2:F:50:VAL:N	2.22	1.01
1:C:25:TYR:CB	2:F:65:GLY:CA	2.38	1.01
1:A:352:PRO:CB	2:D:272:ALA:HB3	1.90	1.01
1:K:44:GLY:CA	2:N:69:ALA:CB	2.38	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:199:GLY:C	3:G:203:ALA:HB2	1.86	1.01
1:A:11:GLY:HA3	2:F:50:VAL:CA	1.89	1.01
1:I:11:GLY:CA	2:N:50:VAL:O	2.07	1.01
1:K:224:ALA:HB1	1:K:405:ALA:HB3	1.42	1.00
1:K:208:GLY:O	1:K:507:CYS:O	1.79	1.00
3:O:199:GLY:C	3:O:203:ALA:HB2	1.86	0.99
1:C:352:PRO:CB	2:F:269:GLU:CB	2.39	0.99
1:B:224:ALA:HB2	1:B:405:ALA:HB3	1.45	0.99
1:J:224:ALA:HB1	1:J:405:ALA:HB3	1.41	0.99
1:K:259:GLY:N	2:M:296:GLU:HA	1.36	0.99
1:I:24:MET:CA	2:L:66:LEU:N	2.25	0.98
1:A:11:GLY:HA3	2:F:50:VAL:N	1.78	0.98
1:B:11:GLY:HA3	2:D:49:GLU:HA	1.45	0.98
1:I:267:VAL:N	2:N:124:ARG:CA	2.22	0.98
1:C:292:SER:CB	2:E:292:ALA:HB3	1.93	0.98
1:I:25:TYR:O	2:L:65:GLY:HA2	1.62	0.98
1:A:259:GLY:H	2:F:296:GLU:CA	1.75	0.97
1:B:224:ALA:HB1	1:B:405:ALA:HB3	1.42	0.97
2:D:134:GLY:HA2	2:D:430:ARG:O	1.61	0.97
1:C:224:ALA:HB2	1:C:405:ALA:HB3	1.45	0.97
1:K:25:TYR:CB	2:N:65:GLY:HA2	1.94	0.97
3:G:199:GLY:O	3:G:203:ALA:HB2	1.63	0.97
1:I:224:ALA:HB2	1:I:405:ALA:HB3	1.45	0.96
2:L:334:GLU:CB	2:L:361:LEU:CB	2.44	0.96
2:F:149:LYS:O	2:F:333:THR:HA	1.66	0.96
1:A:224:ALA:HB2	1:A:405:ALA:HB3	1.46	0.96
2:F:427:GLN:CB	1:K:126:GLY:CA	2.43	0.96
1:I:259:GLY:O	2:N:296:GLU:O	1.82	0.96
1:J:224:ALA:HB2	1:J:405:ALA:HB3	1.45	0.96
1:K:259:GLY:C	2:M:296:GLU:C	2.33	0.96
3:O:199:GLY:O	3:O:203:ALA:HB2	1.63	0.96
2:L:150:LEU:HA	2:L:335:GLY:O	1.66	0.96
1:I:11:GLY:HA2	2:N:50:VAL:H	0.81	0.96
1:A:11:GLY:CA	2:F:50:VAL:O	2.13	0.95
1:C:259:GLY:H	2:E:296:GLU:N	1.64	0.95
1:B:11:GLY:HA3	2:D:49:GLU:CB	1.96	0.95
1:B:263:THR:CB	2:D:124:ARG:C	2.39	0.95
1:K:224:ALA:HB2	1:K:405:ALA:HB3	1.46	0.95
2:F:150:LEU:HA	2:F:335:GLY:O	1.66	0.95
3:G:148:LYS:O	3:G:152:GLU:CB	2.15	0.95
2:D:150:LEU:HA	2:D:335:GLY:O	1.67	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:150:LEU:HA	2:N:335:GLY:O	1.67	0.94
1:C:259:GLY:N	2:E:296:GLU:N	1.86	0.94
2:N:149:LYS:O	2:N:333:THR:HA	1.66	0.94
3:O:47:MET:O	3:O:49:ALA:N	2.00	0.94
2:M:150:LEU:HA	2:M:335:GLY:O	1.67	0.94
1:K:259:GLY:H	2:M:296:GLU:CA	1.51	0.94
2:L:149:LYS:O	2:L:333:THR:HA	1.66	0.94
2:E:150:LEU:HA	2:E:335:GLY:O	1.66	0.94
1:K:11:GLY:HA3	2:M:50:VAL:H	1.31	0.94
2:D:149:LYS:O	2:D:333:THR:HA	1.66	0.94
1:C:266:LEU:CB	2:E:124:ARG:HA	1.97	0.93
3:O:148:LYS:O	3:O:152:GLU:CB	2.15	0.93
3:G:47:MET:O	3:G:49:ALA:N	2.00	0.93
1:I:70:PRO:CB	1:I:190:ARG:CB	2.46	0.93
2:N:149:LYS:O	2:N:333:THR:CA	2.16	0.93
2:E:149:LYS:O	2:E:333:THR:HA	1.66	0.93
2:L:149:LYS:O	2:L:333:THR:CA	2.17	0.93
1:I:11:GLY:CA	2:N:50:VAL:CA	2.45	0.93
1:C:44:GLY:HA2	2:F:69:ALA:HB1	1.50	0.93
2:D:149:LYS:O	2:D:333:THR:CA	2.16	0.93
2:F:149:LYS:O	2:F:333:THR:CA	2.16	0.93
2:M:149:LYS:O	2:M:333:THR:HA	1.66	0.93
1:I:25:TYR:O	2:L:65:GLY:CA	2.17	0.93
2:E:149:LYS:O	2:E:333:THR:CA	2.17	0.92
1:B:11:GLY:HA3	2:D:49:GLU:CA	1.98	0.92
3:O:48:GLU:O	3:O:51:LYS:CB	2.18	0.92
3:G:48:GLU:O	3:G:51:LYS:CB	2.18	0.92
1:I:267:VAL:H	2:N:124:ARG:CA	1.83	0.92
2:M:149:LYS:O	2:M:333:THR:CA	2.17	0.92
1:I:260:ASN:CB	2:N:298:ALA:O	2.19	0.91
1:C:208:GLY:CA	1:C:507:CYS:O	2.19	0.91
3:G:47:MET:O	3:G:48:GLU:C	2.09	0.91
3:G:174:ALA:O	3:G:175:GLN:C	2.09	0.90
3:G:135:GLU:C	3:G:137:LEU:N	2.17	0.90
3:G:49:ALA:O	3:G:52:ALA:HB3	1.72	0.90
3:O:174:ALA:O	3:O:175:GLN:C	2.09	0.90
1:I:25:TYR:CA	2:L:65:GLY:HA2	2.02	0.90
4:P:75:ALA:C	4:P:75:ALA:HA	1.95	0.89
3:O:141:ALA:O	3:O:145:THR:CB	2.20	0.89
1:I:419:PHE:CB	1:I:497:GLN:O	2.20	0.89
1:B:25:TYR:C	2:E:65:GLY:HA2	1.97	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:263:THR:CB	2:L:125:ARG:CA	2.51	0.89
5:C:600:ADP:O3'	2:E:360:ARG:HA	1.73	0.88
3:O:49:ALA:O	3:O:52:ALA:HB3	1.72	0.88
1:I:25:TYR:CB	2:L:64:THR:O	2.21	0.88
3:G:141:ALA:O	3:G:145:THR:CB	2.21	0.88
3:O:51:LYS:CB	3:O:136:ALA:HB1	2.04	0.88
3:O:135:GLU:C	3:O:137:LEU:N	2.17	0.88
1:K:259:GLY:C	2:M:296:GLU:HA	1.81	0.88
1:J:24:MET:CB	2:M:66:LEU:HA	2.03	0.88
2:F:295:TYR:CB	2:F:332:ILE:CB	2.52	0.87
1:C:11:GLY:HA3	2:E:50:VAL:H	0.86	0.87
2:M:295:TYR:CB	2:M:332:ILE:CB	2.52	0.87
2:N:295:TYR:CB	2:N:332:ILE:CB	2.53	0.87
1:I:419:PHE:N	1:I:496:GLN:HA	1.89	0.87
2:D:295:TYR:CB	2:D:332:ILE:CB	2.53	0.86
2:L:295:TYR:CB	2:L:332:ILE:CB	2.53	0.86
1:I:25:TYR:C	2:L:65:GLY:HA2	1.98	0.86
2:L:153:PHE:O	2:L:339:LEU:N	2.08	0.86
4:P:74:ILE:O	4:P:75:ALA:CA	2.19	0.86
2:L:150:LEU:CA	2:L:335:GLY:O	2.24	0.86
2:F:153:PHE:O	2:F:339:LEU:N	2.09	0.86
1:I:217:PRO:O	1:I:431:PHE:CB	2.24	0.86
1:A:11:GLY:HA2	2:F:50:VAL:N	1.87	0.86
2:M:153:PHE:O	2:M:339:LEU:N	2.09	0.86
1:I:12:PRO:N	2:N:49:GLU:CB	2.38	0.85
1:J:263:THR:CB	2:L:125:ARG:N	2.40	0.85
2:E:295:TYR:CB	2:E:332:ILE:CB	2.53	0.85
2:M:150:LEU:CA	2:M:335:GLY:O	2.24	0.85
2:F:150:LEU:CA	2:F:335:GLY:O	2.24	0.85
2:N:153:PHE:O	2:N:339:LEU:N	2.09	0.85
2:E:150:LEU:CA	2:E:335:GLY:O	2.24	0.85
2:D:150:LEU:CA	2:D:335:GLY:O	2.24	0.85
1:I:267:VAL:CA	2:N:124:ARG:CB	2.50	0.84
3:O:47:MET:O	3:O:48:GLU:C	2.09	0.84
3:O:199:GLY:O	3:O:203:ALA:CB	2.25	0.84
2:D:153:PHE:O	2:D:339:LEU:N	2.09	0.84
2:N:150:LEU:CA	2:N:335:GLY:O	2.24	0.84
1:I:352:PRO:CB	2:L:269:GLU:O	2.26	0.84
1:B:419:PHE:O	1:B:496:GLN:CA	2.23	0.84
2:M:140:VAL:CB	2:M:435:SER:CB	2.56	0.83
1:I:25:TYR:CB	2:L:65:GLY:HA2	2.08	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:GLY:O	2:D:430:ARG:N	2.11	0.83
2:E:153:PHE:O	2:E:339:LEU:N	2.09	0.83
3:O:158:THR:O	3:O:161:VAL:CB	2.27	0.83
1:B:263:THR:CB	2:D:125:ARG:N	2.42	0.83
1:C:352:PRO:CB	2:F:269:GLU:C	2.51	0.83
1:J:475:ALA:HB3	4:P:100:PHE:CB	2.05	0.83
1:C:344:MET:CB	2:F:272:ALA:HA	2.09	0.82
3:G:158:THR:O	3:G:161:VAL:CB	2.27	0.82
1:A:259:GLY:O	2:F:296:GLU:C	2.21	0.82
1:B:10:ALA:N	2:D:50:VAL:CB	2.41	0.82
1:C:18:GLY:O	1:C:19:MET:CB	2.28	0.82
3:G:199:GLY:O	3:G:203:ALA:CB	2.26	0.82
3:O:167:VAL:O	3:O:168:VAL:C	2.19	0.82
1:I:266:LEU:CA	2:N:124:ARG:CB	2.57	0.82
3:O:163:ALA:C	3:O:163:ALA:HA	2.04	0.82
1:A:189:VAL:HA	1:A:308:THR:CB	2.10	0.82
3:O:196:ARG:C	3:O:196:ARG:HA	2.05	0.82
1:I:18:GLY:O	1:I:19:MET:CB	2.27	0.81
1:K:231:GLY:HA2	5:K:600:ADP:H5'1	1.61	0.81
2:E:81:ARG:N	2:E:81:ARG:HA	1.94	0.81
1:C:292:SER:CB	2:E:292:ALA:CB	2.59	0.80
1:K:18:GLY:O	1:K:19:MET:CB	2.27	0.80
1:A:43:ASP:C	2:D:69:ALA:CB	2.54	0.80
1:A:259:GLY:O	2:F:296:GLU:O	1.99	0.80
3:G:167:VAL:O	3:G:168:VAL:C	2.19	0.80
2:L:134:GLY:HA2	2:L:430:ARG:O	1.81	0.80
3:O:167:VAL:O	3:O:169:ILE:N	2.14	0.80
1:J:18:GLY:O	1:J:19:MET:CB	2.28	0.80
1:K:44:GLY:HA2	2:N:69:ALA:HB2	1.62	0.80
1:J:224:ALA:HB1	1:J:405:ALA:CB	2.12	0.80
1:K:44:GLY:CA	2:N:69:ALA:HB2	2.12	0.80
1:B:18:GLY:O	1:B:19:MET:CB	2.28	0.79
3:G:167:VAL:O	3:G:169:ILE:N	2.14	0.79
2:N:134:GLY:O	2:N:429:ASN:HA	1.82	0.79
3:O:194:LEU:C	3:O:194:LEU:HA	2.03	0.79
1:A:224:ALA:HB1	1:A:405:ALA:CB	2.12	0.79
1:C:224:ALA:HB1	1:C:405:ALA:CB	2.12	0.79
1:B:224:ALA:HB1	1:B:405:ALA:CB	2.12	0.79
3:G:132:ARG:N	3:G:134:ALA:HB3	1.98	0.79
3:G:132:ARG:C	3:G:134:ALA:N	2.37	0.79
1:I:267:VAL:H	2:N:124:ARG:CB	1.90	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:199:GLY:C	3:G:203:ALA:CB	2.56	0.79
1:I:71:LEU:CB	1:I:72:ALA:HA	2.12	0.79
1:K:52:TYR:C	1:K:295:PRO:CB	2.56	0.79
1:K:259:GLY:C	2:M:296:GLU:CA	2.38	0.79
1:I:224:ALA:HB1	1:I:405:ALA:CB	2.12	0.79
1:K:224:ALA:HB1	1:K:405:ALA:CB	2.13	0.79
3:O:199:GLY:C	3:O:203:ALA:CB	2.56	0.79
1:C:52:TYR:HA	1:C:295:PRO:CB	2.13	0.78
3:G:194:LEU:C	3:G:194:LEU:HA	2.04	0.78
3:O:132:ARG:C	3:O:134:ALA:N	2.37	0.78
3:G:4:VAL:C	3:G:4:VAL:HA	2.07	0.78
3:O:132:ARG:N	3:O:134:ALA:HB3	1.98	0.78
1:A:44:GLY:HA2	2:D:69:ALA:CB	2.13	0.78
3:G:45:GLU:O	3:G:46:ALA:C	2.27	0.78
1:A:18:GLY:O	1:A:19:MET:CB	2.28	0.78
3:O:45:GLU:O	3:O:46:ALA:C	2.27	0.78
1:A:12:PRO:N	2:F:49:GLU:CB	2.47	0.77
3:G:28:LEU:O	3:G:31:LYS:CB	2.32	0.77
3:G:196:ARG:C	3:G:196:ARG:HA	2.05	0.77
1:A:81:ASN:HA	1:A:282:MET:O	1.84	0.77
3:O:28:LEU:O	3:O:31:LYS:CB	2.32	0.77
2:F:51:SER:O	2:F:52:GLU:CB	2.33	0.77
1:C:224:ALA:CB	1:C:405:ALA:CB	2.58	0.76
2:M:51:SER:O	2:M:52:GLU:CB	2.33	0.76
2:L:51:SER:O	2:L:52:GLU:CB	2.33	0.76
3:O:135:GLU:O	3:O:136:ALA:C	2.28	0.76
2:D:51:SER:O	2:D:52:GLU:CB	2.33	0.76
1:K:11:GLY:HA3	2:M:50:VAL:N	2.00	0.76
3:G:135:GLU:O	3:G:136:ALA:C	2.28	0.76
1:B:10:ALA:C	2:D:50:VAL:H	1.94	0.75
2:E:80:ALA:C	2:E:80:ALA:HA	2.06	0.75
3:G:39:PHE:O	3:G:42:LEU:CB	2.34	0.75
2:N:51:SER:O	2:N:52:GLU:CB	2.33	0.75
1:C:52:TYR:CA	1:C:295:PRO:CB	2.65	0.75
3:O:39:PHE:O	3:O:42:LEU:CB	2.34	0.75
1:I:224:ALA:CB	1:I:405:ALA:CB	2.58	0.75
1:I:259:GLY:O	2:N:297:ARG:N	2.18	0.75
2:E:149:LYS:CB	2:E:332:ILE:O	2.35	0.75
1:I:24:MET:CB	2:L:66:LEU:N	2.49	0.75
4:P:65:GLY:CA	4:P:66:ARG:CB	2.65	0.75
2:E:51:SER:O	2:E:52:GLU:CB	2.33	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:LYS:CB	2:F:332:ILE:O	2.35	0.75
3:G:163:ALA:C	3:G:163:ALA:HA	2.04	0.75
2:L:149:LYS:CB	2:L:332:ILE:O	2.35	0.75
1:B:224:ALA:CB	1:B:405:ALA:CB	2.58	0.74
2:L:359:SER:C	2:L:361:LEU:N	2.39	0.74
1:C:56:SER:CB	2:E:30:GLY:O	2.35	0.74
1:J:419:PHE:O	1:J:496:GLN:CB	2.35	0.74
3:O:140:VAL:O	3:O:144:GLU:CB	2.35	0.74
1:J:263:THR:CB	2:L:125:ARG:O	2.35	0.74
2:E:81:ARG:C	2:E:81:ARG:HA	2.05	0.74
1:I:24:MET:CB	2:L:66:LEU:CA	2.65	0.74
4:P:75:ALA:C	4:P:75:ALA:CB	2.60	0.74
2:M:149:LYS:CB	2:M:332:ILE:O	2.35	0.74
3:G:140:VAL:O	3:G:144:GLU:CB	2.35	0.74
1:K:69:LEU:CB	1:K:72:ALA:HB2	2.19	0.73
2:N:69:ALA:O	2:N:70:THR:CB	2.36	0.73
1:B:25:TYR:N	2:E:66:LEU:H	1.86	0.73
3:G:142:ASN:O	3:G:146:ARG:CB	2.36	0.73
3:O:48:GLU:C	3:O:51:LYS:H	1.97	0.73
3:O:142:ASN:O	3:O:146:ARG:CB	2.36	0.73
1:C:11:GLY:HA2	2:E:49:GLU:HA	1.70	0.73
1:I:52:TYR:CB	1:I:297:ALA:HB3	2.19	0.73
2:N:149:LYS:CB	2:N:332:ILE:O	2.35	0.73
4:P:75:ALA:HB2	4:P:85:ASP:CB	2.19	0.73
1:A:259:GLY:C	2:F:296:GLU:HA	2.10	0.73
2:D:149:LYS:CB	2:D:332:ILE:O	2.35	0.73
1:I:56:SER:CB	2:N:30:GLY:N	2.52	0.73
2:F:69:ALA:O	2:F:70:THR:CB	2.37	0.73
2:L:69:ALA:O	2:L:70:THR:CB	2.36	0.73
1:C:44:GLY:CA	2:F:69:ALA:CB	2.61	0.73
1:J:419:PHE:C	1:J:496:GLN:HA	2.13	0.73
1:C:11:GLY:CA	2:E:50:VAL:N	2.21	0.72
1:C:259:GLY:O	2:E:296:GLU:C	2.32	0.72
1:A:224:ALA:CB	1:A:405:ALA:CB	2.58	0.72
2:E:69:ALA:O	2:E:70:THR:CB	2.37	0.72
3:G:48:GLU:C	3:G:51:LYS:H	1.97	0.72
3:G:150:ILE:O	3:G:151:GLY:O	2.08	0.72
3:O:150:ILE:O	3:O:151:GLY:O	2.07	0.72
1:I:11:GLY:CA	2:N:50:VAL:CB	2.65	0.72
1:I:25:TYR:H	2:L:65:GLY:C	1.96	0.72
3:O:4:VAL:C	3:O:4:VAL:HA	2.07	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLY:HA2	1:B:302:SER:CB	2.19	0.72
1:C:344:MET:CA	2:F:272:ALA:HB1	2.18	0.72
1:C:267:VAL:O	2:E:125:ARG:HA	1.84	0.72
2:F:359:SER:CB	2:F:362:MET:CB	2.67	0.72
2:D:69:ALA:O	2:D:70:THR:CB	2.36	0.72
2:M:69:ALA:O	2:M:70:THR:CB	2.37	0.72
2:N:65:GLY:O	2:N:66:LEU:CB	2.38	0.71
1:B:24:MET:C	2:E:66:LEU:H	1.96	0.71
1:B:9:ILE:HA	2:D:50:VAL:CB	2.21	0.71
1:K:259:GLY:H	2:M:296:GLU:CB	2.02	0.71
4:P:74:ILE:C	4:P:75:ALA:CA	2.62	0.71
1:C:260:ASN:CB	2:E:298:ALA:HB3	2.21	0.71
4:H:77:LEU:H	4:H:80:ALA:HB3	1.55	0.71
1:I:204:PRO:CB	1:I:435:LEU:CB	2.68	0.71
2:F:65:GLY:O	2:F:66:LEU:CB	2.39	0.70
1:B:11:GLY:CA	2:D:49:GLU:HA	2.20	0.70
2:E:65:GLY:O	2:E:66:LEU:CB	2.38	0.70
1:I:259:GLY:C	2:N:296:GLU:O	2.31	0.70
1:I:225:ALA:N	1:I:405:ALA:O	2.25	0.70
1:K:44:GLY:CA	2:N:69:ALA:HB3	2.07	0.70
1:C:266:LEU:C	2:E:124:ARG:CB	2.64	0.70
1:C:419:PHE:C	1:C:497:GLN:H	1.97	0.70
1:I:56:SER:CB	2:N:30:GLY:O	2.40	0.70
2:L:274:ARG:O	2:L:275:GLU:CB	2.37	0.70
2:M:65:GLY:O	2:M:66:LEU:CB	2.38	0.70
1:A:225:ALA:N	1:A:405:ALA:O	2.25	0.70
2:M:149:LYS:O	2:M:333:THR:C	2.35	0.70
2:N:61:GLU:HA	2:N:229:ILE:CB	2.22	0.70
1:A:71:LEU:CB	1:A:188:PRO:HA	2.22	0.70
2:F:274:ARG:O	2:F:275:GLU:CB	2.37	0.70
1:A:44:GLY:N	2:D:69:ALA:CB	2.54	0.69
1:K:225:ALA:N	1:K:405:ALA:O	2.25	0.69
2:N:274:ARG:O	2:N:275:GLU:CB	2.37	0.69
2:D:65:GLY:O	2:D:66:LEU:CB	2.38	0.69
2:E:149:LYS:O	2:E:333:THR:C	2.35	0.69
2:N:149:LYS:O	2:N:333:THR:C	2.35	0.69
2:F:149:LYS:O	2:F:333:THR:C	2.35	0.69
1:J:225:ALA:N	1:J:405:ALA:O	2.25	0.69
1:A:44:GLY:HA2	2:D:69:ALA:HB1	1.74	0.69
1:C:11:GLY:HA3	2:E:49:GLU:C	2.15	0.69
1:C:225:ALA:N	1:C:405:ALA:O	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:149:LYS:O	2:L:333:THR:C	2.35	0.69
1:A:43:ASP:C	2:D:69:ALA:HB2	2.18	0.69
2:F:427:GLN:O	1:K:126:GLY:N	2.25	0.69
1:I:11:GLY:HA3	2:N:50:VAL:CB	2.23	0.69
1:B:225:ALA:N	1:B:405:ALA:O	2.25	0.69
1:J:24:MET:CB	2:M:66:LEU:CA	2.69	0.69
3:O:156:LYS:C	3:O:158:THR:N	2.44	0.69
2:E:140:VAL:CB	2:E:435:SER:CB	2.71	0.69
1:I:25:TYR:O	2:L:65:GLY:HA3	1.93	0.69
2:L:65:GLY:O	2:L:66:LEU:CB	2.39	0.69
2:M:274:ARG:O	2:M:275:GLU:CB	2.38	0.69
3:O:156:LYS:O	3:O:157:THR:C	2.33	0.69
1:A:71:LEU:HA	1:A:188:PRO:HA	1.75	0.68
3:O:31:LYS:N	3:O:31:LYS:HA	2.02	0.68
3:O:197:ILE:O	3:O:200:LYS:CB	2.41	0.68
2:D:149:LYS:O	2:D:333:THR:C	2.35	0.68
3:G:156:LYS:C	3:G:158:THR:N	2.44	0.68
4:H:84:HIS:O	4:H:85:ASP:C	2.34	0.68
1:J:224:ALA:CB	1:J:405:ALA:CB	2.58	0.68
1:A:5:VAL:CB	1:A:18:GLY:O	2.42	0.68
3:G:197:ILE:O	3:G:200:LYS:CB	2.40	0.68
1:A:352:PRO:CB	2:D:272:ALA:CB	2.70	0.68
1:J:5:VAL:CB	1:J:18:GLY:O	2.42	0.68
3:G:151:GLY:O	3:G:152:GLU:C	2.36	0.68
1:I:5:VAL:CB	1:I:18:GLY:O	2.42	0.68
1:K:5:VAL:CB	1:K:18:GLY:O	2.42	0.68
1:J:10:ALA:O	2:L:49:GLU:HA	1.93	0.68
3:O:151:GLY:O	3:O:152:GLU:C	2.36	0.68
1:K:224:ALA:CB	1:K:405:ALA:CB	2.58	0.68
1:C:44:GLY:HA2	2:F:69:ALA:HB3	1.70	0.68
1:K:259:GLY:C	2:M:296:GLU:O	2.35	0.68
1:K:189:VAL:O	1:K:304:TYR:CB	2.42	0.67
1:A:11:GLY:CA	2:F:50:VAL:CA	2.68	0.67
2:E:81:ARG:C	2:E:81:ARG:CB	2.67	0.67
2:E:274:ARG:O	2:E:275:GLU:CB	2.37	0.67
1:C:5:VAL:CB	1:C:18:GLY:O	2.42	0.67
3:G:156:LYS:O	3:G:157:THR:C	2.33	0.67
1:A:259:GLY:C	2:F:296:GLU:C	2.63	0.67
1:B:5:VAL:CB	1:B:18:GLY:O	2.42	0.67
1:A:196:GLN:N	1:A:369:ILE:O	2.28	0.67
1:I:419:PHE:H	1:I:496:GLN:HA	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:MET:CA	2:F:66:LEU:HA	2.18	0.67
3:G:31:LYS:N	3:G:31:LYS:HA	2.02	0.67
3:G:151:GLY:HA2	3:G:155:LYS:CB	2.25	0.67
1:C:44:GLY:HA2	2:F:69:ALA:HB2	1.74	0.66
3:O:41:GLY:O	3:O:42:LEU:C	2.38	0.66
2:D:274:ARG:O	2:D:275:GLU:CB	2.38	0.66
3:G:3:GLN:O	3:G:5:SER:N	2.29	0.66
3:G:41:GLY:O	3:G:42:LEU:C	2.38	0.66
3:O:135:GLU:C	3:O:137:LEU:H	2.03	0.66
3:O:151:GLY:HA2	3:O:155:LYS:CB	2.26	0.66
3:O:141:ALA:HA	3:O:144:GLU:CB	2.26	0.66
1:A:44:GLY:CA	2:D:69:ALA:HB1	2.25	0.66
1:K:27:ILE:HA	1:K:71:LEU:H	1.61	0.66
3:G:135:GLU:C	3:G:137:LEU:H	2.03	0.66
1:K:429:SER:C	1:K:431:PHE:H	2.03	0.66
3:O:3:GLN:O	3:O:5:SER:N	2.29	0.66
2:M:61:GLU:O	2:M:227:PRO:CB	2.44	0.66
1:A:44:GLY:CA	2:D:69:ALA:CB	2.74	0.66
3:G:141:ALA:HA	3:G:144:GLU:CB	2.26	0.65
4:H:65:GLY:HA2	4:H:66:ARG:CB	2.26	0.65
1:A:44:GLY:HA2	2:D:69:ALA:HB3	1.78	0.65
2:L:334:GLU:O	2:L:361:LEU:CB	2.45	0.65
3:O:158:THR:C	3:O:161:VAL:CB	2.70	0.65
1:K:56:SER:CB	2:M:30:GLY:O	2.44	0.65
3:G:158:THR:C	3:G:161:VAL:CB	2.70	0.65
2:L:334:GLU:CA	2:L:361:LEU:CB	2.75	0.65
1:I:260:ASN:N	2:N:296:GLU:HA	1.99	0.65
4:P:65:GLY:HA2	4:P:66:ARG:CB	2.27	0.65
1:J:24:MET:CA	2:M:67:ASP:O	2.38	0.64
3:O:172:ILE:O	3:O:176:ILE:CB	2.45	0.64
3:G:141:ALA:HA	3:G:145:THR:H	1.62	0.64
3:O:150:ILE:C	3:O:151:GLY:O	2.39	0.64
1:A:260:ASN:CB	2:F:298:ALA:O	2.45	0.64
1:A:419:PHE:C	1:A:497:GLN:O	2.41	0.64
2:E:81:ARG:N	2:E:81:ARG:CB	2.60	0.64
1:B:9:ILE:CB	2:D:50:VAL:C	2.70	0.64
3:G:172:ILE:O	3:G:176:ILE:CB	2.45	0.64
3:O:141:ALA:HA	3:O:145:THR:H	1.62	0.63
1:K:11:GLY:CA	2:M:49:GLU:HA	2.28	0.63
3:G:150:ILE:C	3:G:151:GLY:O	2.39	0.63
1:C:11:GLY:CA	2:E:49:GLU:CA	2.77	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:CA	1:A:282:MET:O	2.47	0.63
3:G:18:LEU:O	3:G:21:ALA:HB3	1.99	0.63
2:N:76:VAL:O	2:N:77:GLU:CB	2.47	0.63
3:O:156:LYS:HA	3:O:159:ARG:H	1.64	0.63
1:C:25:TYR:CA	2:F:65:GLY:HA2	2.27	0.62
1:C:266:LEU:C	2:E:124:ARG:CA	2.68	0.62
2:E:76:VAL:O	2:E:77:GLU:CB	2.47	0.62
2:F:76:VAL:O	2:F:77:GLU:CB	2.47	0.62
2:L:76:VAL:O	2:L:77:GLU:CB	2.47	0.62
3:O:148:LYS:O	3:O:149:LYS:O	2.17	0.62
3:G:156:LYS:HA	3:G:159:ARG:H	1.64	0.62
1:K:25:TYR:CB	2:N:65:GLY:CA	2.75	0.62
3:O:18:LEU:O	3:O:21:ALA:HB3	1.99	0.62
3:G:47:MET:C	3:G:49:ALA:N	2.57	0.62
2:E:80:ALA:C	2:E:80:ALA:CB	2.70	0.62
2:D:334:GLU:O	2:D:361:LEU:N	2.31	0.62
3:G:47:MET:C	3:G:49:ALA:H	2.08	0.62
1:I:208:GLY:O	1:I:507:CYS:O	2.18	0.62
2:D:134:GLY:CA	2:D:430:ARG:O	2.42	0.62
2:D:359:SER:C	2:D:361:LEU:N	2.49	0.61
2:D:76:VAL:O	2:D:77:GLU:CB	2.47	0.61
3:G:148:LYS:O	3:G:149:LYS:O	2.17	0.61
4:P:75:ALA:N	4:P:75:ALA:CB	2.56	0.61
3:O:132:ARG:O	3:O:133:TYR:C	2.38	0.61
1:A:266:LEU:CB	2:F:124:ARG:CA	2.78	0.61
1:B:25:TYR:N	2:E:66:LEU:N	2.48	0.61
1:I:419:PHE:HA	1:I:420:PRO:C	2.25	0.61
2:M:76:VAL:O	2:M:77:GLU:CB	2.47	0.61
3:O:44:ARG:C	3:O:47:MET:CB	2.72	0.61
3:O:47:MET:C	3:O:49:ALA:H	2.09	0.61
2:L:134:GLY:O	2:L:430:ARG:N	2.34	0.61
3:O:47:MET:C	3:O:49:ALA:N	2.57	0.61
3:O:170:PRO:O	3:O:174:ALA:HB2	2.00	0.61
2:F:61:GLU:HA	2:F:229:ILE:CB	2.31	0.61
1:C:344:MET:CB	2:F:272:ALA:C	2.73	0.61
1:C:359:ALA:HB3	2:F:224:ALA:HB1	1.83	0.60
1:C:419:PHE:HA	1:C:420:PRO:C	2.25	0.60
2:E:349:TYR:O	2:E:424:ASN:HA	2.01	0.60
3:G:170:PRO:O	3:G:174:ALA:HB2	2.00	0.60
1:B:419:PHE:HA	1:B:420:PRO:C	2.25	0.60
3:G:135:GLU:O	3:G:137:LEU:N	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:HA	1:A:420:PRO:C	2.25	0.60
3:O:45:GLU:C	3:O:47:MET:N	2.58	0.60
1:I:12:PRO:O	1:I:13:ALA:HB3	2.01	0.60
1:K:419:PHE:HA	1:K:420:PRO:C	2.25	0.60
1:C:12:PRO:O	1:C:13:ALA:HB3	2.02	0.60
1:A:199:LEU:O	1:A:200:ASP:C	2.45	0.60
3:G:44:ARG:C	3:G:47:MET:CB	2.72	0.60
1:A:12:PRO:O	1:A:13:ALA:HB3	2.02	0.60
1:C:259:GLY:O	2:E:297:ARG:N	2.35	0.60
3:G:160:ARG:O	3:G:164:LEU:CB	2.50	0.60
1:J:12:PRO:O	1:J:13:ALA:HB3	2.02	0.60
1:J:419:PHE:HA	1:J:420:PRO:C	2.25	0.60
1:K:12:PRO:O	1:K:13:ALA:HB3	2.02	0.59
1:A:259:GLY:C	2:F:296:GLU:CA	2.69	0.59
3:G:132:ARG:O	3:G:133:TYR:C	2.37	0.59
3:G:135:GLU:HA	3:G:138:ILE:N	2.16	0.59
1:C:266:LEU:CB	2:E:124:ARG:CA	2.78	0.59
1:J:9:ILE:CA	2:L:50:VAL:O	2.48	0.59
1:B:12:PRO:O	1:B:13:ALA:HB3	2.01	0.59
1:C:11:GLY:C	2:E:49:GLU:CB	2.75	0.59
3:O:135:GLU:HA	3:O:138:ILE:N	2.17	0.59
4:H:77:LEU:N	4:H:80:ALA:HB3	2.18	0.59
3:O:160:ARG:O	3:O:164:LEU:CB	2.50	0.59
2:F:427:GLN:O	1:K:126:GLY:CA	2.50	0.59
1:I:429:SER:CB	1:I:431:PHE:H	2.16	0.59
3:O:135:GLU:O	3:O:137:LEU:N	2.33	0.59
1:I:25:TYR:N	2:L:65:GLY:HA2	2.18	0.58
2:L:359:SER:C	2:L:361:LEU:H	2.07	0.58
4:H:84:HIS:C	4:H:86:VAL:N	2.53	0.58
3:G:167:VAL:C	3:G:169:ILE:N	2.61	0.58
1:A:43:ASP:O	2:D:69:ALA:HB3	2.04	0.58
1:I:189:VAL:HA	1:I:308:THR:CB	2.34	0.58
2:L:134:GLY:CA	2:L:430:ARG:O	2.51	0.58
1:A:56:SER:CB	2:F:30:GLY:N	2.67	0.58
1:C:11:GLY:CA	2:E:49:GLU:HA	2.34	0.57
3:O:186:ARG:O	3:O:190:ASP:CB	2.53	0.57
2:D:134:GLY:HA2	2:D:430:ARG:C	2.30	0.57
1:K:241:LEU:O	1:K:245:SER:N	2.31	0.57
2:E:134:GLY:O	2:E:429:ASN:HA	2.04	0.57
1:K:260:ASN:CB	2:M:298:ALA:O	2.52	0.57
3:O:167:VAL:C	3:O:167:VAL:HA	2.16	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:N	1:A:282:MET:O	2.36	0.57
3:G:165:GLU:O	3:G:166:GLN:C	2.47	0.57
3:G:45:GLU:C	3:G:47:MET:N	2.58	0.57
4:P:74:ILE:C	4:P:75:ALA:HA	2.16	0.57
3:O:167:VAL:C	3:O:169:ILE:N	2.61	0.56
2:D:359:SER:C	2:D:362:MET:H	2.13	0.56
3:G:186:ARG:O	3:G:190:ASP:CB	2.53	0.56
1:J:23:ARG:O	2:M:68:LEU:HA	2.05	0.56
1:K:11:GLY:HA3	2:M:49:GLU:CA	2.35	0.56
3:O:48:GLU:O	3:O:51:LYS:N	2.38	0.56
1:A:241:LEU:O	1:A:245:SER:N	2.31	0.56
1:C:241:LEU:O	1:C:245:SER:N	2.31	0.56
3:G:189:GLU:CB	3:G:189:GLU:HA	2.18	0.56
1:J:263:THR:CB	2:L:124:ARG:C	2.78	0.56
4:P:62:LEU:O	4:P:63:MET:CB	2.46	0.56
1:I:132:GLY:HA3	1:I:371:LEU:C	2.30	0.56
1:K:419:PHE:CB	1:K:497:GLN:O	2.54	0.56
3:G:137:LEU:O	3:G:140:VAL:CB	2.54	0.56
1:I:24:MET:CB	2:L:66:LEU:HA	2.29	0.56
3:O:165:GLU:O	3:O:166:GLN:C	2.47	0.56
3:G:132:ARG:N	3:G:134:ALA:CB	2.68	0.56
1:J:241:LEU:O	1:J:245:SER:N	2.32	0.56
1:C:352:PRO:CB	2:F:269:GLU:O	2.54	0.56
1:I:241:LEU:O	1:I:245:SER:N	2.31	0.56
3:G:52:ALA:CB	3:G:52:ALA:C	2.74	0.55
3:O:138:ILE:C	3:O:139:ARG:O	2.45	0.55
3:O:158:THR:HA	3:O:161:VAL:CB	2.37	0.55
3:O:52:ALA:CB	3:O:52:ALA:C	2.74	0.55
3:O:137:LEU:O	3:O:140:VAL:CB	2.54	0.55
3:O:142:ASN:CB	3:O:142:ASN:HA	2.16	0.55
2:D:334:GLU:CB	2:D:361:LEU:CB	2.84	0.55
3:G:48:GLU:O	3:G:51:LYS:N	2.39	0.55
3:G:138:ILE:C	3:G:139:ARG:O	2.45	0.55
3:G:194:LEU:C	3:G:194:LEU:CB	2.73	0.55
3:O:55:GLN:CB	3:O:133:TYR:CB	2.85	0.55
1:A:199:LEU:O	1:A:200:ASP:O	2.24	0.55
3:G:142:ASN:CB	3:G:142:ASN:HA	2.17	0.55
1:I:71:LEU:HA	1:I:189:VAL:H	1.72	0.55
1:K:429:SER:C	1:K:431:PHE:N	2.60	0.55
3:O:136:ALA:O	3:O:140:VAL:CB	2.55	0.55
1:I:71:LEU:CB	1:I:72:ALA:CA	2.83	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:334:GLU:O	2:L:361:LEU:CA	2.54	0.54
1:C:260:ASN:N	2:E:296:GLU:HA	2.22	0.54
3:G:146:ARG:O	3:G:147:LEU:C	2.50	0.54
3:O:137:LEU:O	3:O:140:VAL:N	2.40	0.54
1:B:241:LEU:O	1:B:245:SER:N	2.31	0.54
3:G:158:THR:HA	3:G:161:VAL:CB	2.37	0.54
1:A:11:GLY:CA	2:F:50:VAL:CB	2.85	0.54
3:G:132:ARG:C	3:G:134:ALA:H	2.13	0.54
2:E:334:GLU:O	2:E:360:ARG:N	2.39	0.54
3:G:137:LEU:O	3:G:140:VAL:N	2.40	0.54
1:A:557:GLU:C	1:A:559:PHE:N	2.66	0.54
3:G:136:ALA:O	3:G:140:VAL:CB	2.55	0.54
1:J:557:GLU:C	1:J:559:PHE:N	2.66	0.54
1:C:259:GLY:H	2:E:296:GLU:H	1.51	0.54
1:I:225:ALA:O	1:I:406:PHE:HA	2.07	0.54
1:I:404:GLY:O	1:I:430:LEU:CB	2.56	0.54
1:K:225:ALA:O	1:K:406:PHE:HA	2.07	0.54
3:G:43:VAL:O	3:G:44:ARG:C	2.51	0.54
1:J:429:SER:C	1:J:431:PHE:H	2.17	0.54
3:O:7:THR:O	3:O:9:MET:N	2.41	0.54
3:O:132:ARG:N	3:O:134:ALA:CB	2.68	0.54
3:O:146:ARG:O	3:O:147:LEU:C	2.50	0.54
1:A:225:ALA:O	1:A:406:PHE:HA	2.08	0.53
2:E:153:PHE:CB	2:E:338:GLN:HA	2.38	0.53
1:J:296:VAL:HA	1:J:333:ALA:HB1	1.90	0.53
1:B:224:ALA:CA	1:B:405:ALA:HB3	2.37	0.53
1:B:225:ALA:O	1:B:406:PHE:HA	2.07	0.53
1:C:225:ALA:O	1:C:406:PHE:HA	2.08	0.53
1:K:11:GLY:CA	2:M:50:VAL:H	2.14	0.53
1:K:224:ALA:CA	1:K:405:ALA:HB3	2.37	0.53
3:O:132:ARG:C	3:O:134:ALA:H	2.13	0.53
1:A:81:ASN:HA	1:A:282:MET:C	2.33	0.53
1:A:296:VAL:HA	1:A:333:ALA:HB1	1.90	0.53
3:G:138:ILE:O	3:G:139:ARG:O	2.27	0.53
1:K:11:GLY:HA2	2:M:49:GLU:HA	1.89	0.53
1:J:227:PRO:HA	1:J:384:VAL:CB	2.39	0.53
1:A:233:GLY:HA2	5:A:600:ADP:O1A	2.09	0.53
1:B:296:VAL:HA	1:B:333:ALA:HB1	1.90	0.53
1:B:557:GLU:C	1:B:559:PHE:N	2.66	0.53
2:L:153:PHE:CB	2:L:338:GLN:HA	2.39	0.53
3:O:145:THR:O	3:O:149:LYS:CB	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HA	1:A:384:VAL:CB	2.39	0.53
1:C:25:TYR:N	2:F:66:LEU:N	2.14	0.53
1:I:557:GLU:C	1:I:559:PHE:N	2.66	0.53
2:M:153:PHE:CB	2:M:338:GLN:HA	2.39	0.53
3:O:198:LYS:O	3:O:199:GLY:C	2.52	0.53
1:I:352:PRO:CB	2:L:272:ALA:HB3	2.39	0.53
3:O:42:LEU:O	3:O:45:GLU:CB	2.57	0.53
1:B:86:GLY:O	1:B:302:SER:HA	2.09	0.53
1:C:557:GLU:C	1:C:559:PHE:N	2.66	0.53
2:D:153:PHE:CB	2:D:338:GLN:HA	2.39	0.53
3:G:166:GLN:O	3:G:169:ILE:CB	2.57	0.53
1:C:296:VAL:HA	1:C:333:ALA:HB1	1.90	0.53
1:C:352:PRO:C	2:F:269:GLU:CB	2.81	0.53
1:I:227:PRO:HA	1:I:384:VAL:CB	2.39	0.53
1:K:557:GLU:C	1:K:559:PHE:N	2.66	0.53
2:N:153:PHE:CB	2:N:338:GLN:HA	2.39	0.53
3:O:138:ILE:O	3:O:139:ARG:O	2.27	0.53
2:F:153:PHE:CB	2:F:338:GLN:HA	2.39	0.53
3:G:198:LYS:O	3:G:199:GLY:C	2.52	0.53
1:B:227:PRO:HA	1:B:384:VAL:CB	2.39	0.52
3:G:145:THR:O	3:G:149:LYS:CB	2.57	0.52
1:A:224:ALA:CA	1:A:405:ALA:HB3	2.37	0.52
1:C:227:PRO:HA	1:C:384:VAL:CB	2.39	0.52
1:I:296:VAL:HA	1:I:333:ALA:HB1	1.91	0.52
1:A:43:ASP:C	2:D:69:ALA:HB3	2.34	0.52
2:L:359:SER:CA	2:L:362:MET:H	2.22	0.52
1:A:71:LEU:CA	1:A:188:PRO:HA	2.39	0.52
1:C:420:PRO:N	1:C:497:GLN:H	2.07	0.52
1:J:225:ALA:O	1:J:406:PHE:HA	2.08	0.52
1:K:69:LEU:CA	1:K:72:ALA:HB2	2.40	0.52
1:I:25:TYR:N	2:L:65:GLY:C	2.60	0.52
3:O:166:GLN:O	3:O:169:ILE:CB	2.57	0.52
3:O:173:ARG:O	3:O:177:ARG:CB	2.58	0.52
1:K:227:PRO:HA	1:K:384:VAL:CB	2.40	0.52
1:A:44:GLY:N	2:D:69:ALA:HB1	2.22	0.52
1:A:233:GLY:HA2	5:A:600:ADP:PA	2.49	0.52
3:G:42:LEU:O	3:G:45:GLU:CB	2.57	0.52
1:I:259:GLY:O	2:N:298:ALA:N	2.42	0.52
3:O:43:VAL:O	3:O:44:ARG:C	2.51	0.52
1:A:52:TYR:O	1:A:53:GLU:CB	2.58	0.52
2:E:150:LEU:C	2:E:335:GLY:O	2.53	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:MET:CB	2:M:66:LEU:C	2.83	0.52
2:N:62:GLU:HA	2:N:227:PRO:CB	2.39	0.52
1:C:52:TYR:O	1:C:53:GLU:CB	2.58	0.52
2:F:150:LEU:C	2:F:335:GLY:O	2.53	0.52
2:M:150:LEU:C	2:M:335:GLY:O	2.53	0.52
3:O:167:VAL:C	3:O:169:ILE:H	2.17	0.52
1:I:52:TYR:O	1:I:53:GLU:CB	2.58	0.52
1:A:419:PHE:O	1:A:497:GLN:O	2.27	0.51
1:B:429:SER:C	1:B:431:PHE:H	2.19	0.51
1:I:25:TYR:CB	2:L:65:GLY:CA	2.84	0.51
1:K:52:TYR:O	1:K:53:GLU:CB	2.58	0.51
3:O:194:LEU:C	3:O:194:LEU:CB	2.73	0.51
1:B:71:LEU:O	1:B:188:PRO:HA	2.10	0.51
2:D:150:LEU:C	2:D:335:GLY:O	2.53	0.51
1:I:224:ALA:CA	1:I:405:ALA:HB3	2.37	0.51
1:I:263:THR:O	2:N:124:ARG:HA	2.10	0.51
3:O:141:ALA:CA	3:O:145:THR:H	2.22	0.51
1:K:296:VAL:HA	1:K:333:ALA:HB1	1.90	0.51
2:L:150:LEU:C	2:L:335:GLY:O	2.52	0.51
1:B:52:TYR:O	1:B:53:GLU:CB	2.59	0.51
1:C:11:GLY:CA	2:E:49:GLU:CB	2.88	0.51
3:O:171:GLY:O	3:O:174:ALA:HB3	2.11	0.51
1:B:224:ALA:HB2	1:B:405:ALA:CB	2.31	0.51
3:G:7:THR:O	3:G:9:MET:N	2.42	0.51
3:G:141:ALA:CA	3:G:145:THR:H	2.22	0.51
3:G:173:ARG:O	3:G:177:ARG:CB	2.58	0.51
2:M:359:SER:CB	2:M:362:MET:CB	2.88	0.51
3:O:205:GLU:CB	3:O:205:GLU:N	2.67	0.51
1:B:9:ILE:CA	2:D:50:VAL:CB	2.87	0.51
3:G:171:GLY:O	3:G:174:ALA:HB3	2.11	0.51
2:L:134:GLY:C	2:L:430:ARG:O	2.54	0.51
1:I:346:ALA:HB2	2:L:272:ALA:CB	2.40	0.51
2:N:150:LEU:C	2:N:335:GLY:O	2.53	0.51
4:H:84:HIS:C	4:H:86:VAL:H	2.10	0.51
1:A:132:GLY:HA3	1:A:371:LEU:O	2.11	0.50
3:G:167:VAL:C	3:G:169:ILE:H	2.18	0.50
3:G:183:LEU:O	3:G:186:ARG:CB	2.59	0.50
3:O:183:LEU:O	3:O:186:ARG:CB	2.59	0.50
1:C:73:VAL:O	1:C:186:THR:HA	2.12	0.50
1:I:217:PRO:C	1:I:431:PHE:CB	2.84	0.50
2:L:130:PHE:CB	2:L:370:LYS:O	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:148:LYS:O	3:O:152:GLU:CA	2.59	0.50
1:I:418:HIS:HA	1:I:496:GLN:CB	2.42	0.50
1:J:52:TYR:O	1:J:53:GLU:CB	2.58	0.50
1:A:73:VAL:O	1:A:186:THR:HA	2.12	0.50
1:J:224:ALA:CA	1:J:405:ALA:HB3	2.37	0.50
3:G:205:GLU:CB	3:G:205:GLU:N	2.66	0.50
1:J:224:ALA:HB2	1:J:405:ALA:CB	2.31	0.50
1:B:73:VAL:O	1:B:186:THR:HA	2.12	0.49
1:J:73:VAL:O	1:J:186:THR:HA	2.11	0.49
1:K:73:VAL:O	1:K:186:THR:HA	2.12	0.49
1:K:231:GLY:CA	5:K:600:ADP:H5'1	2.37	0.49
2:L:150:LEU:CB	2:L:335:GLY:O	2.60	0.49
2:N:149:LYS:O	2:N:333:THR:CB	2.59	0.49
4:P:84:HIS:O	4:P:85:ASP:C	2.48	0.49
1:J:9:ILE:HA	2:L:50:VAL:CB	2.42	0.49
1:C:259:GLY:C	2:E:296:GLU:C	2.80	0.49
2:F:149:LYS:O	2:F:333:THR:CB	2.59	0.49
3:G:146:ARG:O	3:G:149:LYS:N	2.45	0.49
1:I:11:GLY:C	2:N:50:VAL:O	2.54	0.49
1:J:70:PRO:O	1:J:71:LEU:C	2.55	0.49
1:C:11:GLY:HA3	2:E:49:GLU:CA	2.42	0.49
2:E:149:LYS:O	2:E:333:THR:CB	2.59	0.49
3:G:148:LYS:O	3:G:152:GLU:CA	2.59	0.49
2:D:149:LYS:O	2:D:333:THR:CB	2.59	0.49
2:E:150:LEU:CB	2:E:335:GLY:O	2.61	0.49
3:O:49:ALA:O	3:O:52:ALA:CB	2.53	0.49
3:O:146:ARG:O	3:O:149:LYS:N	2.45	0.49
2:N:150:LEU:CB	2:N:335:GLY:O	2.61	0.49
3:O:142:ASN:CB	3:O:142:ASN:N	2.67	0.49
2:D:150:LEU:CB	2:D:335:GLY:O	2.60	0.49
1:I:475:ALA:HB1	2:L:398:ILE:O	2.13	0.49
1:K:216:PHE:HA	1:K:429:SER:CB	2.43	0.49
2:M:150:LEU:CB	2:M:335:GLY:O	2.61	0.49
1:B:21:GLY:O	2:E:68:LEU:CB	2.61	0.49
3:O:198:LYS:O	3:O:199:GLY:O	2.31	0.49
1:I:71:LEU:CB	1:I:188:PRO:CB	2.87	0.49
3:O:134:ALA:O	4:P:16:ALA:HB2	2.13	0.49
1:I:24:MET:HA	2:L:66:LEU:HA	0.57	0.49
2:L:149:LYS:O	2:L:333:THR:CB	2.59	0.49
3:O:134:ALA:O	3:O:137:LEU:CB	2.61	0.49
2:M:149:LYS:O	2:M:333:THR:CB	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:198:LYS:O	3:G:199:GLY:O	2.31	0.48
4:H:65:GLY:CA	4:H:66:ARG:CB	2.91	0.48
1:I:73:VAL:O	1:I:186:THR:HA	2.12	0.48
1:C:208:GLY:O	1:C:507:CYS:CA	2.61	0.48
1:C:224:ALA:CA	1:C:405:ALA:HB3	2.37	0.48
1:I:440:ARG:HA	1:I:444:ALA:O	2.14	0.48
1:J:440:ARG:HA	1:J:444:ALA:O	2.14	0.48
1:J:471:VAL:CB	4:P:98:ILE:O	2.61	0.48
2:N:349:TYR:HA	2:N:350:PRO:C	2.38	0.48
3:O:3:GLN:O	3:O:6:PRO:N	2.46	0.48
3:O:163:ALA:C	3:O:163:ALA:CB	2.79	0.48
3:O:200:LYS:HA	3:O:203:ALA:HB3	1.96	0.48
3:G:134:ALA:O	3:G:137:LEU:CB	2.62	0.48
1:K:259:GLY:N	2:M:296:GLU:CB	2.68	0.48
3:O:138:ILE:O	3:O:142:ASN:CB	2.62	0.48
2:F:150:LEU:CB	2:F:335:GLY:O	2.61	0.48
3:G:3:GLN:O	3:G:6:PRO:N	2.47	0.48
1:I:24:MET:CB	2:L:66:LEU:CB	2.92	0.48
3:O:48:GLU:CB	3:O:51:LYS:CB	2.92	0.48
3:G:135:GLU:HA	3:G:138:ILE:H	1.79	0.48
2:F:349:TYR:HA	2:F:350:PRO:C	2.38	0.48
1:I:404:GLY:O	1:I:430:LEU:N	2.47	0.48
2:M:349:TYR:HA	2:M:350:PRO:C	2.39	0.48
2:D:349:TYR:HA	2:D:350:PRO:C	2.38	0.48
3:G:153:GLU:O	3:G:154:ILE:O	2.32	0.47
2:M:61:GLU:HA	2:M:229:ILE:CB	2.44	0.47
3:O:153:GLU:O	3:O:154:ILE:O	2.32	0.47
3:G:4:VAL:CA	3:G:5:SER:N	2.68	0.47
2:L:349:TYR:HA	2:L:350:PRO:C	2.38	0.47
3:O:179:ILE:O	3:O:180:GLN:C	2.55	0.47
1:A:440:ARG:HA	1:A:444:ALA:O	2.14	0.47
1:K:233:GLY:CA	5:K:600:ADP:C8	2.97	0.47
2:F:427:GLN:C	1:K:126:GLY:HA2	2.40	0.47
3:G:48:GLU:CB	3:G:51:LYS:CB	2.92	0.47
3:G:4:VAL:C	3:G:6:PRO:N	2.71	0.47
3:G:138:ILE:O	3:G:142:ASN:CB	2.62	0.47
4:H:77:LEU:O	4:H:78:LYS:C	2.35	0.47
1:K:259:GLY:CA	2:M:296:GLU:C	2.60	0.47
1:K:440:ARG:HA	1:K:444:ALA:O	2.14	0.47
1:B:25:TYR:CB	2:E:64:THR:O	2.63	0.47
1:C:266:LEU:O	2:E:124:ARG:CB	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:TYR:N	2:L:65:GLY:CA	2.77	0.47
3:O:135:GLU:HA	3:O:138:ILE:H	1.80	0.47
4:P:77:LEU:O	4:P:78:LYS:C	2.37	0.47
1:C:440:ARG:HA	1:C:444:ALA:O	2.14	0.47
1:B:440:ARG:HA	1:B:444:ALA:O	2.14	0.47
1:C:266:LEU:CB	2:E:124:ARG:CB	2.93	0.47
1:C:352:PRO:O	2:F:269:GLU:CB	2.63	0.47
2:E:349:TYR:HA	2:E:350:PRO:C	2.39	0.47
3:G:167:VAL:C	3:G:167:VAL:HA	2.16	0.47
3:G:200:LYS:HA	3:G:203:ALA:HB3	1.96	0.47
2:D:359:SER:CA	2:D:362:MET:H	2.27	0.46
1:I:346:ALA:HB2	2:L:272:ALA:HB2	1.97	0.46
3:O:200:LYS:CA	3:O:203:ALA:HB3	2.45	0.46
3:G:49:ALA:O	3:G:52:ALA:CB	2.53	0.46
1:I:132:GLY:HA3	1:I:371:LEU:O	2.16	0.46
2:L:334:GLU:C	2:L:361:LEU:CB	2.88	0.46
1:A:43:ASP:O	2:D:69:ALA:CB	2.63	0.46
1:B:23:ARG:O	2:E:67:ASP:O	2.34	0.46
1:A:198:LYS:HA	1:A:368:VAL:HA	1.98	0.46
1:B:10:ALA:O	2:D:49:GLU:HA	2.16	0.46
2:F:427:GLN:O	1:K:126:GLY:HA2	2.15	0.46
1:I:419:PHE:O	1:I:495:LEU:O	2.34	0.46
1:A:56:SER:CB	2:F:30:GLY:H	2.28	0.46
3:G:200:LYS:CA	3:G:203:ALA:HB3	2.45	0.46
1:A:224:ALA:HB2	1:A:405:ALA:CB	2.31	0.46
1:C:359:ALA:CB	2:F:224:ALA:HB1	2.46	0.46
1:K:419:PHE:N	1:K:496:GLN:HA	2.31	0.46
1:C:268:GLU:CB	2:E:126:LYS:CB	2.94	0.46
2:F:427:GLN:C	1:K:126:GLY:CA	2.89	0.46
3:G:27:LEU:CB	3:G:27:LEU:C	2.80	0.45
3:G:179:ILE:O	3:G:180:GLN:C	2.56	0.45
1:I:419:PHE:H	1:I:496:GLN:CA	2.27	0.45
3:O:52:ALA:O	3:O:55:GLN:O	2.34	0.45
1:A:197:ARG:O	1:A:369:ILE:N	2.38	0.45
1:I:11:GLY:N	2:N:50:VAL:O	2.47	0.45
3:G:35:LEU:O	3:G:38:GLU:CB	2.65	0.45
3:O:7:THR:O	3:O:8:ARG:O	2.30	0.45
3:O:35:LEU:O	3:O:38:GLU:CB	2.65	0.45
3:G:7:THR:O	3:G:8:ARG:O	2.30	0.45
3:G:52:ALA:O	3:G:55:GLN:O	2.34	0.45
1:J:71:LEU:O	1:J:188:PRO:HA	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:142:ASN:CB	3:G:142:ASN:N	2.67	0.45
1:K:44:GLY:N	2:N:69:ALA:HB2	2.32	0.45
1:K:296:VAL:CA	1:K:333:ALA:HB1	2.47	0.45
4:P:94:VAL:O	4:P:95:ARG:C	2.58	0.45
3:G:148:LYS:C	3:G:149:LYS:O	2.60	0.45
3:G:151:GLY:O	3:G:152:GLU:O	2.35	0.45
1:A:11:GLY:HA3	2:F:50:VAL:CB	2.42	0.45
1:J:208:GLY:O	1:J:507:CYS:CB	2.65	0.45
1:I:24:MET:CA	2:L:66:LEU:H	1.93	0.45
1:A:44:GLY:CA	2:D:69:ALA:HB3	2.44	0.45
1:C:296:VAL:CA	1:C:333:ALA:HB1	2.47	0.45
1:I:56:SER:CB	2:N:30:GLY:CA	2.95	0.45
1:C:388:GLY:C	1:C:390:ASP:H	2.26	0.44
3:G:141:ALA:HB1	3:G:145:THR:CB	2.47	0.44
1:J:296:VAL:CA	1:J:333:ALA:HB1	2.47	0.44
1:K:26:ASP:O	1:K:71:LEU:N	2.50	0.44
1:A:263:THR:CB	2:F:123:ALA:O	2.66	0.44
2:D:153:PHE:O	2:D:338:GLN:HA	2.17	0.44
3:G:163:ALA:C	3:G:163:ALA:CB	2.79	0.44
1:K:388:GLY:C	1:K:390:ASP:H	2.25	0.44
3:O:4:VAL:C	3:O:6:PRO:N	2.71	0.44
3:O:141:ALA:HB1	3:O:145:THR:CB	2.47	0.44
1:A:388:GLY:C	1:A:390:ASP:H	2.25	0.44
1:B:296:VAL:CA	1:B:333:ALA:HB1	2.47	0.44
1:C:314:ARG:HA	1:C:318:PHE:O	2.18	0.44
1:C:419:PHE:C	1:C:497:GLN:N	2.58	0.44
3:G:45:GLU:O	3:G:47:MET:N	2.50	0.44
4:H:76:GLY:C	4:H:80:ALA:HB3	2.43	0.44
1:K:11:GLY:HA3	2:M:49:GLU:HA	1.94	0.44
3:O:27:LEU:CB	3:O:27:LEU:C	2.80	0.44
1:B:388:GLY:C	1:B:390:ASP:H	2.25	0.44
3:G:175:GLN:O	3:G:177:ARG:N	2.51	0.44
3:G:189:GLU:CB	3:G:189:GLU:N	2.69	0.44
1:J:314:ARG:HA	1:J:318:PHE:O	2.18	0.44
1:A:314:ARG:HA	1:A:318:PHE:O	2.18	0.44
1:J:10:ALA:O	2:L:49:GLU:CA	2.65	0.44
1:J:25:TYR:O	2:M:65:GLY:HA2	2.17	0.44
3:O:151:GLY:O	3:O:152:GLU:O	2.35	0.44
3:O:175:GLN:O	3:O:177:ARG:N	2.51	0.44
4:P:84:HIS:C	4:P:86:VAL:N	2.70	0.44
1:A:296:VAL:CA	1:A:333:ALA:HB1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ARG:HA	1:B:318:PHE:O	2.18	0.44
1:I:86:GLY:O	1:I:305:VAL:CB	2.66	0.44
1:I:296:VAL:CA	1:I:333:ALA:HB1	2.47	0.44
1:K:233:GLY:HA2	5:K:600:ADP:C8	2.52	0.44
1:I:25:TYR:CB	2:L:64:THR:C	2.90	0.44
1:K:314:ARG:HA	1:K:318:PHE:O	2.18	0.44
2:E:153:PHE:O	2:E:338:GLN:HA	2.18	0.44
1:J:388:GLY:C	1:J:390:ASP:H	2.26	0.44
2:L:153:PHE:O	2:L:338:GLN:HA	2.18	0.44
1:K:224:ALA:HB2	1:K:405:ALA:CB	2.32	0.43
1:B:80:LEU:C	1:B:82:GLY:H	2.26	0.43
1:C:80:LEU:C	1:C:82:GLY:H	2.26	0.43
2:N:153:PHE:O	2:N:338:GLN:HA	2.18	0.43
3:O:177:ARG:C	3:O:179:ILE:N	2.72	0.43
1:A:266:LEU:C	2:F:124:ARG:CB	2.90	0.43
1:I:314:ARG:HA	1:I:318:PHE:O	2.18	0.43
2:M:153:PHE:O	2:M:338:GLN:HA	2.18	0.43
4:P:59:VAL:O	4:P:60:GLU:C	2.61	0.43
3:O:189:GLU:CB	3:O:189:GLU:N	2.69	0.43
1:I:255:CYS:HA	1:I:290:ASN:CB	2.49	0.43
1:J:75:LEU:O	1:J:184:TYR:HA	2.19	0.43
1:A:80:LEU:C	1:A:82:GLY:H	2.27	0.43
2:F:258:THR:HA	2:F:259:ASP:HA	1.85	0.43
1:B:241:LEU:O	1:B:245:SER:CB	2.67	0.43
3:G:177:ARG:C	3:G:179:ILE:N	2.72	0.43
4:H:59:VAL:O	4:H:60:GLU:C	2.61	0.43
2:D:334:GLU:CA	2:D:361:LEU:CB	2.97	0.43
3:O:159:ARG:C	3:O:161:VAL:N	2.77	0.43
3:O:189:GLU:O	3:O:190:ASP:C	2.62	0.43
1:A:255:CYS:HA	1:A:290:ASN:CB	2.49	0.43
1:C:292:SER:CB	2:E:292:ALA:HB1	2.45	0.43
3:G:175:GLN:O	3:G:178:PHE:N	2.51	0.43
1:I:56:SER:CB	2:N:30:GLY:H	2.29	0.43
1:I:388:GLY:C	1:I:390:ASP:H	2.25	0.43
1:J:241:LEU:O	1:J:245:SER:CB	2.67	0.43
1:K:75:LEU:O	1:K:184:TYR:HA	2.19	0.43
3:O:45:GLU:O	3:O:47:MET:N	2.50	0.43
3:O:135:GLU:O	3:O:139:ARG:CB	2.67	0.43
2:E:258:THR:HA	2:E:259:ASP:HA	1.85	0.43
3:G:135:GLU:O	3:G:139:ARG:CB	2.67	0.43
1:K:189:VAL:CB	1:K:304:TYR:CB	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:140:VAL:O	3:O:144:GLU:N	2.47	0.43
1:A:241:LEU:O	1:A:245:SER:CB	2.67	0.42
1:B:9:ILE:CB	2:D:52:GLU:N	2.82	0.42
1:K:208:GLY:C	1:K:507:CYS:O	2.57	0.42
2:L:359:SER:C	2:L:362:MET:H	2.26	0.42
3:O:189:GLU:CB	3:O:189:GLU:HA	2.18	0.42
1:B:255:CYS:HA	1:B:290:ASN:CB	2.49	0.42
1:J:80:LEU:C	1:J:82:GLY:H	2.26	0.42
1:K:255:CYS:HA	1:K:290:ASN:CB	2.49	0.42
2:F:153:PHE:O	2:F:338:GLN:HA	2.18	0.42
2:F:427:GLN:CB	1:K:126:GLY:HA2	2.43	0.42
1:K:241:LEU:O	1:K:245:SER:CB	2.67	0.42
2:M:334:GLU:O	2:M:360:ARG:N	2.49	0.42
3:O:148:LYS:C	3:O:149:LYS:O	2.59	0.42
3:O:174:ALA:O	3:O:175:GLN:O	2.37	0.42
1:B:75:LEU:O	1:B:184:TYR:HA	2.19	0.42
1:C:241:LEU:O	1:C:245:SER:CB	2.67	0.42
1:I:241:LEU:O	1:I:245:SER:CB	2.67	0.42
1:K:208:GLY:O	1:K:507:CYS:C	2.58	0.42
1:C:208:GLY:C	1:C:507:CYS:O	2.63	0.42
1:J:255:CYS:HA	1:J:290:ASN:CB	2.49	0.42
2:D:149:LYS:C	2:D:334:GLU:H	2.14	0.42
2:D:189:VAL:O	2:D:217:SER:HA	2.20	0.42
2:E:189:VAL:O	2:E:217:SER:HA	2.20	0.42
4:H:77:LEU:H	4:H:80:ALA:CB	2.28	0.42
2:L:189:VAL:O	2:L:217:SER:HA	2.20	0.42
2:N:360:ARG:C	2:N:362:MET:N	2.38	0.42
1:K:12:PRO:N	2:M:49:GLU:CB	2.83	0.42
1:A:11:GLY:N	2:F:50:VAL:O	2.53	0.42
1:C:75:LEU:O	1:C:184:TYR:HA	2.19	0.42
1:K:80:LEU:C	1:K:82:GLY:H	2.27	0.42
1:A:267:VAL:CB	2:F:125:ARG:HA	2.50	0.42
2:F:189:VAL:O	2:F:217:SER:HA	2.20	0.42
3:G:189:GLU:O	3:G:190:ASP:C	2.62	0.42
4:H:94:VAL:O	4:H:95:ARG:C	2.58	0.42
3:O:4:VAL:CA	3:O:5:SER:N	2.68	0.42
1:A:133:MET:O	1:A:148:LEU:HA	2.20	0.42
1:A:266:LEU:CB	2:F:124:ARG:HA	2.49	0.42
1:B:25:TYR:O	2:E:65:GLY:HA3	2.02	0.42
3:G:48:GLU:C	3:G:51:LYS:CB	2.92	0.42
1:I:75:LEU:O	1:I:184:TYR:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:11:GLY:CA	2:M:49:GLU:CA	2.95	0.42
3:O:3:GLN:O	3:O:4:VAL:C	2.63	0.42
1:A:75:LEU:O	1:A:184:TYR:HA	2.19	0.41
1:A:221:GLY:O	1:A:366:GLY:HA2	2.20	0.41
1:B:227:PRO:CB	1:B:384:VAL:CB	2.98	0.41
1:J:133:MET:O	1:J:148:LEU:HA	2.20	0.41
3:O:175:GLN:O	3:O:178:PHE:N	2.51	0.41
1:B:22:ALA:HA	2:E:68:LEU:CB	2.50	0.41
1:C:133:MET:O	1:C:148:LEU:HA	2.20	0.41
2:F:334:GLU:O	2:F:360:ARG:N	2.53	0.41
1:I:80:LEU:C	1:I:82:GLY:H	2.27	0.41
2:M:189:VAL:O	2:M:217:SER:HA	2.20	0.41
3:O:48:GLU:O	3:O:51:LYS:CA	2.67	0.41
1:C:255:CYS:HA	1:C:290:ASN:CB	2.49	0.41
1:J:10:ALA:O	2:L:50:VAL:N	2.47	0.41
1:K:227:PRO:CB	1:K:384:VAL:CB	2.99	0.41
3:G:43:VAL:O	3:G:45:GLU:N	2.54	0.41
2:L:359:SER:O	2:L:360:ARG:C	2.60	0.41
3:O:11:LEU:O	3:O:12:LEU:C	2.64	0.41
3:G:149:LYS:O	3:G:150:ILE:C	2.63	0.41
1:K:133:MET:O	1:K:148:LEU:HA	2.21	0.41
2:N:189:VAL:O	2:N:217:SER:HA	2.20	0.41
1:B:133:MET:O	1:B:148:LEU:HA	2.20	0.41
1:B:221:GLY:O	1:B:366:GLY:HA2	2.21	0.41
2:D:149:LYS:CB	2:D:333:THR:HA	2.51	0.41
3:G:3:GLN:O	3:G:4:VAL:C	2.63	0.41
1:I:133:MET:O	1:I:148:LEU:HA	2.21	0.41
3:O:20:LEU:O	3:O:21:ALA:C	2.64	0.41
1:B:141:PHE:O	1:B:143:PHE:O	2.39	0.41
1:B:263:THR:CB	2:D:124:ARG:CA	2.97	0.41
2:F:149:LYS:CB	2:F:333:THR:HA	2.51	0.41
1:K:221:GLY:O	1:K:366:GLY:HA2	2.21	0.41
1:C:221:GLY:O	1:C:366:GLY:HA2	2.21	0.41
2:F:149:LYS:C	2:F:334:GLU:H	2.14	0.41
1:I:227:PRO:CB	1:I:384:VAL:CB	2.99	0.41
1:J:221:GLY:O	1:J:366:GLY:HA2	2.20	0.41
1:A:259:GLY:C	2:F:296:GLU:O	2.61	0.41
1:C:141:PHE:O	1:C:143:PHE:O	2.39	0.41
2:D:130:PHE:CB	2:D:370:LYS:O	2.68	0.41
3:G:159:ARG:C	3:G:161:VAL:N	2.77	0.41
1:I:346:ALA:HB2	2:L:272:ALA:HB1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:PHE:O	1:K:143:PHE:O	2.39	0.41
2:M:149:LYS:C	2:M:334:GLU:H	2.14	0.41
2:N:149:LYS:CB	2:N:333:THR:HA	2.51	0.41
3:O:40:PHE:O	3:O:43:VAL:CB	2.69	0.41
3:O:43:VAL:O	3:O:45:GLU:N	2.54	0.41
1:A:227:PRO:CB	1:A:384:VAL:CB	2.99	0.41
3:G:146:ARG:O	3:G:149:LYS:CB	2.69	0.41
1:C:44:GLY:CA	2:F:69:ALA:HB2	2.42	0.40
1:C:227:PRO:CB	1:C:384:VAL:CB	2.99	0.40
3:G:48:GLU:O	3:G:51:LYS:CA	2.68	0.40
3:G:174:ALA:O	3:G:175:GLN:O	2.36	0.40
1:I:221:GLY:O	1:I:366:GLY:HA2	2.21	0.40
2:N:258:THR:HA	2:N:259:ASP:HA	1.85	0.40
4:H:63:MET:CB	4:H:64:ARG:HA	2.52	0.40
1:I:226:ILE:O	1:I:384:VAL:N	2.55	0.40
2:M:149:LYS:CB	2:M:333:THR:HA	2.51	0.40
3:O:146:ARG:O	3:O:149:LYS:CB	2.69	0.40
1:A:226:ILE:O	1:A:384:VAL:N	2.55	0.40
3:G:40:PHE:O	3:G:43:VAL:CB	2.69	0.40
1:J:263:THR:CB	2:L:126:LYS:N	2.77	0.40
3:O:149:LYS:O	3:O:150:ILE:C	2.64	0.40
4:P:75:ALA:C	4:P:75:ALA:HB1	2.42	0.40
1:C:226:ILE:O	1:C:384:VAL:N	2.54	0.40
1:I:141:PHE:O	1:I:143:PHE:O	2.39	0.40
1:J:227:PRO:CB	1:J:384:VAL:CB	2.99	0.40
1:K:233:GLY:HA2	5:K:600:ADP:O1A	2.21	0.40
2:L:149:LYS:CB	2:L:333:THR:HA	2.51	0.40
1:B:263:THR:CB	2:D:124:ARG:HA	2.51	0.40
1:J:141:PHE:O	1:J:143:PHE:O	2.39	0.40
1:J:226:ILE:O	1:J:384:VAL:N	2.55	0.40

All (2) 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:J:6:ILE:CB	2:M:24:ALA:O[5_555]	2.04	0.16
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	2.10	0.10

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	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	3	21
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	3	21
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	3	22
1	I	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	3	23
1	J	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	3	21
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	3	22
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	6	31
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	6	31
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	6	31
2	L	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	6	31
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	6	31
2	N	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	5	29
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	89 (87%)	11 (11%)	2 (2%)	6	31
4	P	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	6	31
All	All	6472/6990 (93%)	5808 (90%)	443 (7%)	221 (3%)	3	21

All (221) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO
1	A	256	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	260	ASN
1	A	325	ASP
1	A	394	PRO
1	A	395	VAL
1	A	558	GLU
1	B	12	PRO
1	B	19	MET
1	B	53	GLU
1	B	143	PHE
1	B	227	PRO
1	B	256	GLY
1	B	260	ASN
1	B	325	ASP
1	B	394	PRO
1	B	395	VAL
1	B	558	GLU
1	C	12	PRO
1	C	19	MET
1	C	53	GLU
1	C	143	PHE
1	C	227	PRO
1	C	256	GLY
1	C	260	ASN
1	C	325	ASP
1	C	394	PRO
1	C	395	VAL
1	C	558	GLU
2	D	52	GLU
2	D	79	VAL
2	D	316	MET
2	D	356	PRO
2	D	427	GLN
2	E	52	GLU
2	E	79	VAL
2	E	316	MET
2	E	356	PRO
2	E	427	GLN
2	F	52	GLU
2	F	316	MET
2	F	356	PRO
2	F	427	GLN
3	G	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	4	VAL
3	G	43	VAL
3	G	47	MET
3	G	48	GLU
3	G	140	VAL
3	G	149	LYS
3	G	152	GLU
3	G	161	VAL
3	G	172	ILE
3	G	174	ALA
4	H	85	ASP
4	H	100	PHE
1	I	12	PRO
1	I	19	MET
1	I	53	GLU
1	I	143	PHE
1	I	227	PRO
1	I	256	GLY
1	I	260	ASN
1	I	325	ASP
1	I	394	PRO
1	I	395	VAL
1	I	558	GLU
1	J	12	PRO
1	J	19	MET
1	J	53	GLU
1	J	143	PHE
1	J	227	PRO
1	J	256	GLY
1	J	260	ASN
1	J	325	ASP
1	J	394	PRO
1	J	395	VAL
1	J	558	GLU
1	K	12	PRO
1	K	19	MET
1	K	53	GLU
1	K	71	LEU
1	K	143	PHE
1	K	227	PRO
1	K	256	GLY
1	K	260	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	325	ASP
1	K	394	PRO
1	K	395	VAL
1	K	558	GLU
2	L	52	GLU
2	L	79	VAL
2	L	316	MET
2	L	356	PRO
2	L	427	GLN
2	M	52	GLU
2	M	316	MET
2	M	356	PRO
2	M	427	GLN
2	N	52	GLU
2	N	316	MET
2	N	356	PRO
2	N	361	LEU
2	N	427	GLN
3	O	3	GLN
3	O	4	VAL
3	O	43	VAL
3	O	47	MET
3	O	48	GLU
3	O	140	VAL
3	O	149	LYS
3	O	152	GLU
3	O	161	VAL
3	O	172	ILE
3	O	174	ALA
3	O	200	LYS
4	P	85	ASP
4	P	100	PHE
1	A	88	GLN
1	A	255	CYS
1	A	431	PHE
1	B	71	LEU
1	B	88	GLN
1	B	255	CYS
1	C	88	GLN
1	C	255	CYS
2	D	26	ASP
2	D	428	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	26	ASP
2	E	428	GLN
2	F	26	ASP
2	F	428	GLN
3	G	2	SER
3	G	6	PRO
3	G	150	ILE
3	G	151	GLY
3	G	185	GLN
3	G	200	LYS
1	I	88	GLN
1	I	255	CYS
1	J	71	LEU
1	J	88	GLN
1	J	255	CYS
1	J	430	LEU
1	K	88	GLN
1	K	255	CYS
2	L	26	ASP
2	L	428	GLN
2	M	26	ASP
2	M	79	VAL
2	M	428	GLN
2	N	26	ASP
2	N	428	GLN
3	O	2	SER
3	O	6	PRO
3	O	13	GLN
3	O	150	ILE
3	O	151	GLY
3	O	185	GLN
1	A	109	HIS
1	B	109	HIS
1	C	109	HIS
3	G	13	GLN
3	G	139	ARG
3	G	155	LYS
3	G	162	ASN
3	G	165	GLU
1	I	109	HIS
1	J	109	HIS
1	K	109	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	79	VAL
3	O	139	ARG
3	O	155	LYS
3	O	162	ASN
3	O	165	GLU
1	A	200	ASP
2	F	79	VAL
3	G	45	GLU
3	G	186	ARG
3	O	45	GLU
3	O	137	LEU
3	O	186	ARG
1	A	374	GLU
1	B	70	PRO
1	B	374	GLU
1	C	71	LEU
1	C	374	GLU
2	D	317	PRO
2	E	317	PRO
2	F	317	PRO
3	G	53	LEU
3	G	137	LEU
3	G	197	ILE
1	I	374	GLU
1	J	374	GLU
1	K	374	GLU
2	L	317	PRO
2	M	317	PRO
2	N	317	PRO
3	O	53	LEU
3	O	197	ILE
2	D	355	LEU
2	E	355	LEU
2	F	355	LEU
2	L	355	LEU
2	M	355	LEU
2	N	355	LEU
1	A	388	GLY
1	B	388	GLY
1	C	388	GLY
3	G	179	ILE
1	I	388	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	388	GLY
1	K	388	GLY
3	O	179	ILE
3	G	168	VAL
3	O	168	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ADP	A	600	-	28,29,29	1.23	2 (7%)	43,45,45	0.69	1 (2%)
5	ADP	C	600	-	28,29,29	1.02	2 (7%)	43,45,45	0.80	3 (6%)
5	ADP	I	600	-	28,29,29	1.22	2 (7%)	43,45,45	0.69	1 (2%)
5	ADP	K	600	-	28,29,29	1.02	2 (7%)	43,45,45	0.80	3 (6%)

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	ADP	A	600	-	-	2/16/32/32	0/3/3/3
5	ADP	C	600	-	-	0/16/32/32	0/3/3/3
5	ADP	I	600	-	-	2/16/32/32	0/3/3/3
5	ADP	K	600	-	-	0/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	ADP	PA-O3A	4.08	1.63	1.59
5	I	600	ADP	PA-O3A	4.04	1.63	1.59
5	K	600	ADP	PB-O2B	-2.52	1.45	1.54
5	C	600	ADP	PB-O2B	-2.52	1.45	1.54
5	A	600	ADP	PB-O2B	-2.43	1.45	1.54
5	I	600	ADP	PB-O2B	-2.42	1.45	1.54
5	C	600	ADP	PA-O1A	-2.36	1.42	1.50
5	K	600	ADP	PA-O1A	-2.35	1.42	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ADP	O3B-PB-O2B	2.38	116.72	107.80
5	C	600	ADP	O3B-PB-O2B	2.38	116.71	107.80
5	A	600	ADP	O3A-PA-O1A	2.10	117.02	110.70
5	I	600	ADP	O3A-PA-O1A	2.09	116.99	110.70
5	C	600	ADP	O5'-PA-O1A	2.07	117.14	108.94
5	K	600	ADP	O5'-PA-O1A	2.07	117.13	108.94
5	K	600	ADP	O4'-C4'-C3'	-2.05	101.08	105.15
5	C	600	ADP	O4'-C4'-C3'	-2.05	101.09	105.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

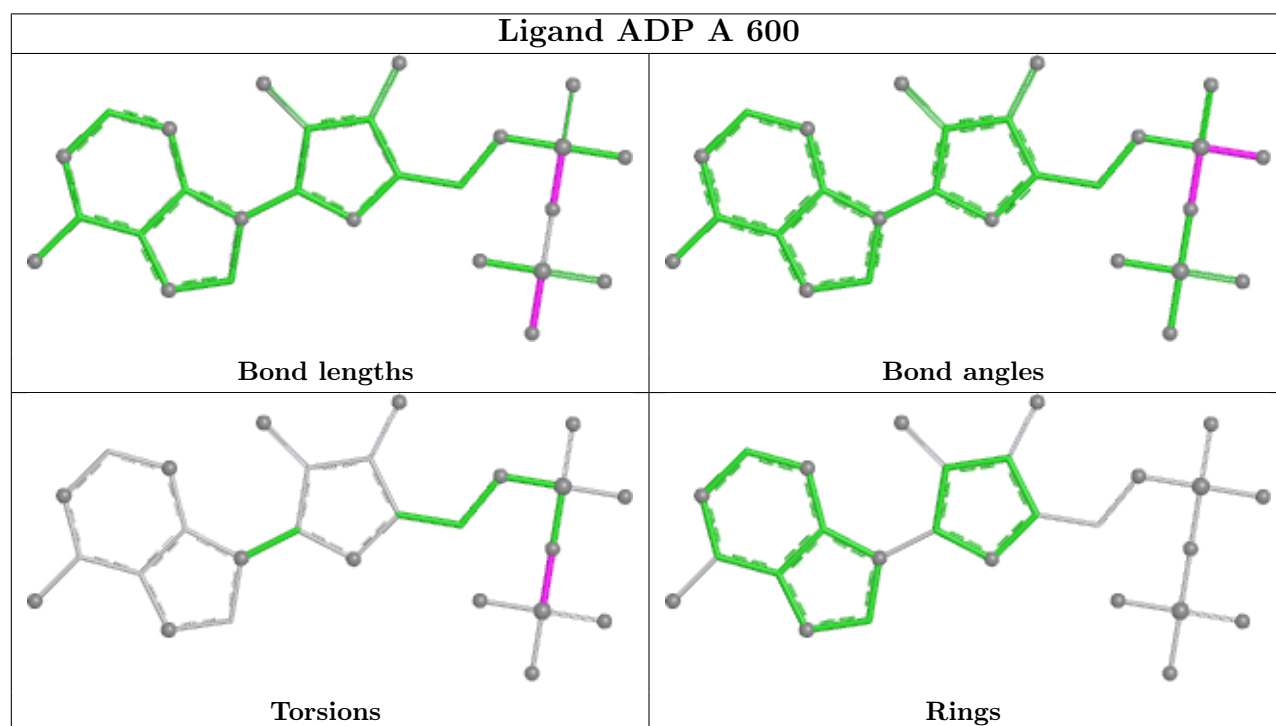
Mol	Chain	Res	Type	Atoms
5	A	600	ADP	PA-O3A-PB-O2B
5	A	600	ADP	PA-O3A-PB-O3B
5	I	600	ADP	PA-O3A-PB-O2B
5	I	600	ADP	PA-O3A-PB-O3B

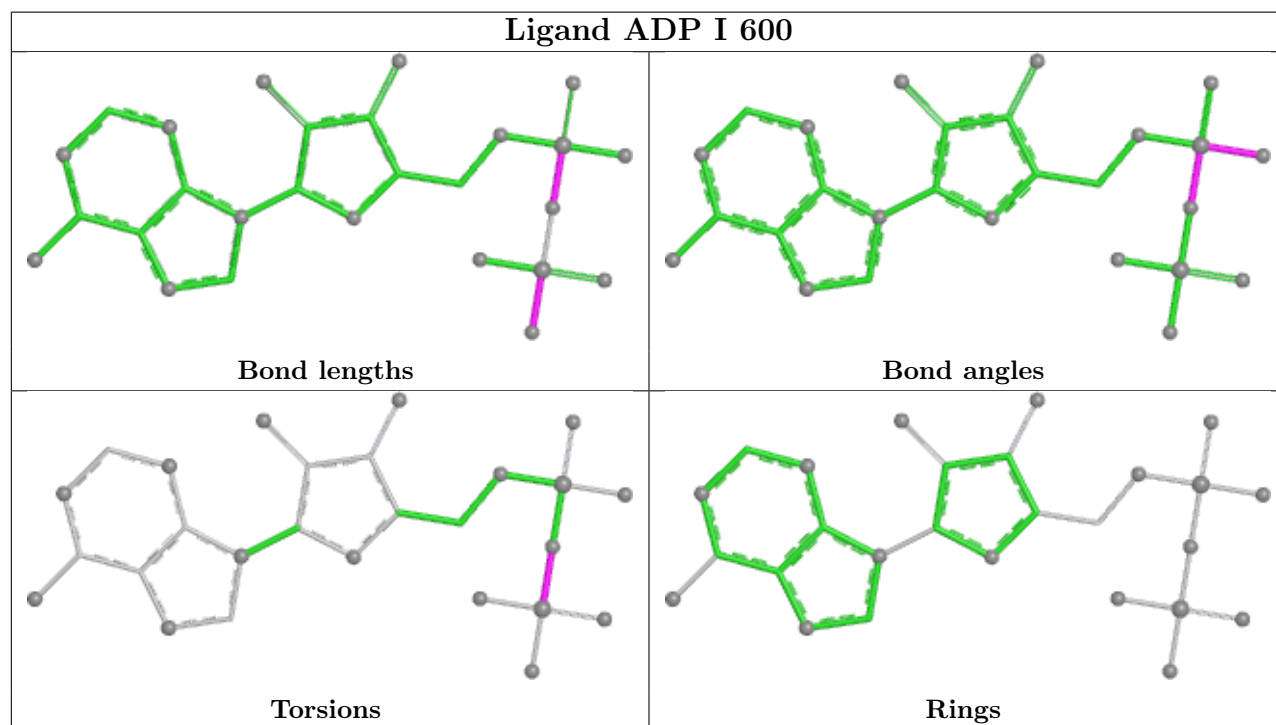
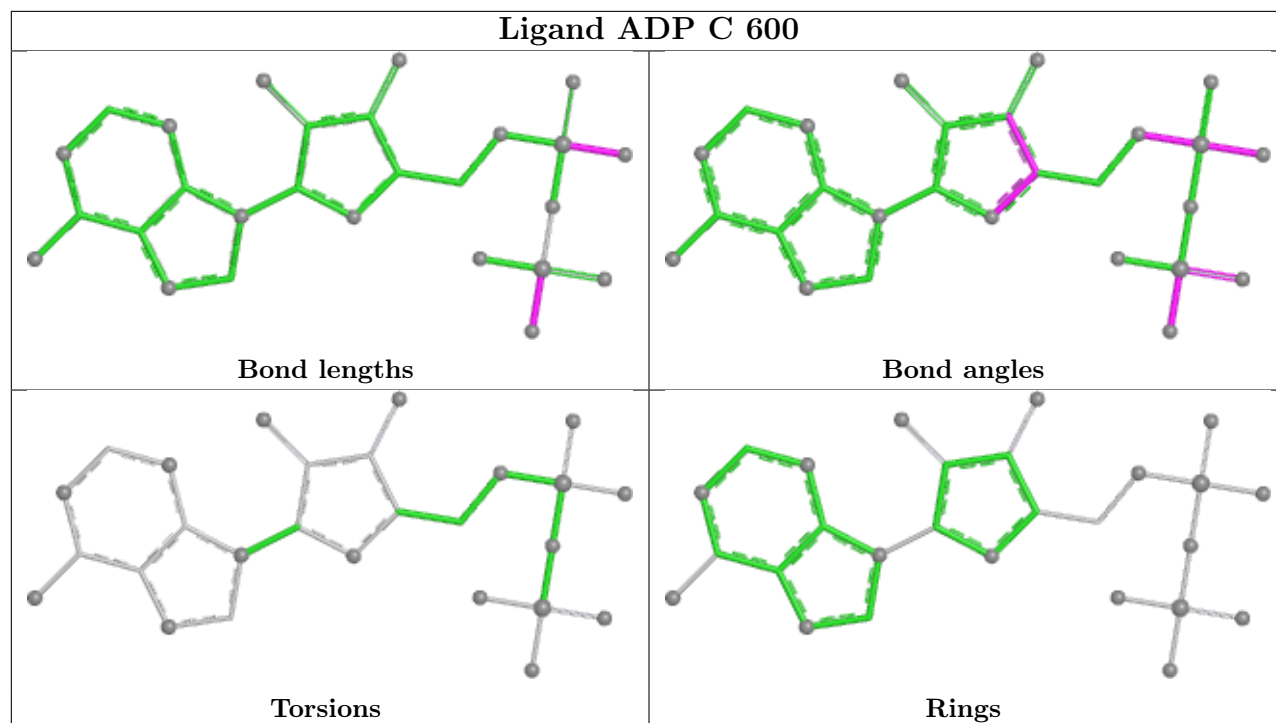
There are no ring outliers.

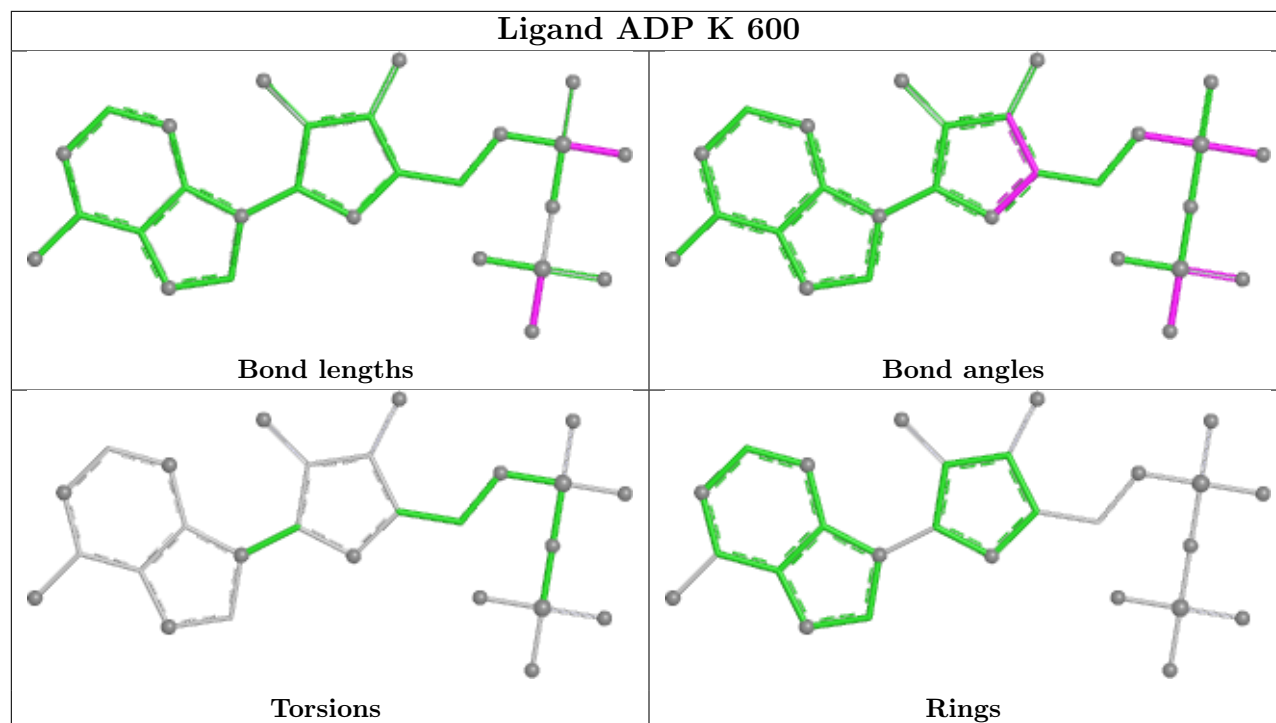
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ADP	2	0
5	C	600	ADP	1	0
5	K	600	ADP	5	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	561/578 (97%)	2.02	229 (40%) 0 2	103, 162, 214, 214	0
1	B	561/578 (97%)	1.50	147 (26%) 1 5	79, 130, 144, 144	0
1	C	561/578 (97%)	2.31	259 (46%) 0 1	137, 189, 210, 210	0
1	I	561/578 (97%)	2.58	293 (52%) 0 1	172, 172, 232, 232	0
1	J	561/578 (97%)	1.34	144 (25%) 1 5	50, 58, 104, 104	0
1	K	561/578 (97%)	2.63	300 (53%) 0 1	146, 177, 189, 189	0
2	D	450/478 (94%)	1.77	153 (34%) 1 4	118, 118, 188, 188	0
2	E	450/478 (94%)	2.07	196 (43%) 0 2	122, 130, 162, 162	0
2	F	450/478 (94%)	2.50	230 (51%) 0 1	109, 217, 217, 217	0
2	L	450/478 (94%)	1.71	134 (29%) 1 4	98, 98, 158, 158	0
2	M	450/478 (94%)	2.25	185 (41%) 0 2	99, 99, 148, 148	0
2	N	450/478 (94%)	2.84	248 (55%) 0 1	158, 250, 250, 250	0
3	G	129/223 (57%)	0.63	16 (12%) 8 13	34, 34, 49, 49	0
3	O	129/223 (57%)	0.69	13 (10%) 12 16	84, 85, 85, 85	0
4	H	104/104 (100%)	2.50	46 (44%) 0 2	110, 110, 134, 134	0
4	P	104/104 (100%)	1.83	33 (31%) 1 4	94, 94, 141, 141	0
All	All	6532/6990 (93%)	2.06	2626 (40%) 0 2	34, 137, 232, 250	0

All (2626) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	24	SER	24.0
4	P	85	ASP	22.8
2	L	122	VAL	20.5
2	M	121	PRO	19.5
2	M	302	GLU	19.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	192	ALA	17.2
1	K	293	ASN	16.7
2	D	102	GLY	16.4
1	I	145	HIS	16.1
2	L	121	PRO	15.8
4	H	76	GLY	15.8
1	K	393	GLU	15.3
1	K	394	PRO	15.2
2	F	224	ALA	15.1
1	I	372	GLY	14.9
1	K	576	ALA	14.8
2	M	363	ASN	14.8
2	M	301	VAL	14.5
4	P	104	LEU	14.2
2	M	122	VAL	14.1
1	I	12	PRO	14.1
2	M	300	VAL	13.8
1	B	110	ALA	13.6
2	M	299	GLY	13.6
1	J	266	LEU	13.4
1	A	201	PRO	13.3
2	F	225	ASP	13.0
2	E	120	ASN	12.9
1	I	424	TRP	12.9
1	I	296	VAL	12.9
2	E	150	LEU	12.8
1	K	117	TRP	12.7
2	N	118	PRO	12.6
1	C	165	GLU	12.6
2	D	121	PRO	12.6
2	E	168	ALA	12.6
1	I	78	GLY	12.5
1	K	345	PRO	12.4
1	B	109	HIS	12.3
2	M	360	ARG	12.2
1	A	296	VAL	12.2
1	K	324	ALA	12.1
2	N	334	GLU	11.9
1	I	63	PRO	11.9
2	L	77	GLU	11.9
1	C	1	MET	11.8
4	H	25	SER	11.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	463	TYR	11.6
1	B	387	PRO	11.5
1	I	139	PRO	11.5
2	E	165	ALA	11.4
1	K	383	ALA	11.3
2	N	165	ALA	11.3
1	C	36	VAL	11.3
1	K	297	ALA	11.2
2	N	191	PHE	11.2
1	A	12	PRO	11.1
2	E	335	GLY	11.1
1	K	141	PHE	11.1
2	D	75	LEU	11.0
1	I	232	SER	11.0
2	N	117	LEU	11.0
2	N	80	ALA	11.0
1	K	349	GLY	11.0
2	M	168	ALA	10.9
1	C	502	GLU	10.9
2	F	201	LEU	10.6
2	M	361	LEU	10.6
1	K	140	GLU	10.6
2	E	172	THR	10.5
1	C	47	ALA	10.5
2	F	216	ARG	10.5
2	N	164	ALA	10.3
2	F	221	LEU	10.3
1	I	140	GLU	10.1
2	M	11	ILE	10.1
1	I	180	GLU	10.1
1	B	471	VAL	10.0
2	M	359	SER	10.0
2	M	172	THR	10.0
2	F	141	MET	10.0
1	C	379	THR	9.7
2	N	359	SER	9.7
2	N	141	MET	9.7
1	B	388	GLY	9.7
1	K	416	ARG	9.6
1	B	12	PRO	9.6
1	I	373	GLY	9.6
1	A	403	VAL	9.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	128	GLU	9.6
1	C	37	GLY	9.6
1	I	224	ALA	9.5
2	N	190	VAL	9.5
1	I	576	ALA	9.3
2	E	164	ALA	9.3
1	B	45	ASP	9.2
3	G	53	LEU	9.2
2	F	86	LYS	9.1
4	H	98	ILE	9.1
1	A	192	ALA	9.1
1	J	12	PRO	9.0
2	F	187	PHE	9.0
1	J	493	ASP	9.0
1	J	474	ASP	9.0
2	N	137	THR	9.0
2	M	362	MET	8.9
1	J	387	PRO	8.8
1	C	292	SER	8.8
2	D	119	LEU	8.7
2	N	341	ARG	8.7
1	K	382	GLY	8.6
1	I	138	VAL	8.6
2	M	80	ALA	8.6
2	E	119	LEU	8.6
2	N	66	LEU	8.6
1	A	61	GLY	8.6
2	F	278	PRO	8.6
2	F	332	ILE	8.5
2	M	402	ASP	8.5
1	I	563	PHE	8.5
2	D	360	ARG	8.5
2	E	118	PRO	8.5
2	N	67	ASP	8.5
4	H	16	ALA	8.4
2	N	419	GLU	8.4
1	C	388	GLY	8.4
1	B	266	LEU	8.4
2	L	302	GLU	8.4
2	M	198	GLN	8.4
1	C	151	PRO	8.3
2	N	278	PRO	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2	ILE	8.3
1	J	471	VAL	8.3
1	K	296	VAL	8.3
1	B	111	LEU	8.2
2	M	42	VAL	8.2
1	K	122	MET	8.2
2	N	140	VAL	8.2
1	J	395	VAL	8.1
2	F	83	GLY	8.1
1	A	395	VAL	8.1
2	M	117	LEU	8.1
1	I	382	GLY	8.0
1	I	55	THR	8.0
1	K	77	PRO	8.0
1	C	270	PRO	7.9
4	H	38	GLU	7.9
2	D	122	VAL	7.8
1	I	84	TYR	7.8
1	I	291	THR	7.8
4	H	29	ALA	7.8
2	N	331	TYR	7.8
2	F	136	SER	7.7
2	M	25	LYS	7.7
1	B	194	PRO	7.7
2	N	220	PHE	7.7
2	N	335	GLY	7.7
1	A	200	ASP	7.7
2	E	28	ALA	7.6
2	L	56	VAL	7.6
1	A	134	VAL	7.6
1	J	267	VAL	7.6
2	N	184	GLU	7.6
1	C	288	ILE	7.6
2	E	141	MET	7.6
2	N	297	ARG	7.6
1	K	258	ARG	7.6
1	J	263	THR	7.6
1	I	77	PRO	7.6
2	F	121	PRO	7.6
1	A	14	VAL	7.5
1	K	114	GLU	7.5
2	F	122	VAL	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	421	PHE	7.5
3	G	54	ASP	7.5
1	I	26	ASP	7.4
2	D	109	GLU	7.4
1	I	146	LYS	7.4
4	P	98	ILE	7.4
2	F	154	SER	7.3
4	P	64	ARG	7.3
2	N	198	GLN	7.3
1	C	258	ARG	7.3
1	B	270	PRO	7.3
2	N	238	ALA	7.3
2	D	310	GLN	7.2
2	N	121	PRO	7.2
2	M	70	THR	7.2
1	J	2	ILE	7.2
1	I	497	GLN	7.2
1	A	193	ARG	7.2
2	F	189	VAL	7.1
1	C	183	MET	7.1
1	K	417	ARG	7.1
1	C	400	LEU	7.1
1	K	78	GLY	7.1
4	P	78	LYS	7.1
1	K	372	GLY	7.0
1	K	237	THR	7.0
2	N	161	ASN	7.0
2	M	401	GLU	7.0
2	F	274	ARG	7.0
2	L	301	VAL	7.0
1	C	256	GLY	7.0
2	N	242	ALA	7.0
2	L	21	VAL	7.0
1	I	183	MET	7.0
1	K	240	SER	7.0
1	I	22	ALA	6.9
2	N	429	ASN	6.9
2	F	186	PRO	6.9
1	K	195	VAL	6.9
2	E	29	TYR	6.9
2	F	331	TYR	6.9
2	L	97	GLY	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	201	LEU	6.9
2	F	298	ALA	6.9
1	A	210	ARG	6.8
1	C	237	THR	6.8
2	N	115	THR	6.8
1	J	416	ARG	6.8
1	B	267	VAL	6.8
1	A	554	VAL	6.8
2	D	77	GLU	6.8
2	D	117	LEU	6.8
2	N	79	VAL	6.8
2	F	299	GLY	6.8
1	K	295	PRO	6.8
2	F	362	MET	6.8
1	A	218	VAL	6.7
1	C	73	VAL	6.7
2	F	297	ARG	6.7
1	A	147	ILE	6.7
2	M	69	ALA	6.7
2	E	122	VAL	6.7
1	C	393	GLU	6.7
1	A	267	VAL	6.7
1	I	218	VAL	6.7
2	N	366	VAL	6.7
1	J	394	PRO	6.6
1	K	193	ARG	6.6
1	I	219	ALA	6.6
2	N	225	ASP	6.6
1	A	207	THR	6.6
2	N	82	LEU	6.6
2	N	168	ALA	6.6
2	N	224	ALA	6.6
1	A	13	ALA	6.6
1	K	256	GLY	6.6
2	M	235	PRO	6.6
2	F	137	THR	6.6
1	A	222	GLY	6.6
2	F	188	ALA	6.6
1	I	499	ALA	6.5
1	K	575	LYS	6.5
1	B	139	PRO	6.5
1	K	74	GLU	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	228	THR	6.5
1	J	494	PHE	6.5
1	I	134	VAL	6.5
1	J	206	LEU	6.5
2	L	229	ILE	6.5
1	K	387	PRO	6.5
1	I	290	ASN	6.5
2	M	426	GLY	6.5
1	C	425	ASN	6.5
1	K	294	MET	6.5
2	F	363	ASN	6.5
2	L	183	LYS	6.5
2	N	258	THR	6.5
1	C	356	ALA	6.4
1	K	201	PRO	6.4
2	E	351	PRO	6.4
1	K	451	ARG	6.4
1	K	360	ALA	6.4
4	P	69	PRO	6.4
4	P	89	TYR	6.4
2	L	28	ALA	6.4
1	I	234	LYS	6.4
1	J	23	ARG	6.4
2	M	243	GLU	6.4
1	I	144	THR	6.3
2	N	174	ARG	6.3
1	C	337	ILE	6.3
1	I	1	MET	6.3
2	L	137	THR	6.3
1	I	433	SER	6.3
2	N	310	GLN	6.3
4	H	53	PRO	6.3
1	J	3	GLN	6.3
2	L	75	LEU	6.3
2	L	300	VAL	6.2
1	A	55	THR	6.2
2	N	122	VAL	6.2
2	M	317	PRO	6.2
3	O	143	THR	6.2
1	I	343	GLU	6.2
2	F	365	GLY	6.1
2	N	289	THR	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.1
1	I	345	PRO	6.1
2	N	17	PRO	6.1
1	K	385	SER	6.1
1	C	144	THR	6.1
1	C	150	PRO	6.1
2	F	142	ASN	6.1
1	B	324	ALA	6.1
1	A	422	ILE	6.1
1	C	29	LYS	6.1
2	N	193	ALA	6.0
1	A	170	GLU	6.0
1	K	311	GLU	6.0
2	M	209	GLU	6.0
2	M	83	GLY	6.0
2	N	218	VAL	6.0
1	I	223	THR	6.0
1	K	183	MET	6.0
1	K	418	HIS	6.0
1	K	359	ALA	6.0
2	N	421	PHE	6.0
2	N	383	TYR	6.0
2	N	78	ASP	6.0
2	N	205	ILE	6.0
2	F	10	GLY	6.0
2	E	117	LEU	6.0
2	N	185	GLU	6.0
1	C	315	ASP	6.0
1	A	162	PRO	6.0
1	K	108	VAL	6.0
2	M	383	TYR	6.0
1	J	207	THR	5.9
1	I	416	ARG	5.9
2	F	359	SER	5.9
4	H	75	ALA	5.9
2	E	315	SER	5.9
1	I	13	ALA	5.9
1	A	150	PRO	5.9
1	I	54	ASP	5.9
2	F	21	VAL	5.9
1	K	194	PRO	5.9
2	E	32	ILE	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	456	LYS	5.8
1	C	35	LEU	5.8
2	N	336	GLN	5.8
1	K	520	LEU	5.8
2	E	137	THR	5.8
2	M	77	GLU	5.8
2	N	83	GLY	5.8
1	B	390	ASP	5.8
4	P	82	GLN	5.8
2	E	325	ILE	5.8
2	F	88	MET	5.8
2	D	45	GLY	5.7
1	C	235	THR	5.7
1	K	400	LEU	5.7
2	M	141	MET	5.7
1	K	118	ALA	5.7
2	E	462	TYR	5.7
2	E	333	THR	5.7
2	N	277	ILE	5.7
1	K	510	LYS	5.7
1	C	4	GLY	5.7
2	L	123	ALA	5.7
4	P	75	ALA	5.7
1	A	209	MET	5.6
1	I	412	SER	5.6
1	C	194	PRO	5.6
1	C	201	PRO	5.6
2	F	119	LEU	5.6
2	D	222	ASN	5.6
1	K	76	GLY	5.6
2	N	360	ARG	5.6
2	F	172	THR	5.6
2	M	165	ALA	5.6
1	C	220	MET	5.6
2	F	336	GLN	5.6
1	K	348	GLU	5.6
1	A	219	ALA	5.6
2	E	70	THR	5.6
2	F	401	GLU	5.6
2	M	365	GLY	5.6
1	J	345	PRO	5.6
1	I	85	ASP	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	394	PRO	5.5
1	K	47	ALA	5.5
1	K	266	LEU	5.5
1	I	147	ILE	5.5
2	F	277	ILE	5.5
1	K	395	VAL	5.5
1	I	536	ILE	5.5
2	D	120	ASN	5.5
1	A	458	LEU	5.5
2	N	339	LEU	5.5
1	I	233	GLY	5.5
1	C	422	ILE	5.5
1	C	398	SER	5.5
1	I	137	THR	5.5
1	I	348	GLU	5.5
1	C	193	ARG	5.5
1	I	136	GLY	5.4
2	F	164	ALA	5.4
1	A	74	GLU	5.4
2	F	205	ILE	5.4
2	F	16	GLY	5.4
1	B	114	GLU	5.4
1	I	560	PRO	5.4
2	F	348	ILE	5.4
2	F	287	MET	5.4
1	B	499	ALA	5.4
2	M	146	ARG	5.4
3	O	142	ASN	5.4
1	K	259	GLY	5.4
1	I	370	THR	5.3
1	J	388	GLY	5.4
2	L	282	GLY	5.4
1	C	273	THR	5.3
1	A	385	SER	5.3
2	F	215	SER	5.3
1	K	492	GLU	5.3
1	C	352	PRO	5.3
1	I	164	GLY	5.3
2	F	24	ALA	5.3
2	F	165	ALA	5.3
2	E	88	MET	5.3
1	C	424	TRP	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	431	SER	5.3
1	C	359	ALA	5.3
2	M	137	THR	5.3
1	K	519	ILE	5.3
2	L	421	PHE	5.3
2	D	101	ASP	5.3
1	B	195	VAL	5.3
2	F	449	GLY	5.3
2	M	224	ALA	5.3
1	A	180	GLU	5.3
1	I	325	ASP	5.3
2	E	374	ASP	5.3
2	L	278	PRO	5.3
2	L	260	MET	5.3
1	I	289	ALA	5.2
1	I	434	ALA	5.2
1	I	400	LEU	5.2
1	I	474	ASP	5.2
2	M	229	ILE	5.2
2	L	215	SER	5.2
1	A	229	PRO	5.2
1	C	171	PRO	5.2
1	K	229	PRO	5.2
2	D	62	GLU	5.2
2	N	276	GLU	5.2
1	B	531	LYS	5.2
2	N	12	THR	5.2
2	N	333	THR	5.2
2	D	325	ILE	5.2
2	N	86	LYS	5.2
1	C	296	VAL	5.2
1	C	376	GLY	5.2
2	F	273	ALA	5.2
1	A	54	ASP	5.2
1	I	566	ALA	5.2
1	K	291	THR	5.1
2	F	117	LEU	5.1
1	A	238	GLN	5.1
2	M	442	LEU	5.1
1	K	220	MET	5.1
2	D	224	ALA	5.1
1	C	531	LYS	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	259	ASP	5.1
2	D	64	THR	5.1
2	N	288	TYR	5.1
4	H	97	THR	5.1
2	E	80	ALA	5.1
2	E	331	TYR	5.1
1	I	381	VAL	5.1
2	E	24	ALA	5.1
2	L	80	ALA	5.1
1	C	389	GLY	5.1
2	F	195	GLY	5.1
2	N	309	THR	5.1
1	C	166	TYR	5.1
1	C	321	ALA	5.1
2	E	30	GLY	5.1
1	J	327	THR	5.1
1	J	507	CYS	5.1
1	K	298	ALA	5.0
1	K	190	ARG	5.0
3	G	188	ARG	5.0
1	A	320	VAL	5.0
1	C	217	PRO	5.0
1	C	395	VAL	5.0
2	F	366	VAL	5.0
1	C	380	ILE	5.0
3	O	144	GLU	5.0
1	A	291	THR	5.0
1	K	367	LYS	5.0
1	K	346	ALA	5.0
2	N	340	SER	5.0
1	I	403	VAL	5.0
1	I	246	ASN	5.0
1	C	46	THR	5.0
1	I	379	THR	5.0
2	D	326	PRO	5.0
2	M	205	ILE	5.0
1	K	230	PHE	5.0
1	A	166	TYR	5.0
2	E	56	VAL	5.0
2	D	364	ASN	5.0
2	D	193	ALA	5.0
1	A	256	GLY	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	401	GLU	5.0
1	J	559	PHE	5.0
1	C	3	GLN	5.0
2	F	280	ARG	5.0
1	C	240	SER	5.0
1	C	143	PHE	5.0
1	K	261	GLU	5.0
2	D	28	ALA	5.0
2	N	173	VAL	5.0
4	H	62	LEU	4.9
1	A	152	ASP	4.9
1	K	292	SER	4.9
2	L	15	SER	4.9
2	N	142	ASN	4.9
2	F	26	ASP	4.9
1	C	355	ALA	4.9
1	I	324	ALA	4.9
1	I	209	MET	4.9
2	D	447	PRO	4.9
1	I	127	ASP	4.9
1	K	325	ASP	4.9
1	K	226	ILE	4.9
1	J	255	CYS	4.9
2	F	295	TYR	4.9
1	C	77	PRO	4.9
2	N	452	LYS	4.9
2	L	27	LEU	4.9
2	N	27	LEU	4.9
2	D	235	PRO	4.9
2	F	243	GLU	4.9
2	E	449	GLY	4.9
2	N	202	SER	4.9
2	M	310	GLN	4.9
2	M	81	ARG	4.9
1	C	28	CYS	4.8
2	M	128	GLU	4.8
1	I	45	ASP	4.8
1	J	478	ASP	4.8
2	E	142	ASN	4.8
2	M	71	THR	4.8
1	I	163	ALA	4.8
2	N	160	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	22	GLU	4.8
2	F	244	TYR	4.8
1	A	172	VAL	4.8
1	K	110	ALA	4.8
2	M	164	ALA	4.8
2	F	87	GLU	4.8
2	M	242	ALA	4.8
1	A	424	TRP	4.8
1	B	140	GLU	4.8
2	L	461	LYS	4.8
2	E	379	SER	4.8
2	N	287	MET	4.8
2	E	375	HIS	4.8
2	E	332	ILE	4.8
2	F	260	MET	4.8
2	F	310	GLN	4.8
1	I	256	GLY	4.8
1	K	389	GLY	4.8
1	A	293	ASN	4.8
2	E	121	PRO	4.8
1	A	333	ALA	4.8
1	K	388	GLY	4.8
1	I	135	LEU	4.8
1	J	189	VAL	4.8
1	B	192	ALA	4.7
1	A	45	ASP	4.7
2	L	281	ARG	4.7
2	L	52	GLU	4.7
2	N	432	ILE	4.7
1	C	405	ALA	4.7
1	A	435	LEU	4.7
1	B	470	LEU	4.7
1	J	254	GLY	4.7
2	E	289	THR	4.7
1	C	205	PHE	4.7
2	D	142	ASN	4.7
2	M	238	ALA	4.7
1	I	193	ARG	4.7
2	N	290	ASP	4.7
2	E	12	THR	4.7
2	D	80	ALA	4.7
1	K	551	ALA	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	330	GLY	4.7
2	M	131	ILE	4.7
1	K	550	ARG	4.7
1	C	68	GLY	4.7
1	B	278	GLY	4.6
1	C	368	VAL	4.6
1	K	376	GLY	4.6
2	N	282	GLY	4.6
1	K	79	MET	4.6
1	C	385	SER	4.6
1	A	194	PRO	4.6
1	J	210	ARG	4.6
2	E	37	ASP	4.6
1	C	81	ASN	4.6
2	M	129	GLN	4.6
1	I	119	TRP	4.6
1	B	77	PRO	4.6
1	B	473	PRO	4.6
1	B	486	VAL	4.6
1	J	140	GLU	4.6
2	D	302	GLU	4.6
1	A	144	THR	4.6
1	I	143	PHE	4.6
1	I	181	LEU	4.6
2	D	223	LYS	4.6
2	M	314	LEU	4.6
1	A	552	ARG	4.6
2	N	18	LEU	4.6
1	A	379	THR	4.6
1	A	299	ARG	4.6
1	I	172	VAL	4.6
2	F	173	VAL	4.6
1	C	86	GLY	4.6
1	I	165	GLU	4.6
2	N	286	TYR	4.6
1	B	108	VAL	4.6
1	B	349	GLY	4.6
2	E	149	LYS	4.6
1	C	291	THR	4.6
2	D	240	THR	4.6
1	K	560	PRO	4.6
1	A	375	GLU	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	128	GLU	4.6
1	B	507	CYS	4.6
1	K	186	THR	4.5
1	K	235	THR	4.5
2	L	29	TYR	4.5
2	F	168	ALA	4.5
1	I	300	GLU	4.5
2	F	315	SER	4.5
1	B	519	ILE	4.5
2	F	318	ASP	4.5
2	N	139	ASP	4.5
2	N	226	ASP	4.5
2	N	169	ARG	4.5
1	B	163	ALA	4.5
1	C	238	GLN	4.5
2	M	26	ASP	4.5
1	I	299	ARG	4.5
2	E	339	LEU	4.5
2	E	398	ILE	4.5
2	F	319	ASP	4.5
1	A	181	LEU	4.5
1	B	9	ILE	4.5
2	N	76	VAL	4.5
2	N	87	GLU	4.5
1	K	411	ALA	4.5
1	A	319	SER	4.5
2	N	136	SER	4.5
3	O	55	GLN	4.5
2	F	364	ASN	4.5
2	L	360	ARG	4.4
1	C	454	ILE	4.4
1	J	195	VAL	4.4
1	C	311	GLU	4.4
1	I	371	LEU	4.4
1	J	58	LEU	4.4
1	I	66	SER	4.4
1	K	213	ASP	4.4
2	M	228	THR	4.4
2	F	242	ALA	4.4
1	B	407	TRP	4.4
1	K	308	THR	4.4
1	C	169	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	429	ASN	4.4
2	M	142	ASN	4.4
2	N	370	LYS	4.4
2	F	11	ILE	4.4
1	K	26	ASP	4.4
2	M	28	ALA	4.4
2	N	63	THR	4.4
1	K	373	GLY	4.4
1	B	559	PHE	4.4
2	M	318	ASP	4.4
2	N	296	GLU	4.4
1	K	227	PRO	4.4
1	K	323	MET	4.4
2	L	431	SER	4.4
2	N	379	SER	4.4
1	I	42	LEU	4.4
2	E	310	GLN	4.4
2	N	119	LEU	4.4
2	N	411	TYR	4.3
1	K	228	GLY	4.3
1	I	559	PHE	4.3
1	K	91	LEU	4.3
2	E	281	ARG	4.3
1	C	501	HIS	4.3
1	K	442	ASN	4.3
4	H	23	ALA	4.3
1	A	60	VAL	4.3
1	C	172	VAL	4.3
2	D	44	GLY	4.3
1	I	141	PHE	4.3
2	E	252	HIS	4.3
1	I	242	ALA	4.3
2	F	193	ALA	4.3
2	D	432	ILE	4.3
1	A	223	THR	4.3
1	I	492	GLU	4.3
3	O	54	ASP	4.3
2	F	96	ILE	4.3
1	A	57	GLY	4.3
2	F	357	SER	4.3
1	C	300	GLU	4.3
1	I	190	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	148	LEU	4.3
2	N	68	LEU	4.3
1	C	70	PRO	4.3
1	I	237	THR	4.3
1	C	264	ASP	4.3
1	K	459	GLN	4.3
1	A	208	GLY	4.3
1	K	164	GLY	4.3
1	A	560	PRO	4.2
1	A	307	VAL	4.2
1	K	22	ALA	4.2
1	K	471	VAL	4.2
1	A	457	LEU	4.2
1	K	54	ASP	4.2
2	D	67	ASP	4.2
1	J	134	VAL	4.2
2	L	164	ALA	4.2
2	F	204	PHE	4.2
2	F	239	LEU	4.2
2	M	334	GLU	4.2
2	N	239	LEU	4.2
2	D	63	THR	4.2
1	J	63	PRO	4.2
2	E	82	LEU	4.2
4	P	84	HIS	4.2
2	E	207	GLU	4.2
2	L	346	LYS	4.2
1	A	553	TYR	4.2
1	A	88	GLN	4.2
2	E	148	GLN	4.2
2	N	132	GLN	4.2
1	K	420	PRO	4.2
2	F	145	VAL	4.2
1	J	475	ALA	4.2
1	K	350	TYR	4.2
2	E	299	GLY	4.2
1	C	85	ASP	4.2
2	L	124	ARG	4.2
1	I	185	HIS	4.2
2	F	329	THR	4.2
1	I	409	LEU	4.2
2	N	382	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	218	VAL	4.2
2	L	273	ALA	4.2
2	N	114	ILE	4.2
2	M	339	LEU	4.2
1	A	559	PHE	4.2
2	F	403	ALA	4.2
1	J	418	HIS	4.1
1	J	303	ILE	4.1
2	L	297	ARG	4.1
4	H	66	ARG	4.1
1	A	243	LYS	4.1
4	H	30	GLN	4.1
1	C	549	GLY	4.1
1	A	87	ILE	4.1
2	M	218	VAL	4.1
1	K	242	ALA	4.1
2	F	226	ASP	4.1
2	L	259	ASP	4.1
1	I	21	GLY	4.1
1	A	62	GLU	4.1
2	N	243	GLU	4.1
3	O	146	ARG	4.1
1	C	230	PHE	4.1
1	I	207	THR	4.1
1	I	507	CYS	4.1
2	D	311	ILE	4.1
2	D	365	GLY	4.1
1	I	557	GLU	4.1
1	B	227	PRO	4.1
1	K	275	PRO	4.1
1	A	136	GLY	4.1
1	C	17	LYS	4.1
2	M	249	HIS	4.1
1	K	290	ASN	4.1
2	F	175	PRO	4.1
2	E	309	THR	4.1
1	A	214	VAL	4.1
1	K	283	HIS	4.1
1	I	347	GLU	4.1
1	C	576	ALA	4.1
1	I	201	PRO	4.1
1	I	498	ASN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	427	GLN	4.1
1	I	40	ILE	4.1
1	K	404	GLY	4.1
1	I	368	VAL	4.1
2	N	295	TYR	4.1
1	C	407	TRP	4.1
1	C	170	GLU	4.0
1	K	310	ALA	4.0
1	B	372	GLY	4.0
1	J	351	PRO	4.0
1	K	351	PRO	4.0
2	D	385	ALA	4.0
1	K	57	GLY	4.0
2	M	38	GLY	4.0
1	I	339	SER	4.0
1	K	412	SER	4.0
1	K	553	TYR	4.0
2	L	411	TYR	4.0
2	N	75	LEU	4.0
1	C	243	LYS	4.0
1	I	380	ILE	4.0
1	J	346	ALA	4.0
1	C	168	VAL	4.0
1	A	167	THR	4.0
1	C	575	LYS	4.0
2	F	12	THR	4.0
2	N	126	LYS	4.0
1	C	87	ILE	4.0
1	K	414	ALA	4.0
2	E	278	PRO	4.0
2	F	17	PRO	4.0
2	F	342	GLU	4.0
2	D	315	SER	4.0
1	A	140	GLU	4.0
1	B	193	ARG	4.0
1	C	348	GLU	4.0
2	F	276	GLU	4.0
2	F	354	PRO	4.0
2	N	200	GLU	4.0
1	B	129	VAL	4.0
1	B	311	GLU	4.0
1	C	268	GLU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	302	GLU	4.0
1	J	495	LEU	4.0
2	E	201	LEU	4.0
2	L	68	LEU	4.0
1	B	364	ARG	4.0
2	N	171	ALA	4.0
2	F	115	THR	4.0
1	I	182	LYS	3.9
1	J	234	LYS	3.9
1	C	227	PRO	3.9
2	F	312	PRO	3.9
1	I	155	GLY	3.9
1	A	225	ALA	3.9
1	C	289	ALA	3.9
1	C	310	ALA	3.9
2	D	43	ARG	3.9
1	I	425	ASN	3.9
1	J	14	VAL	3.9
1	K	257	GLU	3.9
1	K	441	GLU	3.9
2	D	48	ILE	3.9
1	K	465	GLN	3.9
1	C	190	ARG	3.9
4	P	86	VAL	3.9
2	F	20	PHE	3.9
2	M	239	LEU	3.9
1	K	386	PRO	3.9
2	M	118	PRO	3.9
2	D	30	GLY	3.9
1	I	74	GLU	3.9
1	J	311	GLU	3.9
4	P	87	GLU	3.9
1	I	297	ALA	3.9
1	J	218	VAL	3.9
2	F	290	ASP	3.9
2	M	37	ASP	3.9
1	C	275	PRO	3.9
1	I	402	ILE	3.9
2	E	269	GLU	3.9
2	F	84	VAL	3.9
2	N	241	VAL	3.9
4	P	71	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	161	LYS	3.9
2	F	402	ASP	3.9
2	F	113	PRO	3.9
2	D	38	GLY	3.9
1	A	143	PHE	3.9
1	C	414	ALA	3.9
1	I	383	ALA	3.9
1	B	112	ASP	3.9
2	E	34	ASP	3.9
1	A	145	HIS	3.9
1	C	485	GLU	3.9
1	K	538	GLU	3.9
2	F	140	VAL	3.9
2	M	15	SER	3.9
2	E	452	LYS	3.8
1	B	520	LEU	3.8
2	F	375	HIS	3.8
2	M	244	TYR	3.8
2	F	130	PHE	3.8
2	F	302	GLU	3.8
1	B	367	LYS	3.8
2	F	143	THR	3.8
2	D	229	ILE	3.8
2	E	326	PRO	3.8
2	F	118	PRO	3.8
4	H	69	PRO	3.8
1	A	340	ARG	3.8
2	M	150	LEU	3.8
4	H	39	ARG	3.8
2	F	255	VAL	3.8
1	C	370	THR	3.8
2	M	240	THR	3.8
2	D	205	ILE	3.8
1	I	376	GLY	3.8
2	D	140	VAL	3.8
2	D	259	ASP	3.8
2	M	34	ASP	3.8
1	C	283	HIS	3.8
1	C	375	GLU	3.8
2	E	69	ALA	3.8
1	A	399	THR	3.8
1	A	349	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	139	PRO	3.8
1	I	473	PRO	3.8
1	C	378	VAL	3.8
2	D	76	VAL	3.8
2	E	47	VAL	3.8
1	K	434	ALA	3.8
2	N	363	ASN	3.8
2	D	85	SER	3.8
2	N	148	GLN	3.8
1	I	44	GLY	3.8
2	N	172	THR	3.8
1	A	51	VAL	3.8
2	E	362	MET	3.8
2	L	417	ALA	3.8
1	C	82	GLY	3.8
1	A	244	TRP	3.8
1	I	197	ARG	3.8
2	F	97	GLY	3.8
2	N	400	GLY	3.8
4	H	55	PRO	3.8
1	A	251	VAL	3.8
2	D	143	THR	3.8
2	L	450	GLU	3.8
1	C	473	PRO	3.7
1	K	246	ASN	3.7
2	E	357	SER	3.7
2	N	455	SER	3.7
2	N	256	ILE	3.7
2	N	423	ILE	3.7
1	C	112	ASP	3.7
1	B	259	GLY	3.7
1	I	417	ARG	3.7
1	J	451	ARG	3.7
1	K	554	VAL	3.7
1	C	239	GLN	3.7
1	K	425	ASN	3.7
2	M	371	THR	3.7
2	N	219	LEU	3.7
1	C	286	VAL	3.7
1	C	320	VAL	3.7
2	D	209	GLU	3.7
2	N	369	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	122	MET	3.7
2	D	175	PRO	3.7
2	E	99	PRO	3.7
2	N	350	PRO	3.7
1	A	429	SER	3.7
1	I	28	CYS	3.7
1	I	365	ALA	3.7
2	E	211	THR	3.7
2	N	96	ILE	3.7
2	L	125	ARG	3.7
2	M	341	ARG	3.7
2	N	81	ARG	3.7
2	N	281	ARG	3.7
1	I	86	GLY	3.7
1	K	169	GLU	3.7
1	C	448	PRO	3.7
2	E	319	ASP	3.7
2	L	324	PRO	3.7
1	I	392	SER	3.7
2	M	438	ILE	3.7
1	C	223	THR	3.7
1	I	552	ARG	3.7
2	E	21	VAL	3.7
2	F	249	HIS	3.7
1	I	88	GLN	3.7
2	E	132	GLN	3.7
1	B	237	THR	3.7
2	F	133	THR	3.7
2	E	173	VAL	3.7
2	L	141	MET	3.7
1	A	78	GLY	3.7
4	P	65	GLY	3.7
1	I	244	TRP	3.7
4	H	101	ASP	3.7
1	I	321	ALA	3.7
1	C	123	VAL	3.7
1	J	305	VAL	3.7
2	F	300	VAL	3.7
2	M	56	VAL	3.7
2	M	12	THR	3.7
2	L	40	GLY	3.7
1	I	227	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	139	PRO	3.7
1	C	252	TYR	3.7
1	I	562	TYR	3.7
2	F	132	GLN	3.7
2	N	194	MET	3.6
4	P	15	LEU	3.6
1	A	303	ILE	3.6
2	L	325	ILE	3.6
2	N	454	ILE	3.6
1	J	62	GLU	3.6
1	I	50	GLN	3.6
1	K	192	ALA	3.6
1	B	478	ASP	3.6
1	A	129	VAL	3.6
2	N	280	ARG	3.6
2	E	154	SER	3.6
2	N	221	LEU	3.6
1	C	402	ILE	3.6
1	I	39	ILE	3.6
1	K	288	ILE	3.6
2	E	135	ILE	3.6
2	E	329	THR	3.6
1	B	562	TYR	3.6
1	A	187	TRP	3.6
1	I	214	VAL	3.6
1	J	22	ALA	3.6
1	K	362	TYR	3.6
1	I	215	LEU	3.6
1	A	248	ASP	3.6
1	K	493	ASP	3.6
1	A	345	PRO	3.6
2	M	133	THR	3.6
1	A	321	ALA	3.6
1	I	405	ALA	3.6
1	K	60	VAL	3.6
2	F	144	LEU	3.6
2	L	382	LEU	3.6
2	N	166	GLN	3.6
1	A	21	GLY	3.6
1	C	45	ASP	3.6
2	N	14	ILE	3.6
1	K	364	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	8	TYR	3.6
2	E	230	GLU	3.6
2	L	49	GLU	3.6
1	A	562	TYR	3.6
1	B	242	ALA	3.6
1	K	72	ALA	3.6
1	K	219	ALA	3.6
2	M	23	ASN	3.6
3	G	162	ASN	3.6
2	E	313	ILE	3.6
1	I	150	PRO	3.5
1	A	551	ALA	3.5
1	A	555	SER	3.5
1	C	290	ASN	3.5
1	B	374	GLU	3.5
1	I	564	GLU	3.5
2	F	109	GLU	3.5
2	F	433	GLU	3.5
1	I	467	ILE	3.5
2	E	336	GLN	3.5
2	F	134	GLY	3.5
1	I	194	PRO	3.5
1	J	420	PRO	3.5
1	A	163	ALA	3.5
2	F	94	ASN	3.5
2	N	384	SER	3.5
1	A	327	THR	3.5
1	C	492	GLU	3.5
1	B	221	GLY	3.5
2	E	314	LEU	3.5
1	K	267	VAL	3.5
1	C	391	MET	3.5
2	N	24	ALA	3.5
2	M	225	ASP	3.5
2	F	337	ILE	3.5
1	A	507	CYS	3.5
1	B	11	GLY	3.5
1	C	396	THR	3.5
2	E	115	THR	3.5
2	E	261	THR	3.5
2	L	336	GLN	3.5
1	K	134	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	345	PRO	3.5
1	C	229	PRO	3.5
1	I	19	MET	3.5
1	A	16	ALA	3.5
2	F	131	ILE	3.5
2	F	252	HIS	3.5
1	A	18	GLY	3.5
1	C	246	ASN	3.5
2	D	426	GLY	3.5
2	L	51	SER	3.5
2	M	455	SER	3.5
1	I	186	THR	3.5
2	N	254	LEU	3.5
1	A	503	VAL	3.5
1	C	471	VAL	3.5
1	K	486	VAL	3.5
2	E	247	PHE	3.5
1	B	346	ALA	3.5
1	K	355	ALA	3.5
1	K	377	ALA	3.5
1	C	145	HIS	3.5
2	M	27	LEU	3.5
2	N	195	GLY	3.5
2	F	74	SER	3.5
1	B	218	VAL	3.5
1	I	202	ASN	3.5
2	M	427	GLN	3.5
2	E	25	LYS	3.5
1	A	515	ILE	3.5
2	L	48	ILE	3.5
1	A	148	LEU	3.5
2	M	144	LEU	3.5
1	A	376	GLY	3.5
1	C	390	ASP	3.5
2	F	155	GLY	3.5
1	A	258	ARG	3.5
1	J	261	GLU	3.5
2	L	20	PHE	3.5
1	I	302	SER	3.5
1	K	243	LYS	3.5
2	E	205	ILE	3.5
2	L	337	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	49	ALA	3.5
1	C	52	TYR	3.5
2	M	295	TYR	3.5
1	K	540	LEU	3.4
2	L	412	LEU	3.4
2	D	91	ARG	3.4
2	D	231	ARG	3.4
2	L	458	HIS	3.4
1	K	200	ASP	3.4
1	K	146	LYS	3.4
2	D	128	GLU	3.4
2	N	275	GLU	3.4
2	E	348	ILE	3.4
2	L	12	THR	3.4
1	I	68	GLY	3.4
1	C	117	TRP	3.4
2	N	252	HIS	3.4
1	A	300	GLU	3.4
2	F	374	ASP	3.4
2	M	7	GLU	3.4
4	P	8	GLU	3.4
2	M	114	ILE	3.4
2	F	235	PRO	3.4
2	N	186	PRO	3.4
2	D	23	ASN	3.4
2	D	288	TYR	3.4
2	E	103	LEU	3.4
2	E	174	ARG	3.4
2	E	282	GLY	3.4
2	N	175	PRO	3.4
2	N	355	LEU	3.4
1	C	293	ASN	3.4
1	C	428	TYR	3.4
1	C	486	VAL	3.4
2	L	231	ARG	3.4
1	A	119	TRP	3.4
1	A	358	LEU	3.4
1	A	383	ALA	3.4
1	K	289	ALA	3.4
2	M	298	ALA	3.4
2	N	435	SER	3.4
1	C	399	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	205	PHE	3.4
2	E	161	ASN	3.4
2	N	116	GLY	3.4
1	A	185	HIS	3.4
2	N	358	LEU	3.4
1	A	169	GLU	3.4
1	B	393	GLU	3.4
2	D	342	GLU	3.4
2	L	243	GLU	3.4
1	I	171	PRO	3.4
1	B	196	GLN	3.4
1	I	316	GLN	3.4
1	I	500	TYR	3.4
2	N	380	ASP	3.4
1	C	251	VAL	3.4
2	D	321	ARG	3.4
2	F	156	SER	3.4
1	A	235	THR	3.4
1	J	233	GLY	3.4
1	K	202	ASN	3.4
1	C	369	ILE	3.4
2	F	152	ILE	3.4
1	C	434	ALA	3.4
2	D	439	ALA	3.4
2	F	123	ALA	3.4
1	C	74	GLU	3.4
2	D	17	PRO	3.4
2	F	356	PRO	3.4
2	F	153	PHE	3.4
2	L	435	SER	3.4
1	C	383	ALA	3.3
1	B	201	PRO	3.3
1	K	180	GLU	3.3
1	C	552	ARG	3.3
2	E	378	VAL	3.3
2	N	268	ARG	3.3
1	A	26	ASP	3.3
1	K	474	ASP	3.3
1	K	207	THR	3.3
2	F	309	THR	3.3
1	A	425	ASN	3.3
1	I	118	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	162	PRO	3.3
1	J	194	PRO	3.3
1	I	353	TYR	3.3
1	J	265	VAL	3.3
1	I	493	ASP	3.3
2	D	137	THR	3.3
2	E	171	ALA	3.3
2	E	266	ALA	3.3
1	I	522	PHE	3.3
2	D	118	PRO	3.3
2	F	378	VAL	3.3
1	A	20	LEU	3.3
1	B	306	GLY	3.3
2	L	126	LYS	3.3
2	N	261	THR	3.3
1	K	187	TRP	3.3
2	N	262	ASN	3.3
2	E	300	VAL	3.3
2	N	127	PRO	3.3
2	N	237	MET	3.3
2	N	463	TYR	3.3
2	E	40	GLY	3.3
1	J	116	LYS	3.3
2	N	259	ASP	3.3
1	A	324	ALA	3.3
4	H	26	ALA	3.3
2	F	79	VAL	3.3
2	M	169	ARG	3.3
3	O	15	ARG	3.3
2	F	317	PRO	3.3
2	N	151	PRO	3.3
2	F	291	LEU	3.3
2	F	436	LEU	3.3
2	F	463	TYR	3.3
1	I	128	GLU	3.3
1	J	208	GLY	3.3
2	M	346	LYS	3.3
1	C	13	ALA	3.3
1	I	177	ASP	3.3
1	I	51	VAL	3.3
2	E	145	VAL	3.3
1	B	233	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	62	GLU	3.3
1	A	130	ARG	3.3
1	C	43	ASP	3.3
2	D	139	ASP	3.3
2	F	150	LEU	3.3
1	A	171	PRO	3.3
1	K	312	TYR	3.3
2	F	263	TYR	3.3
1	J	128	GLU	3.2
2	F	198	GLN	3.2
4	H	81	PHE	3.2
1	J	403	VAL	3.2
2	L	439	ALA	3.2
2	D	88	MET	3.2
2	D	354	PRO	3.2
2	E	416	ASP	3.2
2	F	313	ILE	3.2
1	B	70	PRO	3.2
2	L	175	PRO	3.2
1	K	232	SER	3.2
2	F	85	SER	3.2
2	L	240	THR	3.2
2	N	15	SER	3.2
2	F	222	ASN	3.2
2	M	195	GLY	3.2
2	N	157	GLY	3.2
1	K	32	GLU	3.2
1	C	192	ALA	3.2
1	C	409	LEU	3.2
1	J	434	ALA	3.2
1	K	365	ALA	3.2
2	F	241	VAL	3.2
2	F	439	ALA	3.2
2	M	171	ALA	3.2
2	F	151	PRO	3.2
2	N	324	PRO	3.2
1	A	325	ASP	3.2
1	C	325	ASP	3.2
1	C	493	ASP	3.2
2	F	349	TYR	3.2
4	H	78	LYS	3.2
1	B	406	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	140	GLU	3.2
2	F	185	GLU	3.2
1	C	64	VAL	3.2
1	K	238	GLN	3.2
2	F	339	LEU	3.2
2	M	273	ALA	3.2
1	A	447	TYR	3.2
1	C	274	ASP	3.2
1	K	112	ASP	3.2
1	A	292	SER	3.2
1	C	392	SER	3.2
2	F	63	THR	3.2
2	F	53	GLU	3.2
2	E	272	ALA	3.2
2	N	312	PRO	3.2
2	L	463	TYR	3.2
1	C	91	LEU	3.2
2	D	204	PHE	3.2
1	K	378	VAL	3.2
2	E	73	VAL	3.2
2	N	21	VAL	3.2
2	N	255	VAL	3.2
4	H	35	THR	3.2
4	P	97	THR	3.2
1	A	165	GLU	3.2
1	C	297	ALA	3.2
1	I	391	MET	3.2
1	J	301	ALA	3.2
1	A	50	GLN	3.2
1	A	161	LYS	3.2
1	C	182	LYS	3.2
2	F	126	LYS	3.2
1	I	513	TYR	3.2
1	A	404	GLY	3.2
1	B	230	PHE	3.2
1	K	205	PHE	3.2
1	K	415	PHE	3.2
2	D	103	LEU	3.2
1	B	172	VAL	3.2
1	I	200	ASP	3.2
1	J	129	VAL	3.2
2	M	453	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	253	VAL	3.2
1	A	277	THR	3.2
1	B	326	SER	3.2
2	M	237	MET	3.2
1	B	180	GLU	3.2
1	B	461	GLU	3.2
2	D	266	ALA	3.2
4	P	16	ALA	3.2
1	C	124	LYS	3.2
2	N	129	GLN	3.2
1	B	351	PRO	3.2
1	J	214	VAL	3.2
1	K	251	VAL	3.2
2	F	384	SER	3.1
2	L	36	LYS	3.1
2	M	234	THR	3.1
2	N	307	SER	3.1
2	N	201	LEU	3.1
2	N	227	PRO	3.1
1	I	11	GLY	3.1
1	I	259	GLY	3.1
1	C	530	ILE	3.1
1	B	234	LYS	3.1
2	M	252	HIS	3.1
2	L	156	SER	3.1
2	N	143	THR	3.1
2	N	329	THR	3.1
1	I	31	GLY	3.1
1	J	68	GLY	3.1
1	J	132	GLY	3.1
2	E	102	GLY	3.1
1	B	573	ALA	3.1
1	K	374	GLU	3.1
2	E	221	LEU	3.1
2	L	74	SER	3.1
2	N	204	PHE	3.1
1	A	155	GLY	3.1
2	E	365	GLY	3.1
2	F	330	GLY	3.1
1	C	119	TRP	3.1
1	A	8	LYS	3.1
1	B	365	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	31	ALA	3.1
2	D	249	HIS	3.1
1	J	20	LEU	3.1
2	F	296	GLU	3.1
2	M	296	GLU	3.1
1	B	55	THR	3.1
1	B	125	PRO	3.1
1	K	223	THR	3.1
1	K	239	GLN	3.1
2	D	136	SER	3.1
2	L	391	ASP	3.1
2	D	104	PRO	3.1
2	N	284	PRO	3.1
1	C	209	MET	3.1
1	B	400	LEU	3.1
1	I	58	LEU	3.1
1	I	32	GLU	3.1
1	C	63	PRO	3.1
1	A	79	MET	3.1
1	C	277	THR	3.1
2	E	156	SER	3.1
2	E	356	PRO	3.1
2	N	462	TYR	3.1
1	C	426	GLY	3.1
2	N	299	GLY	3.1
2	D	446	LEU	3.1
1	C	417	ARG	3.1
1	I	375	GLU	3.1
4	H	64	ARG	3.1
1	K	1	MET	3.1
1	K	352	PRO	3.1
2	D	350	PRO	3.1
2	L	317	PRO	3.1
1	K	142	GLY	3.1
2	D	34	ASP	3.1
4	H	4	ILE	3.1
1	B	10	ALA	3.1
1	I	293	ASN	3.1
1	J	333	ALA	3.1
2	D	31	ALA	3.1
2	N	388	ASN	3.1
1	A	173	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	401	ARG	3.1
1	I	123	VAL	3.1
2	N	91	ARG	3.1
1	I	336	GLU	3.1
1	C	21	GLY	3.0
1	C	312	TYR	3.0
1	K	353	TYR	3.0
1	I	390	ASP	3.0
2	N	197	THR	3.0
1	J	225	ALA	3.0
2	L	55	ALA	3.0
2	N	28	ALA	3.0
1	J	574	PHE	3.0
1	B	210	ARG	3.0
1	B	299	ARG	3.0
1	I	265	VAL	3.0
2	F	25	LYS	3.0
2	N	199	ARG	3.0
2	E	49	GLU	3.0
2	E	265	GLU	3.0
1	K	458	LEU	3.0
2	M	132	GLN	3.0
3	O	27	LEU	3.0
1	C	207	THR	3.0
1	K	424	TRP	3.0
2	E	371	THR	3.0
1	K	255	CYS	3.0
1	B	303	ILE	3.0
2	M	138	ILE	3.0
1	B	142	GLY	3.0
1	B	295	PRO	3.0
3	G	134	ALA	3.0
1	B	302	SER	3.0
1	K	43	ASP	3.0
2	L	197	THR	3.0
2	M	329	THR	3.0
1	I	65	VAL	3.0
1	K	314	ARG	3.0
2	L	41	ARG	3.0
2	F	135	ILE	3.0
1	C	334	LEU	3.0
1	B	222	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	52	TYR	3.0
2	N	354	PRO	3.0
1	I	469	GLN	3.0
4	H	11	GLN	3.0
1	J	512	ALA	3.0
1	K	13	ALA	3.0
1	A	396	THR	3.0
1	C	200	ASP	3.0
1	I	179	THR	3.0
1	K	384	VAL	3.0
2	E	140	VAL	3.0
2	F	125	ARG	3.0
1	C	287	LEU	3.0
2	F	161	ASN	3.0
2	L	314	LEU	3.0
1	K	150	PRO	3.0
2	E	45	GLY	3.0
2	N	285	GLY	3.0
2	N	422	PHE	3.0
2	F	111	ARG	3.0
1	I	133	MET	3.0
1	J	396	THR	3.0
2	N	211	THR	3.0
1	I	470	LEU	3.0
1	B	204	PRO	3.0
1	I	431	PHE	3.0
1	J	324	ALA	3.0
1	J	563	PHE	3.0
1	K	321	ALA	3.0
1	K	375	GLU	3.0
2	D	130	PHE	3.0
2	L	397	ALA	3.0
1	K	320	VAL	3.0
2	N	325	ILE	3.0
2	E	355	LEU	3.0
1	B	555	SER	3.0
1	I	43	ASP	3.0
2	D	331	TYR	3.0
2	F	284	PRO	3.0
1	B	290	ASN	3.0
1	I	575	LYS	3.0
2	M	123	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	335	ARG	3.0
2	E	138	ILE	2.9
2	F	100	ILE	2.9
2	F	294	ILE	2.9
1	A	215	LEU	2.9
1	C	281	LEU	2.9
1	I	430	LEU	2.9
1	K	42	LEU	2.9
2	F	358	LEU	2.9
4	H	52	LEU	2.9
1	A	179	THR	2.9
1	C	478	ASP	2.9
2	D	51	SER	2.9
2	F	234	THR	2.9
1	K	11	GLY	2.9
1	K	549	GLY	2.9
1	I	59	LYS	2.9
1	K	473	PRO	2.9
1	J	423	ASN	2.9
1	K	421	ALA	2.9
2	D	388	ASN	2.9
1	C	364	ARG	2.9
1	I	168	VAL	2.9
2	D	450	GLU	2.9
2	F	129	GLN	2.9
2	N	48	ILE	2.9
4	H	82	GLN	2.9
1	A	302	SER	2.9
1	A	350	TYR	2.9
1	K	508	SER	2.9
2	D	199	ARG	2.9
1	I	176	GLU	2.9
1	I	294	MET	2.9
2	L	407	ASN	2.9
1	A	146	LYS	2.9
1	K	82	GLY	2.9
2	E	303	GLY	2.9
2	M	330	GLY	2.9
1	A	428	TYR	2.9
2	M	60	PHE	2.9
1	C	232	SER	2.9
1	I	245	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	26	ASP	2.9
1	K	145	HIS	2.9
1	B	294	MET	2.9
2	E	363	ASN	2.9
2	D	206	GLN	2.9
1	K	124	LYS	2.9
2	M	86	LYS	2.9
1	A	230	PHE	2.9
1	A	473	PRO	2.9
1	C	16	ALA	2.9
1	A	446	ASP	2.9
1	I	509	MET	2.9
1	K	302	SER	2.9
2	M	174	ARG	2.9
2	N	107	THR	2.9
2	N	292	ALA	2.9
2	N	396	VAL	2.9
2	E	26	ASP	2.9
1	A	485	GLU	2.9
1	K	62	GLU	2.9
2	F	184	GLU	2.9
1	A	117	TRP	2.9
2	L	30	GLY	2.9
2	N	147	GLY	2.9
2	D	68	LEU	2.9
2	M	324	PRO	2.9
2	M	404	LEU	2.9
2	N	113	PRO	2.9
2	N	150	LEU	2.9
1	A	224	ALA	2.9
1	I	87	ILE	2.9
2	E	63	THR	2.9
2	F	333	THR	2.9
1	K	45	ASP	2.9
1	B	492	GLU	2.9
1	I	257	GLU	2.9
1	K	33	GLU	2.9
2	N	265	GLU	2.9
2	M	364	ASN	2.9
1	A	142	GLY	2.9
1	B	366	GLY	2.9
4	P	20	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	543	PRO	2.9
3	O	188	ARG	2.9
1	I	79	MET	2.9
2	L	160	ALA	2.9
1	I	326	SER	2.9
2	D	12	THR	2.9
4	P	79	GLU	2.9
4	P	92	GLU	2.9
2	F	425	GLN	2.9
1	A	199	LEU	2.9
1	B	58	LEU	2.9
1	I	2	ILE	2.8
1	A	77	PRO	2.8
1	I	362	TYR	2.8
2	N	11	ILE	2.8
2	N	146	ARG	2.8
3	G	154	ILE	2.8
1	C	475	ALA	2.8
1	J	204	PRO	2.8
2	F	213	ALA	2.8
1	I	120	THR	2.8
1	I	432	THR	2.8
1	K	555	SER	2.8
2	D	371	THR	2.8
1	I	169	GLU	2.8
1	I	266	LEU	2.8
1	K	347	GLU	2.8
1	K	502	GLU	2.8
1	I	329	ARG	2.8
2	D	14	ILE	2.8
2	L	32	ILE	2.8
1	B	500	TYR	2.8
1	I	344	MET	2.8
2	F	28	ALA	2.8
2	N	272	ALA	2.8
1	C	339	SER	2.8
1	C	559	PHE	2.8
1	I	538	GLU	2.8
1	J	53	GLU	2.8
2	F	22	GLU	2.8
2	L	408	ASP	2.8
1	B	49	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	413	GLN	2.8
2	M	46	GLN	2.8
1	K	329	ARG	2.8
2	D	430	ARG	2.8
2	N	65	GLY	2.8
2	F	411	TYR	2.8
1	I	333	ALA	2.8
1	A	116	LYS	2.8
1	C	234	LYS	2.8
1	K	432	THR	2.8
2	M	115	THR	2.8
1	A	348	GLU	2.8
1	C	44	GLY	2.8
1	C	83	ILE	2.8
1	K	37	GLY	2.8
1	K	248	ASP	2.8
1	K	264	ASP	2.8
1	K	539	ILE	2.8
2	F	106	ILE	2.8
2	N	84	VAL	2.8
1	C	362	TYR	2.8
2	F	266	ALA	2.8
2	N	104	PRO	2.8
2	E	23	ASN	2.8
3	G	142	ASN	2.8
2	E	446	LEU	2.8
1	A	309	ILE	2.8
1	C	126	GLY	2.8
1	C	257	GLU	2.8
1	I	208	GLY	2.8
1	K	68	GLY	2.8
1	K	300	GLU	2.8
1	K	366	GLY	2.8
2	E	71	THR	2.8
2	D	336	GLN	2.8
2	F	265	GLU	2.8
2	M	248	GLU	2.8
1	J	264	ASP	2.8
2	N	319	ASP	2.8
1	J	118	ALA	2.8
1	A	368	VAL	2.8
1	I	226	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	21	VAL	2.8
2	M	232	ILE	2.8
2	E	147	GLY	2.8
2	F	116	GLY	2.8
1	B	525	GLU	2.8
1	C	535	SER	2.8
1	C	504	ASP	2.8
2	D	361	LEU	2.8
2	F	231	ARG	2.8
2	M	231	ARG	2.8
2	L	194	MET	2.8
1	C	161	LYS	2.8
1	J	57	GLY	2.8
1	J	531	LYS	2.8
2	E	461	LYS	2.8
2	F	335	GLY	2.8
1	A	346	ALA	2.8
1	C	429	SER	2.8
1	C	432	THR	2.8
3	G	48	GLU	2.8
1	C	540	LEU	2.8
1	J	270	PRO	2.8
1	K	215	LEU	2.8
4	H	71	LEU	2.8
1	I	248	ASP	2.8
2	F	34	ASP	2.8
2	L	26	ASP	2.8
1	A	255	CYS	2.7
1	K	113	ARG	2.7
2	L	120	ASN	2.7
2	L	341	ARG	2.7
1	I	124	LYS	2.7
1	B	91	LEU	2.7
2	D	164	ALA	2.7
2	E	200	GLU	2.7
2	E	361	LEU	2.7
2	M	403	ALA	2.7
1	I	229	PRO	2.7
1	I	387	PRO	2.7
1	J	302	SER	2.7
1	K	90	PRO	2.7
1	K	125	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	175	PRO	2.7
2	N	51	SER	2.7
1	C	545	LEU	2.7
1	K	58	LEU	2.7
2	L	436	LEU	2.7
1	B	538	GLU	2.7
2	E	127	PRO	2.7
1	C	555	SER	2.7
1	I	203	THR	2.7
2	M	220	PHE	2.7
1	A	286	VAL	2.7
1	C	267	VAL	2.7
1	I	443	VAL	2.7
2	F	138	ILE	2.7
2	D	281	ARG	2.7
1	B	567	MET	2.7
2	D	346	LYS	2.7
1	B	81	ASN	2.7
2	D	262	ASN	2.7
2	E	95	GLY	2.7
2	L	339	LEU	2.7
2	N	120	ASN	2.7
1	B	16	ALA	2.7
3	O	163	ALA	2.7
4	P	50	ALA	2.7
1	B	563	PHE	2.7
1	C	336	GLU	2.7
1	J	180	GLU	2.7
1	K	332	GLU	2.7
2	E	191	PHE	2.7
2	M	204	PHE	2.7
2	D	228	THR	2.7
2	N	156	SER	2.7
1	C	54	ASP	2.7
1	J	200	ASP	2.7
1	J	446	ASP	2.7
2	L	457	ASP	2.7
2	M	408	ASP	2.7
2	M	68	LEU	2.7
1	A	290	ASN	2.7
1	C	386	PRO	2.7
1	K	165	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	338	GLN	2.7
2	M	450	GLU	2.7
1	B	146	LYS	2.7
1	K	265	VAL	2.7
2	D	124	ARG	2.7
2	L	91	ARG	2.7
2	L	228	THR	2.7
2	E	27	LEU	2.7
1	A	231	GLY	2.7
1	A	306	GLY	2.7
1	I	126	GLY	2.7
2	D	95	GLY	2.7
1	I	356	ALA	2.7
2	D	168	ALA	2.7
2	L	142	ASN	2.7
2	M	375	HIS	2.7
2	F	350	PRO	2.7
1	K	262	MET	2.7
1	K	299	ARG	2.7
2	M	336	GLN	2.7
1	B	235	THR	2.7
1	K	181	LEU	2.7
1	K	470	LEU	2.7
2	F	75	LEU	2.7
1	J	385	SER	2.7
2	D	359	SER	2.7
2	F	90	GLY	2.7
1	A	43	ASP	2.7
2	D	226	ASP	2.7
2	L	226	ASP	2.7
1	C	110	ALA	2.7
1	I	216	PHE	2.7
1	I	475	ALA	2.7
2	N	131	ILE	2.7
1	I	250	VAL	2.7
2	E	22	GLU	2.7
2	N	381	GLN	2.7
2	M	82	LEU	2.7
1	K	535	SER	2.7
4	H	99	GLY	2.7
1	C	219	ALA	2.6
1	J	112	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	315	ASP	2.6
1	K	331	ALA	2.6
1	C	40	ILE	2.6
1	A	204	PRO	2.6
1	K	123	VAL	2.6
1	K	276	LYS	2.6
2	L	114	ILE	2.6
1	J	188	PRO	2.6
2	N	410	ARG	2.6
1	C	175	LEU	2.6
1	A	278	GLY	2.6
1	B	370	THR	2.6
1	C	137	THR	2.6
1	I	572	GLY	2.6
2	F	240	THR	2.6
2	M	333	THR	2.6
1	A	297	ALA	2.6
1	C	421	ALA	2.6
1	C	505	ALA	2.6
2	N	298	ALA	2.6
1	I	112	ASP	2.6
1	K	85	ASP	2.6
2	L	318	ASP	2.6
2	L	353	ASP	2.6
2	N	232	ILE	2.6
1	A	394	PRO	2.6
1	K	121	PRO	2.6
2	D	150	LEU	2.6
2	N	23	ASN	2.6
2	E	270	ILE	2.6
1	B	464	LEU	2.6
2	D	436	LEU	2.6
1	A	246	ASN	2.6
1	C	536	ILE	2.6
1	I	422	ILE	2.6
2	D	196	ILE	2.6
2	E	160	ALA	2.6
2	N	106	ILE	2.6
1	B	327	THR	2.6
1	J	237	THR	2.6
1	K	396	THR	2.6
2	F	258	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	326	SER	2.6
1	A	506	TYR	2.6
1	B	516	MET	2.6
1	K	326	SER	2.6
2	D	29	TYR	2.6
2	E	283	TYR	2.6
2	N	231	ARG	2.6
1	B	213	ASP	2.6
1	A	347	GLU	2.6
1	C	50	GLN	2.6
1	I	342	GLU	2.6
1	C	146	LYS	2.6
2	M	35	ILE	2.6
1	J	296	VAL	2.6
2	E	193	ALA	2.6
2	E	397	ALA	2.6
1	K	334	LEU	2.6
1	K	457	LEU	2.6
1	I	295	PRO	2.6
1	I	438	TRP	2.6
1	K	407	TRP	2.6
1	C	216	PHE	2.6
1	I	17	LYS	2.6
1	I	374	GLU	2.6
2	E	166	GLN	2.6
2	L	373	GLU	2.6
1	A	9	ILE	2.6
1	C	360	ALA	2.6
1	I	360	ALA	2.6
1	K	503	VAL	2.6
2	L	13	TYR	2.6
1	A	151	PRO	2.6
1	I	277	THR	2.6
1	A	339	SER	2.6
1	J	560	PRO	2.6
2	E	284	PRO	2.6
2	L	186	PRO	2.6
2	M	289	THR	2.6
2	N	356	PRO	2.6
2	D	250	ASP	2.6
1	I	549	GLY	2.6
2	L	22	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	47	VAL	2.6
1	J	262	MET	2.6
4	H	90	MET	2.6
1	I	394	PRO	2.6
2	N	293	THR	2.6
2	D	156	SER	2.5
2	L	422	PHE	2.5
1	A	548	ILE	2.5
1	I	337	ILE	2.5
1	I	132	GLY	2.5
2	D	345	ARG	2.5
2	E	198	GLN	2.5
2	E	401	GLU	2.5
1	A	220	MET	2.5
2	L	280	ARG	2.5
1	I	423	ASN	2.5
2	L	222	ASN	2.5
1	C	184	TYR	2.5
1	I	166	TYR	2.5
2	N	203	TYR	2.5
1	J	352	PRO	2.5
1	J	55	THR	2.5
1	B	435	LEU	2.5
2	F	232	ILE	2.5
1	I	14	VAL	2.5
1	I	73	VAL	2.5
1	B	183	MET	2.5
1	B	190	ARG	2.5
1	A	546	GLU	2.5
1	I	271	GLU	2.5
2	D	7	GLU	2.5
2	D	160	ALA	2.5
2	E	46	GLN	2.5
2	N	318	ASP	2.5
1	B	90	PRO	2.5
1	I	313	PHE	2.5
4	H	73	PRO	2.5
1	I	288	ILE	2.5
1	J	211	ILE	2.5
2	L	14	ILE	2.5
2	F	174	ARG	2.5
2	N	300	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	94	VAL	2.5
4	P	22	GLY	2.5
1	K	356	ALA	2.5
4	H	5	ALA	2.5
2	D	53	GLU	2.5
1	J	562	TYR	2.5
1	C	276	LYS	2.5
2	F	98	LYS	2.5
1	K	28	CYS	2.5
1	A	75	LEU	2.5
1	B	212	LEU	2.5
2	D	459	ILE	2.5
4	H	51	LEU	2.5
1	K	23	ARG	2.5
1	K	443	VAL	2.5
2	D	241	VAL	2.5
2	M	236	ARG	2.5
2	N	426	GLY	2.5
1	C	324	ALA	2.5
2	M	435	SER	2.5
1	A	114	GLU	2.5
1	K	271	GLU	2.5
1	K	469	GLN	2.5
1	I	213	ASP	2.5
2	E	68	LEU	2.5
2	M	358	LEU	2.5
2	N	328	LEU	2.5
1	J	226	ILE	2.5
2	E	167	ILE	2.5
2	N	332	ILE	2.5
2	E	301	VAL	2.5
1	K	21	GLY	2.5
2	E	83	GLY	2.5
2	F	341	ARG	2.5
1	I	110	ALA	2.5
2	L	115	THR	2.5
3	O	52	ALA	2.5
2	E	15	SER	2.5
1	C	271	GLU	2.5
1	I	53	GLU	2.5
2	L	276	GLU	2.5
2	L	446	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	489	ILE	2.5
2	F	57	ILE	2.5
1	I	60	VAL	2.5
2	M	65	GLY	2.5
1	I	158	LYS	2.5
1	K	379	THR	2.5
1	K	511	LYS	2.5
2	L	261	THR	2.5
2	M	154	SER	2.5
1	A	184	TYR	2.5
2	L	7	GLU	2.5
2	L	462	TYR	2.5
2	M	331	TYR	2.5
2	N	7	GLU	2.5
2	M	106	ILE	2.5
1	C	213	ASP	2.5
1	K	171	PRO	2.5
2	N	391	ASP	2.5
1	B	209	MET	2.5
1	K	209	MET	2.5
2	D	369	GLY	2.5
2	L	195	GLY	2.5
2	F	223	LYS	2.5
1	C	482	LEU	2.4
1	J	399	THR	2.4
2	D	258	THR	2.4
2	F	18	LEU	2.4
2	N	89	LEU	2.4
1	B	352	PRO	2.4
1	J	315	ASP	2.4
1	K	381	VAL	2.4
2	M	354	PRO	2.4
2	D	81	ARG	2.4
1	A	382	GLY	2.4
1	I	76	GLY	2.4
2	E	44	GLY	2.4
2	N	279	GLY	2.4
1	K	419	PHE	2.4
2	M	422	PHE	2.4
1	A	46	THR	2.4
1	K	67	THR	2.4
1	K	120	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	147	ILE	2.4
2	F	283	TYR	2.4
2	M	311	ILE	2.4
2	F	217	SER	2.4
1	A	168	VAL	2.4
1	A	249	VAL	2.4
1	A	543	PRO	2.4
1	C	323	MET	2.4
1	C	345	PRO	2.4
2	D	194	MET	2.4
2	D	324	PRO	2.4
1	B	248	ASP	2.4
1	J	221	GLY	2.4
2	F	304	LYS	2.4
1	C	526	ALA	2.4
2	E	328	LEU	2.4
2	N	412	LEU	2.4
1	I	419	PHE	2.4
2	M	100	ILE	2.4
1	B	523	TYR	2.4
2	N	283	TYR	2.4
1	K	88	GLN	2.4
1	K	552	ARG	2.4
2	E	104	PRO	2.4
2	E	202	SER	2.4
2	F	202	SER	2.4
2	F	269	GLU	2.4
2	F	44	GLY	2.4
2	N	149	LYS	2.4
1	A	407	TRP	2.4
1	C	72	ALA	2.4
1	C	225	ALA	2.4
1	K	577	LEU	2.4
2	D	245	LEU	2.4
1	J	187	TRP	2.4
2	N	188	ALA	2.4
1	K	81	ASN	2.4
2	D	348	ILE	2.4
1	A	250	VAL	2.4
1	C	51	VAL	2.4
1	C	167	THR	2.4
1	A	63	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	50	GLN	2.4
2	D	49	GLU	2.4
2	D	166	GLN	2.4
2	D	434	GLU	2.4
2	F	107	THR	2.4
2	F	322	THR	2.4
2	N	46	GLN	2.4
2	N	216	ARG	2.4
1	J	473	PRO	2.4
1	B	508	SER	2.4
2	M	315	SER	2.4
1	A	42	LEU	2.4
1	K	512	ALA	2.4
1	J	202	ASN	2.4
1	C	262	MET	2.4
2	E	169	ARG	2.4
4	P	1	MET	2.4
1	C	186	THR	2.4
1	I	510	LYS	2.4
1	J	227	PRO	2.4
1	K	203	THR	2.4
1	K	217	PRO	2.4
2	D	39	THR	2.4
2	F	197	THR	2.4
2	M	22	GLU	2.4
2	N	206	GLN	2.4
1	I	287	LEU	2.4
1	I	292	SER	2.4
1	I	358	LEU	2.4
1	J	61	GLY	2.4
1	J	319	SER	2.4
4	H	36	LEU	2.4
1	I	355	ALA	2.4
2	E	415	ALA	2.4
2	N	273	ALA	2.4
1	J	337	ILE	2.4
2	D	100	ILE	2.4
2	M	332	ILE	2.4
3	G	201	ILE	2.4
1	A	138	VAL	2.4
1	C	153	VAL	2.4
1	I	340	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	544	VAL	2.4
2	M	13	TYR	2.4
2	N	393	ARG	2.4
1	K	8	LYS	2.4
1	A	53	GLU	2.4
1	A	432	THR	2.4
1	C	55	THR	2.4
1	I	485	GLU	2.4
1	J	435	LEU	2.4
2	F	314	LEU	2.4
2	F	326	PRO	2.4
2	N	326	PRO	2.4
4	P	73	PRO	2.4
1	J	11	GLY	2.4
2	D	71	THR	2.4
2	E	197	THR	2.4
2	M	258	THR	2.4
2	N	40	GLY	2.4
2	M	431	SER	2.4
2	N	152	ILE	2.4
1	J	417	ARG	2.4
1	K	51	VAL	2.4
2	D	78	ASP	2.4
2	E	226	ASP	2.4
4	H	6	ASP	2.4
1	I	276	LYS	2.4
2	F	288	TYR	2.4
1	I	20	LEU	2.4
2	F	448	GLN	2.3
2	N	170	GLN	2.3
1	A	377	ALA	2.3
2	N	418	PHE	2.3
2	L	57	ILE	2.3
4	P	46	ALA	2.3
4	P	102	ILE	2.3
1	I	56	SER	2.3
2	F	72	SER	2.3
1	B	329	ARG	2.3
1	C	191	ARG	2.3
1	I	23	ARG	2.3
2	D	73	VAL	2.3
2	M	173	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	P	66	ARG	2.3
1	A	410	ASP	2.3
1	A	206	LEU	2.3
1	K	148	LEU	2.3
2	F	214	LEU	2.3
1	B	275	PRO	2.3
1	I	270	PRO	2.3
2	E	354	PRO	2.3
1	C	261	GLU	2.3
1	C	469	GLN	2.3
1	K	316	GLN	2.3
2	D	157	GLY	2.3
2	F	279	GLY	2.3
2	F	422	PHE	2.3
2	M	206	GLN	2.3
2	F	238	ALA	2.3
4	H	92	GLU	2.3
2	E	322	THR	2.3
1	I	338	SER	2.3
1	J	56	SER	2.3
1	K	214	VAL	2.3
2	E	51	SER	2.3
1	A	323	MET	2.3
1	C	197	ARG	2.3
2	L	430	ARG	2.3
2	M	41	ARG	2.3
2	M	452	LYS	2.3
2	N	274	ARG	2.3
1	C	127	ASP	2.3
2	E	320	ASP	2.3
2	N	416	ASP	2.3
4	H	67	ASP	2.3
2	F	60	PHE	2.3
2	F	127	PRO	2.3
1	B	442	ASN	2.3
1	K	83	ILE	2.3
1	K	254	GLY	2.3
2	E	152	ILE	2.3
1	J	271	GLU	2.3
2	D	230	GLU	2.3
2	E	273	ALA	2.3
2	N	248	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	265	VAL	2.3
1	C	503	VAL	2.3
1	C	358	LEU	2.3
1	J	19	MET	2.3
2	D	15	SER	2.3
4	H	31	SER	2.3
4	H	77	LEU	2.3
1	A	217	PRO	2.3
1	I	90	PRO	2.3
1	I	351	PRO	2.3
2	L	374	ASP	2.3
1	J	383	ALA	2.3
1	K	16	ALA	2.3
1	A	257	GLU	2.3
1	K	50	GLN	2.3
2	D	24	ALA	2.3
2	E	439	ALA	2.3
1	K	159	GLU	2.3
1	A	154	ARG	2.3
1	A	511	LYS	2.3
2	M	79	VAL	2.3
1	J	401	ARG	2.3
2	E	260	MET	2.3
2	F	81	ARG	2.3
1	B	432	THR	2.3
1	I	273	THR	2.3
2	M	18	LEU	2.3
2	E	418	PHE	2.3
1	C	543	PRO	2.3
1	I	83	ILE	2.3
1	K	204	PRO	2.3
2	F	311	ILE	2.3
2	M	159	PRO	2.3
1	I	349	GLY	2.3
1	K	225	ALA	2.3
2	L	24	ALA	2.3
1	B	568	LYS	2.3
1	J	307	VAL	2.3
1	I	281	LEU	2.3
1	K	507	CYS	2.3
1	K	541	GLN	2.3
2	E	81	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	245	LEU	2.3
2	N	125	ARG	2.3
4	P	19	GLU	2.3
2	E	143	THR	2.3
1	I	439	TYR	2.3
2	D	463	TYR	2.3
2	N	60	PHE	2.3
2	D	96	ILE	2.3
1	I	315	ASP	2.3
1	J	575	LYS	2.3
1	A	400	LEU	2.3
1	C	60	VAL	2.3
1	C	71	LEU	2.3
1	K	135	LEU	2.3
1	B	79	MET	2.3
1	B	122	MET	2.3
1	I	114	GLU	2.3
2	D	448	GLN	2.3
2	L	166	GLN	2.3
1	B	263	THR	2.3
1	B	447	TYR	2.3
1	J	428	TYR	2.3
1	A	211	ILE	2.3
2	D	72	SER	2.3
2	E	57	ILE	2.3
2	E	435	SER	2.3
2	F	325	ILE	2.3
2	L	232	ILE	2.3
2	M	202	SER	2.3
2	N	431	SER	2.3
1	C	231	GLY	2.3
1	B	145	HIS	2.3
1	I	479	ALA	2.3
2	D	452	LYS	2.3
2	M	328	LEU	2.3
3	O	37	ALA	2.3
2	D	318	ASP	2.3
2	E	101	ASP	2.3
2	F	416	ASP	2.3
1	I	397	GLN	2.3
2	E	450	GLU	2.2
4	H	28	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	166	TYR	2.2
2	D	386	TYR	2.2
2	E	204	PHE	2.2
1	A	487	GLY	2.2
1	B	385	SER	2.2
1	C	69	LEU	2.2
1	I	317	GLY	2.2
1	I	458	LEU	2.2
1	J	306	GLY	2.2
2	L	235	PRO	2.2
2	N	315	SER	2.2
1	J	356	ALA	2.2
1	K	73	VAL	2.2
2	M	84	VAL	2.2
2	N	213	ALA	2.2
4	H	37	VAL	2.2
1	C	185	HIS	2.2
1	C	344	MET	2.2
2	F	321	ARG	2.2
2	M	420	ARG	2.2
2	E	290	ASP	2.2
1	K	343	GLU	2.2
2	N	401	GLU	2.2
1	K	216	PHE	2.2
1	K	431	PHE	2.2
1	A	202	ASN	2.2
2	N	110	LYS	2.2
1	A	577	LEU	2.2
1	C	58	LEU	2.2
1	C	142	GLY	2.2
2	E	404	LEU	2.2
2	M	45	GLY	2.2
2	N	16	GLY	2.2
1	C	401	ARG	2.2
1	C	411	ALA	2.2
2	E	31	ALA	2.2
2	E	72	SER	2.2
1	J	363	GLU	2.2
2	L	8	TYR	2.2
2	L	25	LYS	2.2
1	A	58	LEU	2.2
1	A	241	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	148	LEU	2.2
2	E	364	ASN	2.2
1	C	49	VAL	2.2
1	I	486	VAL	2.2
1	A	355	ALA	2.2
1	C	78	GLY	2.2
1	A	391	MET	2.2
1	B	344	MET	2.2
1	C	444	ALA	2.2
1	K	55	THR	2.2
1	K	197	ARG	2.2
2	D	236	ARG	2.2
2	E	41	ARG	2.2
2	F	228	THR	2.2
2	L	321	ARG	2.2
1	K	497	GLN	2.2
1	A	228	GLY	2.2
1	B	86	GLY	2.2
1	C	202	ASN	2.2
1	C	242	ALA	2.2
1	I	298	ALA	2.2
1	I	323	MET	2.2
1	I	414	ALA	2.2
1	K	18	GLY	2.2
1	K	475	ALA	2.2
2	F	171	ALA	2.2
2	F	268	ARG	2.2
2	L	403	ALA	2.2
2	M	387	ALA	2.2
2	N	306	GLY	2.2
1	I	235	THR	2.2
3	G	157	THR	2.2
1	C	328	SER	2.2
2	M	307	SER	2.2
1	A	494	PHE	2.2
2	M	348	ILE	2.2
1	B	239	GLN	2.2
1	C	571	GLN	2.2
1	K	571	GLN	2.2
1	B	348	GLU	2.2
1	I	441	GLU	2.2
1	A	127	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	506	TYR	2.2
2	E	334	GLU	2.2
2	F	62	GLU	2.2
1	I	251	VAL	2.2
1	K	36	VAL	2.2
1	K	236	VAL	2.2
2	M	390	VAL	2.2
1	C	294	MET	2.2
1	I	41	ARG	2.2
2	E	43	ARG	2.2
2	E	92	ARG	2.2
1	I	72	ALA	2.2
2	L	258	THR	2.2
1	K	66	SER	2.2
1	K	392	SER	2.2
2	F	379	SER	2.2
1	K	241	LEU	2.2
1	K	281	LEU	2.2
4	P	77	LEU	2.2
2	M	349	TYR	2.2
2	N	427	GLN	2.2
2	F	275	GLU	2.2
1	A	41	ARG	2.2
1	J	244	TRP	2.2
2	N	73	VAL	2.2
2	E	10	GLY	2.2
2	E	134	GLY	2.2
2	L	330	GLY	2.2
2	M	260	MET	2.2
4	H	63	MET	2.2
1	A	280	PRO	2.2
1	I	225	ALA	2.2
1	K	10	ALA	2.2
2	N	159	PRO	2.2
2	L	94	ASN	2.2
1	B	211	ILE	2.2
2	M	96	ILE	2.2
1	K	111	LEU	2.2
2	M	304	LYS	2.2
1	I	555	SER	2.2
1	A	362	TYR	2.2
1	A	397	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	38	GLU	2.2
1	J	108	VAL	2.2
2	F	462	TYR	2.2
2	N	59	VAL	2.2
2	N	189	VAL	2.2
1	C	24	MET	2.2
1	J	323	MET	2.2
1	I	57	GLY	2.1
1	K	278	GLY	2.1
1	K	521	ALA	2.1
2	D	320	ASP	2.1
4	H	83	GLY	2.1
1	B	394	PRO	2.1
2	M	17	PRO	2.1
2	M	350	PRO	2.1
1	A	402	ILE	2.1
1	I	369	ILE	2.1
2	N	20	PHE	2.1
1	I	482	LEU	2.1
1	J	470	LEU	2.1
2	L	424	ASN	2.1
1	I	67	THR	2.1
1	K	286	VAL	2.1
2	L	315	SER	2.1
2	M	379	SER	2.1
1	I	364	ARG	2.1
1	K	477	GLN	2.1
2	E	58	GLN	2.1
3	G	55	GLN	2.1
2	L	53	GLU	2.1
1	C	224	ALA	2.1
1	I	222	GLY	2.1
1	K	244	TRP	2.1
2	M	147	GLY	2.1
1	A	139	PRO	2.1
1	B	85	ASP	2.1
1	K	162	PRO	2.1
2	F	353	ASP	2.1
2	M	113	PRO	2.1
1	B	287	LEU	2.1
1	C	226	ILE	2.1
1	K	269	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	M	233	LEU	2.1
2	N	304	LYS	2.1
2	L	23	ASN	2.1
1	A	186	THR	2.1
1	A	149	VAL	2.1
4	H	45	VAL	2.1
1	A	398	SER	2.1
2	D	141	MET	2.1
2	E	136	SER	2.1
2	E	455	SER	2.1
2	F	251	TYR	2.1
1	B	469	GLN	2.1
2	F	46	GLN	2.1
1	I	18	GLY	2.1
1	J	289	ALA	2.1
4	H	80	ALA	2.1
1	I	217	PRO	2.1
2	E	17	PRO	2.1
2	E	232	ILE	2.1
2	E	304	LYS	2.1
2	M	175	PRO	2.1
1	A	40	ILE	2.1
1	I	27	ILE	2.1
2	E	451	LEU	2.1
2	N	311	ILE	2.1
1	A	274	ASP	2.1
1	A	423	ASN	2.1
1	I	471	VAL	2.1
1	K	260	ASN	2.1
2	D	79	VAL	2.1
2	M	64	THR	2.1
2	M	143	THR	2.1
1	B	57	GLY	2.1
1	C	427	SER	2.1
1	B	479	ALA	2.1
1	C	374	GLU	2.1
1	J	376	GLY	2.1
1	K	231	GLY	2.1
2	E	373	GLU	2.1
2	F	80	ALA	2.1
2	L	242	ALA	2.1
2	M	397	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	397	ALA	2.1
1	I	524	LYS	2.1
2	E	130	PHE	2.1
2	M	221	LEU	2.1
2	M	247	PHE	2.1
1	A	49	VAL	2.1
1	J	220	MET	2.1
1	B	439	TYR	2.1
1	A	409	LEU	2.1
1	C	88	GLN	2.1
1	J	69	LEU	2.1
1	J	472	GLY	2.1
1	K	61	GLY	2.1
2	L	285	GLY	2.1
2	M	58	GLN	2.1
1	B	40	ILE	2.1
1	K	402	ILE	2.1
2	L	312	PRO	2.1
2	L	399	ILE	2.1
2	N	235	PRO	2.1
1	B	14	VAL	2.1
1	B	488	ARG	2.1
1	I	401	ARG	2.1
1	I	478	ASP	2.1
1	I	537	ASP	2.1
2	E	59	VAL	2.1
1	J	299	ARG	2.1
2	E	67	ASP	2.1
2	E	341	ARG	2.1
2	L	92	ARG	2.1
4	P	101	ASP	2.1
1	C	109	HIS	2.1
1	A	135	LEU	2.1
1	J	308	THR	2.1
1	K	517	LYS	2.1
1	K	572	GLY	2.1
2	E	36	LYS	2.1
2	E	133	THR	2.1
2	L	404	LEU	2.1
2	F	432	ILE	2.1
2	M	294	ILE	2.1
2	N	266	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	330	TRP	2.1
1	B	74	GLU	2.1
1	C	53	GLU	2.1
1	C	188	PRO	2.1
1	I	187	TRP	2.1
1	J	117	TRP	2.1
1	K	38	GLU	2.1
1	A	177	ASP	2.1
1	A	390	ASP	2.1
1	I	243	LYS	2.1
1	J	28	CYS	2.1
2	L	201	LEU	2.1
3	G	133	TYR	2.1
3	O	195	LYS	2.1
1	C	313	PHE	2.1
1	C	406	PHE	2.1
1	J	256	GLY	2.1
1	K	143	PHE	2.1
1	K	499	ALA	2.1
2	E	330	GLY	2.1
2	F	157	GLY	2.1
2	F	256	ILE	2.1
2	F	389	GLY	2.1
2	M	116	GLY	2.1
2	N	94	ASN	2.1
1	J	571	GLN	2.1
3	G	166	GLN	2.1
1	C	245	SER	2.1
1	C	343	GLU	2.1
1	J	455	SER	2.1
2	D	357	SER	2.1
2	E	185	GLU	2.1
2	F	200	GLU	2.1
2	M	384	SER	2.1
1	B	307	VAL	2.1
2	D	21	VAL	2.1
2	E	218	VAL	2.1
2	F	56	VAL	2.1
1	A	183	MET	2.0
1	K	516	MET	2.0
2	E	111	ARG	2.0
2	E	321	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	430	LEU	2.0
1	A	2	ILE	2.0
1	A	434	ALA	2.0
1	B	21	GLY	2.0
1	C	10	ALA	2.0
1	J	40	ILE	2.0
1	K	426	GLY	2.0
2	M	369	GLY	2.0
2	M	421	PHE	2.0
1	J	246	ASN	2.0
2	E	228	THR	2.0
2	N	448	GLN	2.0
1	I	311	GLU	2.0
1	A	381	VAL	2.0
2	M	47	VAL	2.0
2	F	281	ARG	2.0
1	I	447	TYR	2.0
1	J	312	TYR	2.0
1	K	337	ILE	2.0
1	K	530	ILE	2.0
2	E	20	PHE	2.0
2	E	414	PHE	2.0
1	I	526	ALA	2.0
1	J	572	GLY	2.0
2	D	225	ASP	2.0
2	D	460	GLY	2.0
2	N	327	ASP	2.0
3	G	141	ALA	2.0
1	C	295	PRO	2.0
1	C	497	GLN	2.0
2	L	356	PRO	2.0
2	M	377	GLN	2.0
2	N	105	PRO	2.0
1	K	46	THR	2.0
2	D	234	THR	2.0
2	E	280	ARG	2.0
2	M	207	GLU	2.0
2	N	420	ARG	2.0
1	I	69	LEU	2.0
1	J	382	GLY	2.0
1	K	208	GLY	2.0
2	D	69	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	330	GLY	2.0
2	F	55	ALA	2.0
2	M	97	GLY	2.0
3	G	136	ALA	2.0
4	P	88	GLY	2.0
4	P	54	ASP	2.0
1	A	227	PRO	2.0
1	K	448	PRO	2.0
2	E	350	PRO	2.0
1	A	417	ARG	2.0
1	C	488	ARG	2.0
1	I	154	ARG	2.0
1	J	67	THR	2.0
1	J	74	GLU	2.0
1	J	400	LEU	2.0
2	E	64	THR	2.0
1	B	319	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

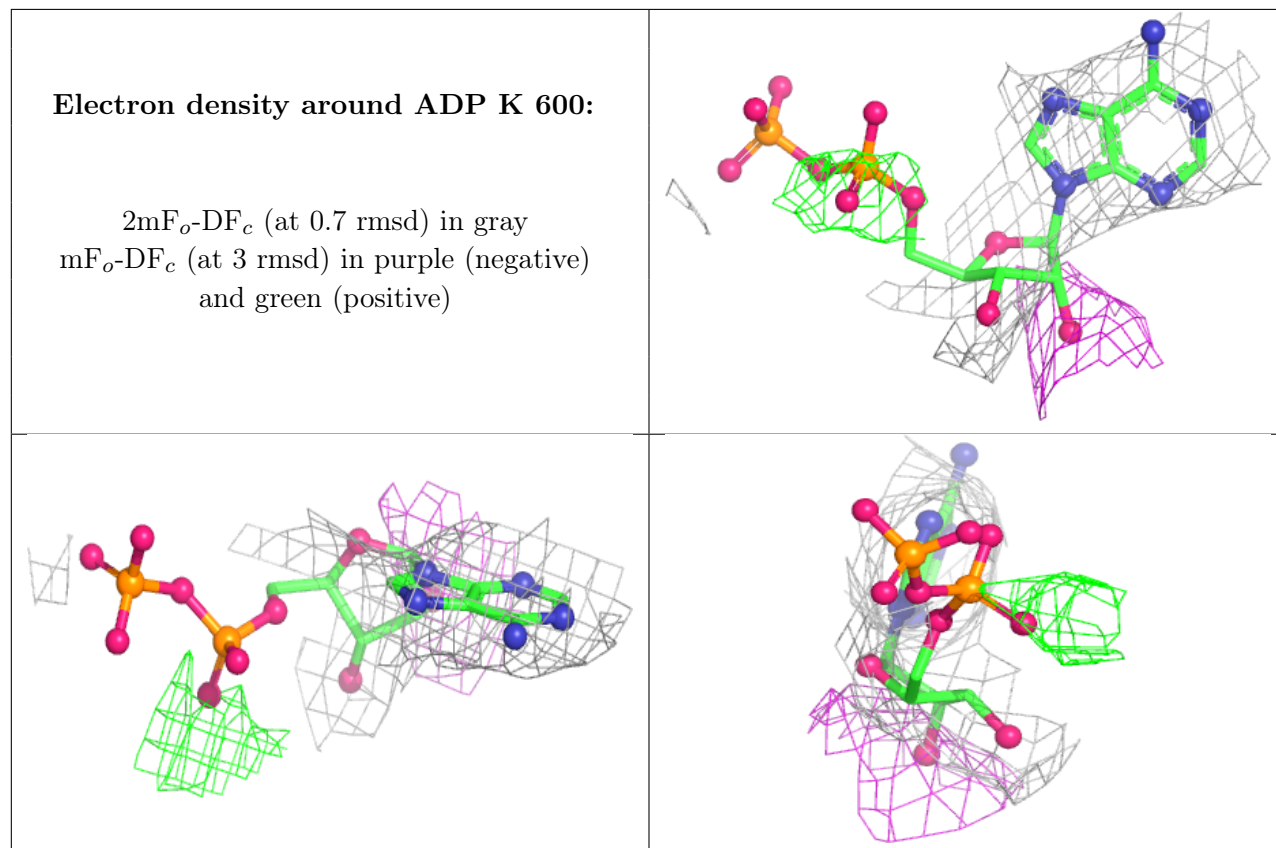
6.4 Ligands [i](#)

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
5	ADP	K	600	27/27	0.72	0.30	112,112,112,112	0
5	ADP	C	600	27/27	0.86	0.14	116,116,116,116	0
5	ADP	A	600	27/27	0.86	0.16	109,109,109,109	0
5	ADP	I	600	27/27	0.87	0.14	110,110,110,110	0

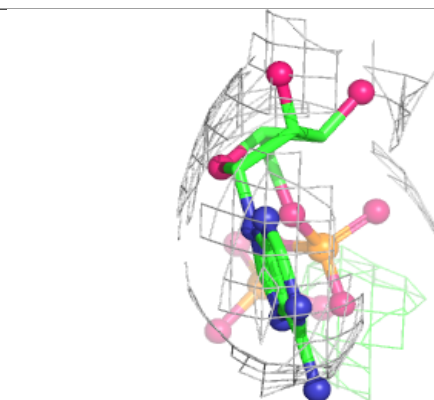
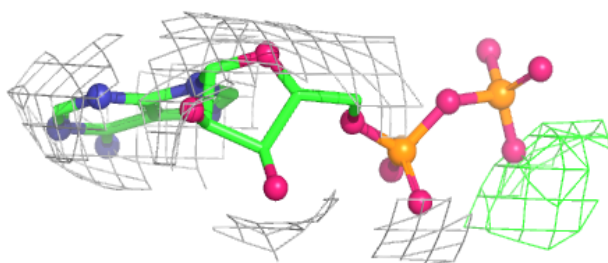
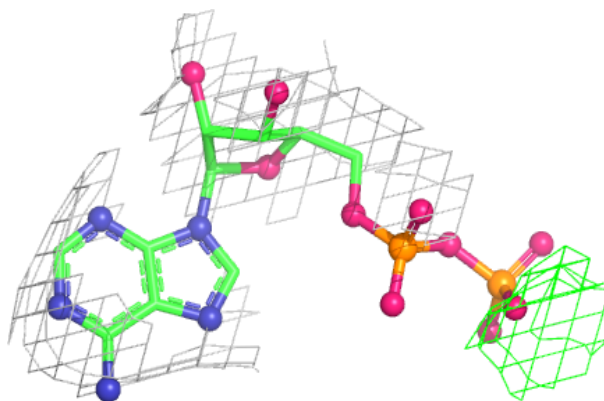
The following is a graphical depiction of the model fit to experimental electron density of all

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.

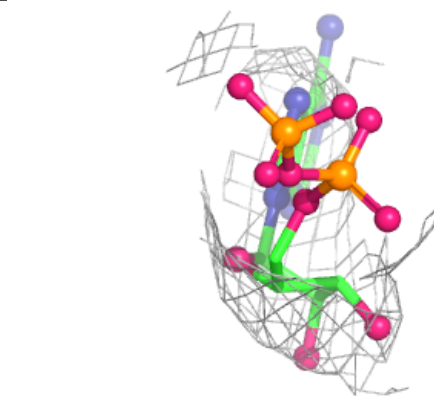
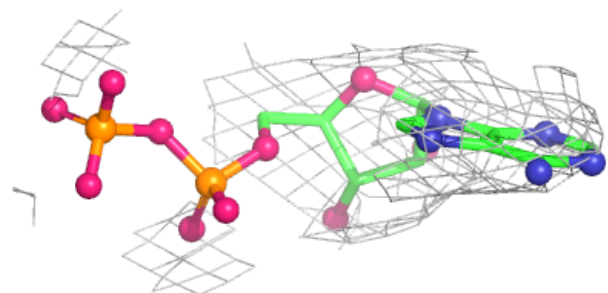
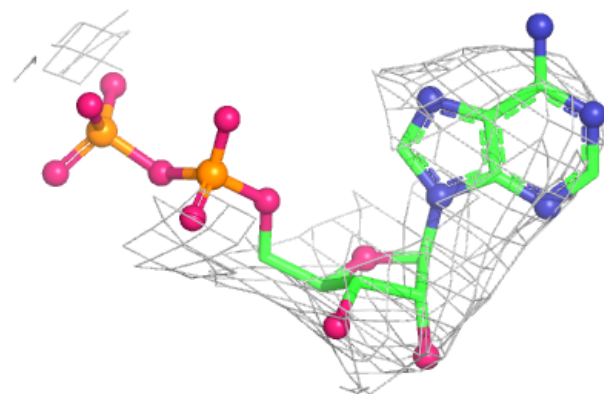


Electron density around ADP C 600:

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

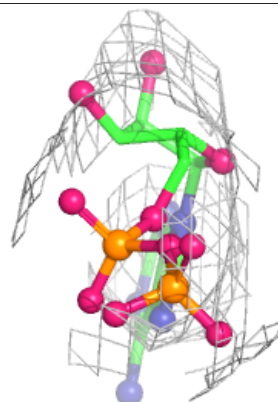
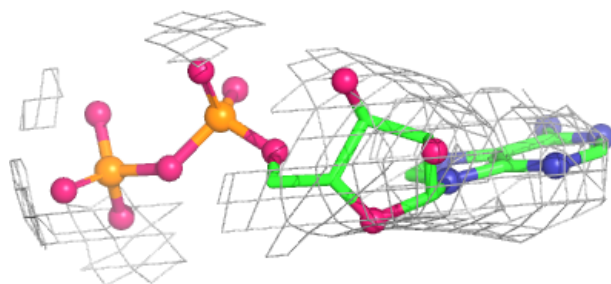
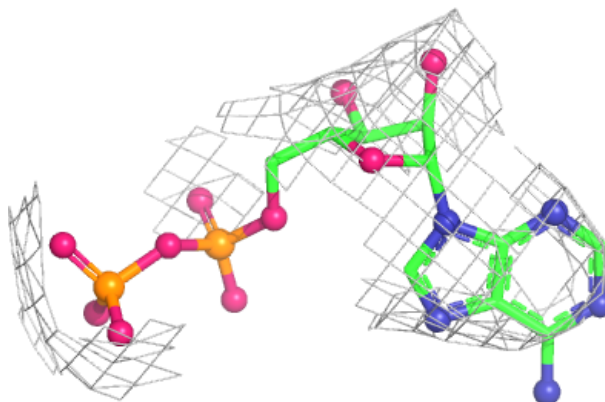
**Electron density around ADP A 600:**

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



Electron density around ADP I 600:

$2mF_o-DF_c$ (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.