



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:02 AM UTC

PDB ID : 4CTS / pdb_00004cts
Title : CRYSTAL STRUCTURE ANALYSIS AND MOLECULAR MODEL OF A
COMPLEX OF CITRATE SYNTHASE WITH OXALOACETATE AND S-
ACETONYL-COENZYME A
Authors : Remington, S.; Wiegand, G.; Huber, R.
Deposited on : 1984-01-27
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

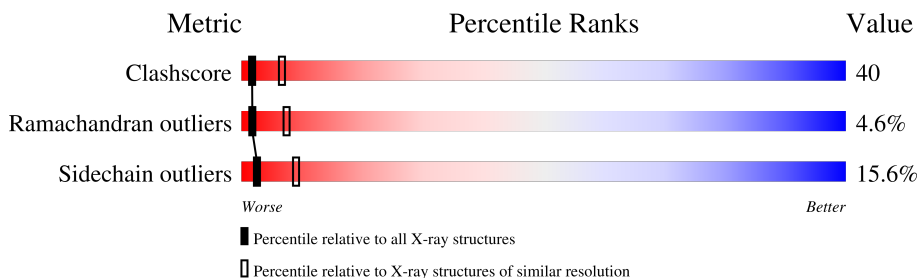
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	22% 38% 29% 11%
1	B	437	23% 38% 28% 11%

2 Entry composition [i](#)

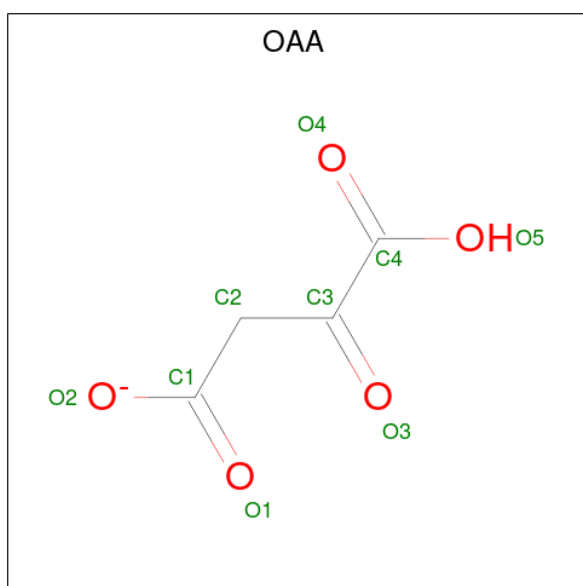
There are 3 unique types of molecules in this entry. The entry contains 7002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	227	0	0
			3444	2200	591	634	19			
1	B	437	Total	C	N	O	S	230	0	0
			3444	2200	591	634	19			

- Molecule 2 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is water.

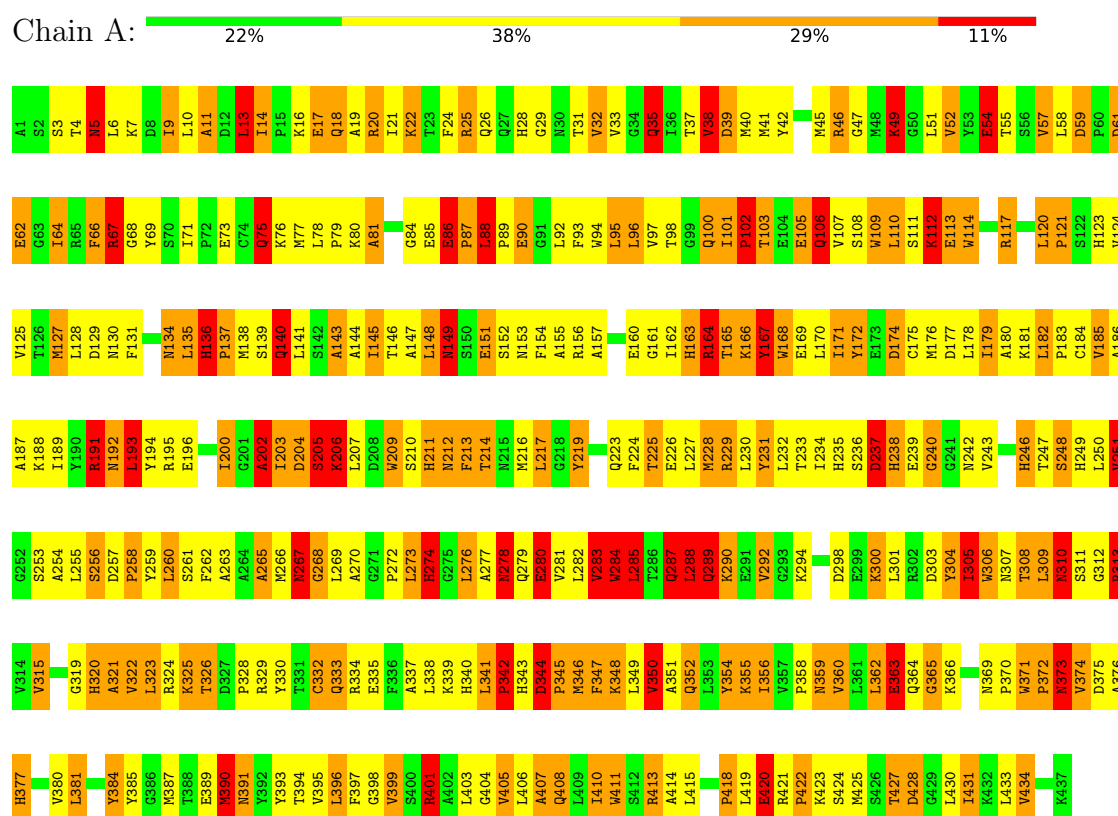
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	47	Total 47	O 47	0	0

3 Residue-property plots

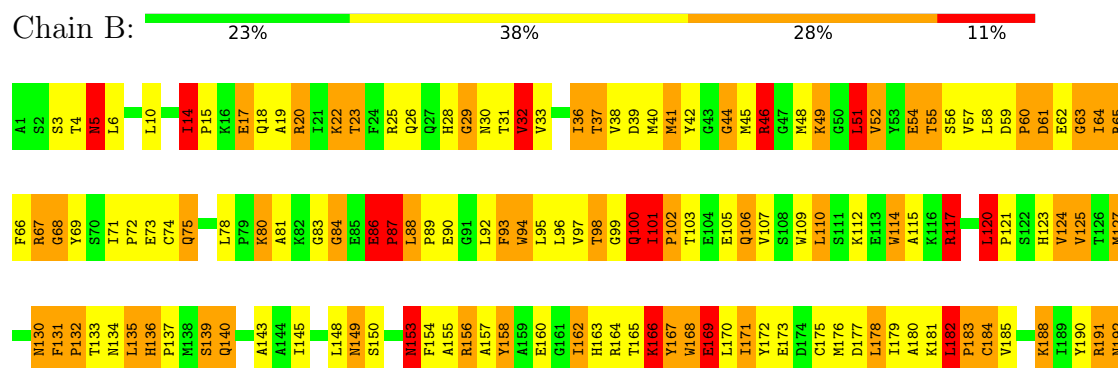
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: CITRATE SYNTHASE



• Molecule 1: CITRATE SYNTHASE



V380	L381	L382	Q383	Y384	G386	G387	T388	E389	M390	N391	Y392	Y393	T394	V395	L396	F397	G398	V399	S400	R401		G404	V405		Q408	L409	I410	W411	S412	R413	A414		F417	P418	L419	E420	R421	P422	K423	S424	M425	S426	T427	D428	G429	L430	I431	K432	L433	V434		K437							
G317	Y318	G319	R320	A321	V322	L323	R324	R325	T326	D327	P328	R329	Y330	T331	C332	Q333	R334	E335	F336	A337	L338	K339	H340	I341	P342	H343	D344	P345	M346	F347	K348	L349	V350		Y354	K355	I356	V357	P358	N359		L362	E363	Q364	G365	K366	A367	K368	N369	P370	W371	P372	N373	Y374	D375	A376	H377	S378	G379
S256	D257	P258	Y259	L260	S261	F262	A263	A264	A265	M266	V267		A270	G271	P272	L273	H274	G275	L276	A277	N278	Q279	E280	V281	L282	V283	W284	L285	T286	Q287	L288	Q289	R290	E291	V292	G293	K294	D295	V296	S297	D298	E299	K300	L301	R302	D303	Y304	I305	W306	N307	T308	L309	N310	S311	G312	R313	V314	V315	P316
L193	L194	R195	E196	G197	S198	S199	I200		I203	D204	S205	K206	L207	D208	W209	S210	H211	N212	F213	T214	N215	M216	L217	G218	Y219	T220	D221	A222	Q223	F224	T225	E226	L227	M228	R229	L230	Y231	L232		H235	S236	D237	H238	E239		N242	V243	S244	A245	H246	T247	S248	H249	L250	V251	G252	S253	A254	L255

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.54Å 101.54Å 224.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.67	42/3528 (1.2%)	2.37	213/4786 (4.5%)
1	B	1.67	50/3528 (1.4%)	2.39	241/4786 (5.0%)
All	All	1.67	92/7056 (1.3%)	2.38	454/9572 (4.7%)

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	1	105
1	B	2	104
All	All	3	209

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	HIS	CE1-NE2	10.89	1.43	1.32
1	B	211	HIS	ND1-CE1	10.52	1.43	1.32
1	B	274	HIS	ND1-CE1	10.47	1.43	1.32
1	A	340	HIS	CE1-NE2	10.44	1.43	1.32
1	A	377	HIS	CE1-NE2	10.31	1.42	1.32
1	B	114	TRP	NE1-CE2	-10.27	1.26	1.37
1	B	377	HIS	CE1-NE2	10.11	1.42	1.32
1	A	249	HIS	CE1-NE2	10.00	1.42	1.32
1	A	235	HIS	CE1-NE2	9.88	1.42	1.32
1	B	320	HIS	CE1-NE2	9.86	1.42	1.32
1	A	235	HIS	ND1-CE1	9.84	1.42	1.32
1	B	249	HIS	ND1-CE1	9.82	1.42	1.32
1	B	377	HIS	ND1-CE1	9.76	1.42	1.32
1	B	235	HIS	CE1-NE2	9.71	1.42	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	HIS	CE1-NE2	9.66	1.42	1.32
1	A	249	HIS	ND1-CE1	9.60	1.42	1.32
1	B	109	TRP	NE1-CE2	-9.57	1.26	1.37
1	B	246	HIS	ND1-CE1	9.57	1.42	1.32
1	A	238	HIS	CE1-NE2	9.54	1.42	1.32
1	A	274	HIS	ND1-CE1	9.45	1.42	1.32
1	A	28	HIS	CE1-NE2	9.36	1.42	1.32
1	A	163	HIS	ND1-CE1	9.30	1.41	1.32
1	A	114	TRP	NE1-CE2	-9.29	1.27	1.37
1	A	168	TRP	NE1-CE2	-9.19	1.27	1.37
1	A	377	HIS	ND1-CE1	9.16	1.41	1.32
1	B	340	HIS	ND1-CE1	9.13	1.41	1.32
1	A	28	HIS	ND1-CE1	9.12	1.41	1.32
1	A	320	HIS	CE1-NE2	9.12	1.41	1.32
1	B	163	HIS	ND1-CE1	9.08	1.41	1.32
1	B	235	HIS	ND1-CE1	9.03	1.41	1.32
1	A	371	TRP	NE1-CE2	-8.95	1.27	1.37
1	B	371	TRP	NE1-CE2	-8.90	1.27	1.37
1	A	163	HIS	CE1-NE2	8.83	1.41	1.32
1	B	163	HIS	CE1-NE2	8.83	1.41	1.32
1	B	249	HIS	CE1-NE2	8.79	1.41	1.32
1	A	343	HIS	ND1-CE1	8.79	1.41	1.32
1	A	109	TRP	NE1-CE2	-8.74	1.27	1.37
1	A	343	HIS	CE1-NE2	8.70	1.41	1.32
1	B	238	HIS	ND1-CE1	8.61	1.41	1.32
1	B	343	HIS	CE1-NE2	8.57	1.41	1.32
1	A	211	HIS	CE1-NE2	8.56	1.41	1.32
1	A	211	HIS	ND1-CE1	8.54	1.41	1.32
1	B	94	TRP	NE1-CE2	-8.53	1.28	1.37
1	B	168	TRP	NE1-CE2	-8.49	1.28	1.37
1	A	209	TRP	NE1-CE2	-8.48	1.28	1.37
1	B	123	HIS	ND1-CE1	8.46	1.41	1.32
1	A	136	HIS	ND1-CE1	8.44	1.41	1.32
1	A	411	TRP	NE1-CE2	-8.35	1.28	1.37
1	B	411	TRP	NE1-CE2	-8.28	1.28	1.37
1	B	123	HIS	CE1-NE2	8.26	1.40	1.32
1	A	246	HIS	ND1-CE1	8.24	1.40	1.32
1	B	136	HIS	CE1-NE2	8.24	1.40	1.32
1	A	136	HIS	CE1-NE2	8.23	1.40	1.32
1	A	94	TRP	NE1-CE2	-8.16	1.28	1.37
1	B	274	HIS	CE1-NE2	8.03	1.40	1.32
1	A	123	HIS	CE1-NE2	7.98	1.40	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	TRP	NE1-CE2	-7.98	1.28	1.37
1	B	306	TRP	NE1-CE2	-7.96	1.28	1.37
1	B	28	HIS	CE1-NE2	7.89	1.40	1.32
1	A	123	HIS	ND1-CE1	7.83	1.40	1.32
1	B	320	HIS	ND1-CE1	7.70	1.40	1.32
1	B	209	TRP	NE1-CE2	-7.61	1.29	1.37
1	B	136	HIS	ND1-CE1	7.59	1.40	1.32
1	B	246	HIS	CE1-NE2	7.54	1.40	1.32
1	B	343	HIS	ND1-CE1	7.50	1.40	1.32
1	B	28	HIS	ND1-CE1	7.39	1.40	1.32
1	A	306	TRP	NE1-CE2	-7.38	1.29	1.37
1	B	84	GLY	N-CA	7.22	1.51	1.45
1	B	4	THR	N-CA	7.16	1.54	1.46
1	A	238	HIS	ND1-CE1	7.06	1.39	1.32
1	A	340	HIS	ND1-CE1	6.92	1.39	1.32
1	A	284	TRP	NE1-CE2	-6.58	1.30	1.37
1	B	211	HIS	CE1-NE2	6.36	1.39	1.32
1	B	238	HIS	CE1-NE2	6.25	1.38	1.32
1	B	379	GLY	C-N	-5.92	1.26	1.33
1	A	117	ARG	NE-CZ	-5.80	1.26	1.33
1	A	172	TYR	C-N	-5.80	1.25	1.34
1	A	274	HIS	CE1-NE2	5.70	1.38	1.32
1	B	235	HIS	C-N	-5.69	1.26	1.33
1	B	433	LEU	C-N	-5.62	1.26	1.33
1	B	340	HIS	N-CA	5.60	1.53	1.46
1	B	117	ARG	C-N	-5.58	1.26	1.33
1	B	290	LYS	C-N	-5.50	1.25	1.33
1	B	283	VAL	CA-CB	5.42	1.60	1.54
1	A	250	LEU	C-N	-5.29	1.28	1.34
1	B	404	GLY	C-N	-5.29	1.27	1.33
1	B	384	TYR	CZ-OH	5.22	1.49	1.38
1	A	364	GLN	N-CA	5.18	1.52	1.46
1	B	246	HIS	CD2-NE2	5.14	1.43	1.37
1	A	123	HIS	CD2-NE2	5.12	1.43	1.37
1	B	56	SER	N-CA	5.12	1.52	1.46
1	A	71	ILE	C-N	-5.11	1.27	1.33

All (454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	GLY	CA-C-N	13.22	133.94	122.17
1	B	83	GLY	C-N-CA	13.22	133.94	122.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	HIS	CA-CB-CG	-11.28	102.52	113.80
1	B	28	HIS	CA-CB-CG	-10.74	103.06	113.80
1	B	356	ILE	N-CA-C	10.29	120.23	111.90
1	A	278	ASN	CA-C-N	10.28	141.17	121.54
1	A	278	ASN	C-N-CA	10.28	141.17	121.54
1	A	22	LYS	N-CA-C	10.08	122.02	111.14
1	A	274	HIS	CA-CB-CG	-10.03	103.77	113.80
1	B	433	LEU	CA-C-N	-9.60	105.79	121.34
1	B	433	LEU	C-N-CA	-9.60	105.79	121.34
1	A	268	GLY	N-CA-C	-9.42	100.71	112.77
1	A	356	ILE	N-CA-C	9.31	119.94	112.12
1	A	267	ASN	N-CA-C	-9.15	102.25	113.50
1	A	248	SER	O-C-N	9.14	131.81	122.12
1	A	35	GLN	N-CA-C	8.98	124.03	109.40
1	B	359	ASN	N-CA-C	-8.75	102.62	113.38
1	A	364	GLN	N-CA-C	8.67	123.95	113.12
1	A	408	GLN	CA-C-N	8.62	132.19	120.38
1	A	408	GLN	C-N-CA	8.62	132.19	120.38
1	B	209	TRP	O-C-N	8.62	131.05	122.09
1	A	288	LEU	N-CA-C	-8.40	101.71	111.03
1	B	3	SER	CA-C-N	8.38	132.76	120.87
1	B	3	SER	C-N-CA	8.38	132.76	120.87
1	A	57	VAL	CA-C-N	8.37	134.76	123.05
1	A	57	VAL	C-N-CA	8.37	134.76	123.05
1	B	396	LEU	O-C-N	8.27	130.93	122.08
1	B	397	PHE	CA-CB-CG	8.26	122.06	113.80
1	A	117	ARG	NE-CZ-NH2	-8.25	111.78	119.20
1	B	120	LEU	N-CA-C	8.23	120.00	109.72
1	B	51	LEU	O-C-N	-8.16	113.71	123.10
1	B	56	SER	N-CA-C	8.12	120.86	108.52
1	B	36	ILE	N-CA-C	7.93	120.36	108.23
1	A	105	GLU	N-CA-C	7.91	119.53	111.07
1	B	267	ASN	N-CA-C	-7.89	103.87	113.97
1	A	101	ILE	N-CA-CB	-7.80	101.51	110.17
1	B	358	PRO	CA-C-N	7.80	135.75	122.26
1	B	358	PRO	C-N-CA	7.80	135.75	122.26
1	A	139	SER	N-CA-C	-7.78	102.70	112.90
1	B	124	VAL	CA-C-N	7.72	130.29	120.56
1	B	124	VAL	C-N-CA	7.72	130.29	120.56
1	A	192	ASN	CA-C-N	-7.70	110.49	122.42
1	A	192	ASN	C-N-CA	-7.70	110.49	122.42
1	A	205	SER	N-CA-CB	-7.69	97.50	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	TRP	N-CA-C	7.68	121.46	110.24
1	B	254	ALA	CA-C-N	7.67	133.01	122.34
1	B	254	ALA	C-N-CA	7.67	133.01	122.34
1	B	283	VAL	CA-CB-CG1	7.62	123.35	110.40
1	B	29	GLY	N-CA-C	-7.62	105.22	114.66
1	B	178	LEU	N-CA-C	-7.60	102.57	112.68
1	B	88	LEU	N-CA-CB	-7.51	97.00	110.37
1	B	165	THR	CA-C-N	7.49	135.84	121.54
1	B	165	THR	C-N-CA	7.49	135.84	121.54
1	B	377	HIS	N-CA-CB	-7.45	100.28	111.15
1	A	340	HIS	CA-CB-CG	-7.45	106.36	113.80
1	A	325	LYS	N-CA-C	7.44	121.05	109.52
1	A	313	ARG	CA-C-N	7.41	132.27	122.93
1	A	313	ARG	C-N-CA	7.41	132.27	122.93
1	A	249	HIS	O-C-N	7.40	129.96	122.12
1	B	221	ASP	CA-CB-CG	-7.38	105.22	112.60
1	B	61	ASP	CA-CB-CG	-7.36	105.24	112.60
1	B	65	ARG	CD-NE-CZ	7.36	134.70	124.40
1	B	372	PRO	N-CA-C	7.33	122.76	111.11
1	B	383	GLN	O-C-N	7.32	129.88	122.12
1	B	213	PHE	CA-CB-CG	7.31	121.11	113.80
1	A	240	GLY	CA-C-N	7.25	128.18	119.99
1	A	240	GLY	C-N-CA	7.25	128.18	119.99
1	B	228	MET	O-C-N	7.24	129.53	122.07
1	A	284	TRP	CA-C-N	-7.20	109.80	122.26
1	A	284	TRP	C-N-CA	-7.20	109.80	122.26
1	B	359	ASN	CA-C-N	7.16	132.09	121.77
1	B	359	ASN	C-N-CA	7.16	132.09	121.77
1	A	363	GLU	O-C-N	7.11	130.26	122.15
1	A	186	ALA	O-C-N	7.11	129.43	122.03
1	A	13	LEU	CA-C-N	7.11	127.25	120.43
1	A	13	LEU	C-N-CA	7.11	127.25	120.43
1	A	344	ASP	N-CA-C	7.10	120.11	110.31
1	A	248	SER	CA-C-N	7.05	129.73	120.28
1	A	248	SER	C-N-CA	7.05	129.73	120.28
1	A	231	TYR	O-C-N	7.05	129.33	122.07
1	B	100	GLN	CA-C-N	7.02	129.50	123.04
1	B	100	GLN	C-N-CA	7.02	129.50	123.04
1	A	124	VAL	O-C-N	7.01	129.44	121.94
1	B	417	PHE	O-C-N	7.01	127.41	121.31
1	B	203	ILE	CA-CB-CG2	6.97	122.36	110.50
1	B	396	LEU	CA-C-O	-6.97	113.40	121.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	LEU	N-CA-CB	6.96	120.07	109.98
1	B	84	GLY	N-CA-C	6.96	121.30	111.42
1	B	123	HIS	CA-C-N	6.95	129.39	120.70
1	B	123	HIS	C-N-CA	6.95	129.39	120.70
1	A	47	GLY	N-CA-C	-6.93	105.92	114.92
1	B	127	MET	O-C-N	6.92	129.29	122.09
1	A	309	LEU	N-CA-C	6.89	118.44	111.07
1	B	302	ARG	CA-C-N	6.89	130.20	120.28
1	B	302	ARG	C-N-CA	6.89	130.20	120.28
1	A	358	PRO	CA-C-N	6.88	133.77	121.66
1	A	358	PRO	C-N-CA	6.88	133.77	121.66
1	A	200	ILE	O-C-N	6.87	128.28	122.09
1	B	380	VAL	O-C-N	6.87	129.57	121.80
1	B	364	GLN	N-CA-C	6.87	121.71	113.12
1	B	281	VAL	N-CA-C	-6.86	102.68	112.35
1	A	14	ILE	O-C-N	6.84	124.80	120.42
1	B	86	GLU	N-CA-C	6.82	118.66	110.07
1	A	369	ASN	CA-C-N	6.80	126.04	118.97
1	A	369	ASN	C-N-CA	6.80	126.04	118.97
1	A	106	GLN	N-CA-C	-6.78	104.58	112.92
1	A	164	ARG	CA-C-N	6.76	129.58	120.65
1	A	164	ARG	C-N-CA	6.76	129.58	120.65
1	B	124	VAL	O-C-N	6.76	128.91	121.94
1	B	427	THR	N-CA-CB	6.75	121.89	110.49
1	A	14	ILE	N-CA-C	6.74	121.09	112.67
1	A	174	ASP	CA-C-N	6.73	129.19	120.44
1	A	174	ASP	C-N-CA	6.73	129.19	120.44
1	A	381	LEU	N-CA-C	-6.73	103.75	112.23
1	B	253	SER	CA-C-N	-6.67	111.08	122.56
1	B	253	SER	C-N-CA	-6.67	111.08	122.56
1	A	22	LYS	N-CA-CB	6.67	119.73	110.07
1	A	121	PRO	N-CA-CB	6.65	109.22	103.31
1	A	147	ALA	CA-C-O	-6.65	113.44	120.55
1	B	371	TRP	CA-C-N	6.64	126.67	119.89
1	B	371	TRP	C-N-CA	6.64	126.67	119.89
1	B	396	LEU	N-CA-CB	6.64	119.91	109.82
1	A	309	LEU	O-C-N	6.64	128.91	122.07
1	B	326	THR	CA-C-N	-6.64	111.78	120.67
1	B	326	THR	C-N-CA	-6.64	111.78	120.67
1	B	359	ASN	N-CA-CB	-6.63	100.65	110.53
1	A	67	ARG	NE-CZ-NH1	-6.63	114.87	121.50
1	B	167	TYR	O-C-N	6.63	129.74	122.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	LEU	N-CA-C	-6.59	104.27	112.90
1	A	179	ILE	O-C-N	6.58	128.52	121.87
1	A	140	GLN	O-C-N	6.56	129.18	122.09
1	A	363	GLU	CA-C-N	6.55	135.11	122.53
1	A	363	GLU	C-N-CA	6.55	135.11	122.53
1	A	422	PRO	N-CA-CB	6.53	110.11	103.25
1	A	22	LYS	CA-C-N	6.51	128.90	120.44
1	A	22	LYS	C-N-CA	6.51	128.90	120.44
1	B	223	GLN	CB-CG-CD	-6.47	101.60	112.60
1	B	252	GLY	CA-C-O	-6.47	114.38	121.05
1	A	370	PRO	N-CA-CB	6.47	110.15	103.23
1	B	417	PHE	CA-C-N	6.45	127.91	119.84
1	B	417	PHE	C-N-CA	6.45	127.91	119.84
1	A	320	HIS	ND1-CG-CD2	6.44	112.54	106.10
1	A	16	LYS	O-C-N	6.43	128.94	122.12
1	A	58	LEU	N-CA-CB	-6.42	100.47	110.55
1	A	278	ASN	O-C-N	6.40	131.10	122.59
1	B	121	PRO	N-CA-CB	6.39	108.98	103.36
1	B	336	PHE	N-CA-C	-6.39	102.84	112.04
1	B	418	PRO	CB-CA-C	-6.39	101.02	111.56
1	A	11	ALA	N-CA-C	6.39	120.17	112.38
1	A	365	GLY	CA-C-N	6.38	128.74	120.44
1	A	365	GLY	C-N-CA	6.38	128.74	120.44
1	A	168	TRP	O-C-N	6.38	131.08	122.59
1	B	371	TRP	CA-C-O	-6.38	114.01	120.96
1	A	280	GLU	N-CA-C	6.36	119.97	112.72
1	B	178	LEU	CA-C-O	-6.35	111.24	120.13
1	B	370	PRO	N-CA-CB	6.35	109.38	103.41
1	A	61	ASP	CA-CB-CG	-6.35	106.25	112.60
1	A	183	PRO	N-CA-CB	6.34	109.36	103.46
1	A	350	VAL	CA-C-N	-6.33	112.51	122.65
1	A	350	VAL	C-N-CA	-6.33	112.51	122.65
1	B	41	MET	N-CA-C	-6.33	105.59	113.38
1	B	371	TRP	N-CA-CB	6.32	117.07	109.74
1	A	340	HIS	CB-CA-C	-6.32	101.01	109.16
1	A	391	ASN	CA-CB-CG	-6.31	106.29	112.60
1	B	153	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	184	CYS	N-CA-C	-6.27	104.52	111.36
1	A	134	ASN	N-CA-C	6.26	120.53	113.02
1	B	230	LEU	N-CA-C	6.25	118.17	111.36
1	B	248	SER	O-C-N	6.25	128.75	122.12
1	A	369	ASN	O-C-N	6.25	130.16	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ARG	CA-C-N	-6.25	110.20	121.14
1	A	401	ARG	C-N-CA	-6.25	110.20	121.14
1	B	167	TYR	CA-C-N	6.24	128.93	120.38
1	B	167	TYR	C-N-CA	6.24	128.93	120.38
1	B	340	HIS	CB-CA-C	-6.24	101.11	109.16
1	A	95	LEU	O-C-N	6.23	128.75	122.08
1	A	224	PHE	N-CA-C	-6.22	105.65	113.18
1	A	373	ASN	N-CA-C	6.22	118.15	109.31
1	B	22	LYS	N-CA-C	6.20	119.02	111.82
1	B	57	VAL	CA-C-N	6.17	130.25	121.42
1	B	57	VAL	C-N-CA	6.17	130.25	121.42
1	B	4	THR	N-CA-C	6.17	119.41	110.28
1	B	153	ASN	CA-CB-CG	-6.16	106.44	112.60
1	B	203	ILE	CA-C-N	-6.16	112.78	121.72
1	B	203	ILE	C-N-CA	-6.16	112.78	121.72
1	B	362	LEU	N-CA-C	-6.16	105.79	113.55
1	B	87	PRO	N-CA-CB	6.14	109.70	103.25
1	B	287	GLN	CA-C-O	-6.13	114.56	121.00
1	B	236	SER	CA-C-N	6.13	131.41	122.77
1	B	236	SER	C-N-CA	6.13	131.41	122.77
1	B	65	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	A	152	SER	N-CA-C	6.12	117.97	109.15
1	B	331	THR	O-C-N	6.12	129.38	122.22
1	A	415	LEU	CA-C-N	6.11	133.39	121.41
1	A	415	LEU	C-N-CA	6.11	133.39	121.41
1	B	375	ASP	N-CA-C	6.10	118.44	111.11
1	B	284	TRP	N-CA-C	-6.09	105.33	112.89
1	B	391	ASN	CA-CB-CG	-6.08	106.52	112.60
1	B	44	GLY	CA-C-N	6.08	131.21	122.40
1	B	44	GLY	C-N-CA	6.08	131.21	122.40
1	B	209	TRP	CA-C-N	6.07	128.74	120.54
1	B	209	TRP	C-N-CA	6.07	128.74	120.54
1	A	231	TYR	CA-C-N	6.06	130.84	120.72
1	A	231	TYR	C-N-CA	6.06	130.84	120.72
1	A	59	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	78	LEU	CA-C-N	6.03	126.38	119.93
1	A	78	LEU	C-N-CA	6.03	126.38	119.93
1	A	147	ALA	O-C-N	6.02	129.46	122.17
1	A	407	ALA	N-CA-C	6.02	121.24	111.37
1	B	358	PRO	CB-CA-C	-6.02	101.62	111.31
1	B	422	PRO	N-CA-CB	6.01	109.56	103.25
1	A	285	LEU	CB-CA-C	6.00	120.09	109.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	GLU	N-CA-CB	5.99	119.62	110.70
1	A	265	ALA	CA-C-O	-5.98	114.21	120.55
1	B	110	LEU	O-C-N	5.97	128.54	122.09
1	B	192	ASN	CA-C-N	-5.95	113.20	122.42
1	B	192	ASN	C-N-CA	-5.95	113.20	122.42
1	A	305	ILE	N-CA-C	5.94	116.60	110.36
1	A	332	CYS	O-C-N	5.94	128.50	122.09
1	B	203	ILE	N-CA-C	5.93	115.89	106.88
1	B	427	THR	OG1-CB-CG2	-5.93	97.44	109.30
1	A	396	LEU	N-CA-CB	5.93	118.83	109.82
1	B	342	PRO	CA-C-N	5.92	132.74	122.56
1	B	342	PRO	C-N-CA	5.92	132.74	122.56
1	B	125	VAL	CA-C-O	-5.92	114.90	121.17
1	B	278	ASN	O-C-N	5.92	130.46	122.59
1	B	369	ASN	CA-CB-CG	-5.90	106.70	112.60
1	B	22	LYS	N-CA-CB	5.89	119.42	110.28
1	B	344	ASP	CA-C-N	5.89	125.27	118.85
1	B	344	ASP	C-N-CA	5.89	125.27	118.85
1	B	331	THR	CA-CB-OG1	5.86	118.38	109.60
1	B	371	TRP	CB-CA-C	5.85	118.67	109.37
1	B	210	SER	O-C-N	5.84	128.16	122.09
1	B	252	GLY	O-C-N	5.83	127.91	122.13
1	A	54	GLU	N-CA-C	5.82	120.42	112.68
1	B	68	GLY	N-CA-C	-5.82	99.39	113.18
1	A	229	ARG	CA-C-N	5.82	128.00	120.44
1	A	229	ARG	C-N-CA	5.82	128.00	120.44
1	B	46	ARG	CD-NE-CZ	5.81	132.53	124.40
1	A	193	LEU	CA-C-N	5.79	132.46	122.09
1	A	193	LEU	C-N-CA	5.79	132.46	122.09
1	A	168	TRP	CA-C-N	5.79	128.51	120.29
1	A	168	TRP	C-N-CA	5.79	128.51	120.29
1	B	182	LEU	O-C-N	5.79	127.98	121.32
1	A	237	ASP	CA-C-N	-5.79	113.83	123.04
1	A	237	ASP	C-N-CA	-5.79	113.83	123.04
1	A	373	ASN	CB-CA-C	-5.78	100.81	114.16
1	A	120	LEU	CA-C-O	-5.76	114.33	119.86
1	B	180	ALA	N-CA-C	5.76	117.23	111.07
1	B	168	TRP	O-C-N	5.76	128.22	122.12
1	B	345	PRO	N-CA-CB	5.74	109.87	103.44
1	A	79	PRO	N-CA-CB	5.73	108.35	103.19
1	A	345	PRO	N-CA-CB	5.72	109.25	103.25
1	A	193	LEU	O-C-N	5.71	128.93	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	A	145	ILE	CB-CA-C	5.71	120.10	112.22
1	A	229	ARG	CD-NE-CZ	5.71	132.39	124.40
1	B	347	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	310	ASN	O-C-N	5.70	130.33	122.46
1	A	310	ASN	CA-CB-CG	-5.70	106.91	112.60
1	B	395	VAL	O-C-N	5.69	127.82	121.90
1	A	95	LEU	CA-C-O	-5.69	114.81	121.07
1	B	336	PHE	O-C-N	5.69	129.98	122.30
1	B	117	ARG	CA-C-N	-5.68	112.51	122.62
1	B	117	ARG	C-N-CA	-5.68	112.51	122.62
1	B	373	ASN	CB-CA-C	-5.67	99.14	110.42
1	B	155	ALA	O-C-N	5.66	128.84	122.22
1	B	217	LEU	N-CA-C	-5.65	105.50	112.90
1	A	87	PRO	N-CA-CB	5.64	109.17	103.25
1	B	99	GLY	N-CA-C	-5.62	107.98	115.40
1	A	180	ALA	CA-C-O	-5.60	114.93	120.70
1	B	310	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	100	GLN	N-CA-CB	-5.59	101.10	110.83
1	B	304	TYR	N-CA-C	-5.58	105.20	112.23
1	B	287	GLN	CA-C-N	5.57	127.75	120.28
1	B	287	GLN	C-N-CA	5.57	127.75	120.28
1	B	272	PRO	CA-C-N	5.57	130.15	120.68
1	B	272	PRO	C-N-CA	5.57	130.15	120.68
1	B	114	TRP	CB-CA-C	-5.57	102.14	110.88
1	A	111	SER	O-C-N	5.57	127.88	122.09
1	A	258	PRO	N-CA-CB	5.54	109.07	103.25
1	A	191	ARG	N-CA-CB	-5.54	101.96	110.16
1	A	202	ALA	N-CA-C	5.54	122.60	110.80
1	B	176	MET	O-C-N	5.54	128.51	122.20
1	B	175	CYS	O-C-N	5.54	127.85	122.09
1	A	165	THR	O-C-N	5.53	127.78	122.03
1	B	64	ILE	N-CA-C	5.53	116.34	107.98
1	B	328	PRO	O-C-N	5.53	128.87	122.17
1	B	19	ALA	O-C-N	5.53	127.76	122.07
1	B	176	MET	CA-C-N	5.52	130.81	121.14
1	B	176	MET	C-N-CA	5.52	130.81	121.14
1	B	399	VAL	CB-CA-C	5.52	119.25	112.02
1	B	313	ARG	N-CA-C	5.51	118.89	110.36
1	A	112	LYS	CA-C-N	5.50	129.98	120.58
1	A	112	LYS	C-N-CA	5.50	129.98	120.58
1	A	362	LEU	N-CA-C	-5.50	106.94	113.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	VAL	CA-C-N	5.48	126.03	119.94
1	A	251	VAL	C-N-CA	5.48	126.03	119.94
1	B	52	VAL	N-CA-C	5.48	116.88	108.71
1	B	391	ASN	CA-C-N	-5.48	111.55	121.14
1	B	391	ASN	C-N-CA	-5.48	111.55	121.14
1	B	375	ASP	CA-C-N	5.48	132.00	121.54
1	B	375	ASP	C-N-CA	5.48	132.00	121.54
1	B	276	LEU	CA-C-N	5.47	131.99	121.54
1	B	276	LEU	C-N-CA	5.47	131.99	121.54
1	A	342	PRO	N-CA-CB	5.47	108.55	103.41
1	A	236	SER	O-C-N	5.46	128.28	122.38
1	B	277	ALA	CA-C-N	5.46	131.98	121.54
1	B	277	ALA	C-N-CA	5.46	131.98	121.54
1	B	117	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	B	329	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	B	244	SER	CA-C-O	-5.45	115.08	121.07
1	A	224	PHE	CA-C-N	-5.45	111.93	122.06
1	A	224	PHE	C-N-CA	-5.45	111.93	122.06
1	B	405	VAL	CA-CB-CG1	5.43	119.64	110.40
1	A	427	THR	N-CA-CB	5.43	117.83	109.91
1	B	136	HIS	N-CA-C	5.42	116.24	109.57
1	B	369	ASN	N-CA-C	5.42	119.45	109.10
1	A	88	LEU	CA-C-N	5.42	125.13	119.82
1	A	88	LEU	C-N-CA	5.42	125.13	119.82
1	B	15	PRO	N-CA-CB	5.41	109.04	103.15
1	B	132	PRO	CA-C-O	-5.41	115.27	121.86
1	B	140	GLN	CA-CB-CG	-5.41	103.29	114.10
1	B	235	HIS	CA-CB-CG	-5.40	108.40	113.80
1	A	24	PHE	CA-C-N	-5.39	112.03	122.06
1	A	24	PHE	C-N-CA	-5.39	112.03	122.06
1	A	390	MET	CA-C-O	-5.39	112.04	119.05
1	A	38	VAL	N-CA-C	5.39	116.76	110.62
1	A	359	ASN	O-C-N	5.39	129.84	122.46
1	B	376	ALA	N-CA-C	5.39	122.27	110.80
1	B	57	VAL	N-CA-C	5.38	115.73	107.77
1	A	242	ASN	O-C-N	5.38	129.70	122.82
1	A	325	LYS	CA-C-N	5.38	128.97	121.02
1	A	325	LYS	C-N-CA	5.38	128.97	121.02
1	B	332	CYS	O-C-N	5.37	127.83	122.08
1	B	248	SER	CA-C-N	5.37	127.42	120.44
1	B	248	SER	C-N-CA	5.37	127.42	120.44
1	B	306	TRP	O-C-N	5.37	127.81	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ASN	CA-C-N	5.37	131.79	121.54
1	B	278	ASN	C-N-CA	5.37	131.79	121.54
1	B	178	LEU	O-C-N	5.36	129.21	122.19
1	A	19	ALA	CA-C-N	5.36	129.70	121.19
1	A	19	ALA	C-N-CA	5.36	129.70	121.19
1	A	86	GLU	N-CA-C	5.35	117.70	110.31
1	A	278	ASN	CA-CB-CG	5.35	117.95	112.60
1	B	357	VAL	N-CA-C	5.35	120.44	108.88
1	A	374	VAL	CA-C-N	5.34	128.42	120.31
1	A	374	VAL	C-N-CA	5.34	128.42	120.31
1	B	347	PHE	CA-C-O	-5.33	115.20	121.07
1	B	307	ASN	N-CA-CB	5.32	119.48	110.49
1	A	101	ILE	N-CA-C	5.32	114.76	108.96
1	A	304	TYR	O-C-N	5.32	127.55	122.07
1	B	372	PRO	N-CA-CB	5.32	107.78	103.32
1	A	88	LEU	N-CA-CB	-5.31	102.14	110.11
1	A	311	SER	O-C-N	5.31	129.17	122.37
1	B	285	LEU	O-C-N	5.31	129.73	122.46
1	A	87	PRO	CA-C-N	5.31	133.79	122.17
1	A	87	PRO	C-N-CA	5.31	133.79	122.17
1	B	274	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	109	TRP	O-C-N	5.30	127.74	122.12
1	B	37	THR	CA-C-O	-5.30	115.24	121.44
1	A	340	HIS	ND1-CG-CD2	5.30	111.40	106.10
1	A	358	PRO	N-CA-CB	5.29	108.38	103.41
1	B	272	PRO	O-C-N	5.28	128.56	122.17
1	A	167	TYR	N-CA-C	5.28	116.72	111.07
1	A	396	LEU	CA-C-N	5.28	127.67	120.54
1	A	396	LEU	C-N-CA	5.28	127.67	120.54
1	B	331	THR	N-CA-CB	5.27	118.33	110.22
1	A	112	LYS	N-CA-C	5.26	117.77	111.71
1	A	337	ALA	O-C-N	5.26	128.75	122.27
1	B	284	TRP	CA-C-N	-5.26	112.39	121.66
1	B	284	TRP	C-N-CA	-5.26	112.39	121.66
1	A	234	ILE	O-C-N	5.26	128.22	122.12
1	A	322	VAL	N-CA-CB	-5.25	102.57	111.23
1	A	341	LEU	N-CA-C	5.25	121.41	109.81
1	A	3	SER	N-CA-C	5.25	117.83	109.65
1	B	169	GLU	CA-C-O	-5.25	115.49	121.00
1	A	237	ASP	O-C-N	-5.24	117.06	123.30
1	B	340	HIS	ND1-CG-CD2	5.24	111.34	106.10
1	B	219	TYR	CA-C-O	-5.24	115.44	121.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	LEU	CA-C-O	-5.24	115.05	120.92
1	B	412	SER	CA-C-N	5.23	131.14	121.52
1	B	412	SER	C-N-CA	5.23	131.14	121.52
1	A	372	PRO	N-CA-C	5.22	123.23	112.47
1	B	179	ILE	CB-CA-C	-5.22	105.09	112.14
1	A	110	LEU	O-C-N	5.21	128.09	122.15
1	B	286	THR	CA-C-N	5.21	127.53	120.65
1	B	286	THR	C-N-CA	5.21	127.53	120.65
1	A	184	CYS	O-C-N	5.19	128.06	122.15
1	A	343	HIS	N-CA-C	5.18	119.32	113.15
1	B	89	PRO	N-CA-C	5.18	120.41	114.20
1	A	200	ILE	CA-C-N	5.17	131.55	121.41
1	A	200	ILE	C-N-CA	5.17	131.55	121.41
1	B	391	ASN	CB-CG-ND2	-5.17	108.64	116.40
1	A	24	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	102	PRO	CA-C-N	5.16	129.73	122.09
1	A	102	PRO	C-N-CA	5.16	129.73	122.09
1	B	245	ALA	N-CA-C	5.16	117.30	111.11
1	B	343	HIS	N-CA-C	5.16	119.21	113.02
1	A	313	ARG	O-C-N	5.16	129.45	122.59
1	A	369	ASN	CA-CB-CG	-5.16	107.44	112.60
1	B	60	PRO	CA-C-N	5.15	127.95	120.79
1	B	60	PRO	C-N-CA	5.15	127.95	120.79
1	B	106	GLN	CA-C-N	5.15	128.80	120.82
1	B	106	GLN	C-N-CA	5.15	128.80	120.82
1	A	326	THR	CA-C-N	-5.15	113.65	120.65
1	A	326	THR	C-N-CA	-5.15	113.65	120.65
1	A	403	LEU	CB-CA-C	-5.15	103.03	110.96
1	B	288	LEU	CA-C-O	-5.14	115.10	120.55
1	A	9	ILE	N-CA-C	-5.14	105.53	110.72
1	B	411	TRP	N-CA-C	5.14	117.79	111.82
1	A	87	PRO	O-C-N	5.14	129.57	122.64
1	B	131	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	246	HIS	CA-C-O	-5.13	115.11	120.55
1	B	19	ALA	CA-C-N	5.13	127.11	120.44
1	B	19	ALA	C-N-CA	5.13	127.11	120.44
1	B	247	THR	O-C-N	5.12	127.56	122.08
1	B	199	SER	N-CA-CB	5.12	117.78	110.06
1	A	18	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	120	LEU	O-C-N	5.11	126.29	121.38
1	A	283	VAL	CB-CA-C	5.11	118.46	111.87
1	A	165	THR	CA-C-O	-5.10	115.65	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	N-CA-C	-5.09	105.42	110.97
1	B	184	CYS	CA-C-N	5.09	128.99	120.64
1	B	184	CYS	C-N-CA	5.09	128.99	120.64
1	B	374	VAL	CA-C-N	5.09	127.41	120.54
1	B	374	VAL	C-N-CA	5.09	127.41	120.54
1	A	360	VAL	N-CA-C	-5.09	105.91	113.39
1	B	245	ALA	CA-C-O	-5.09	115.45	120.90
1	B	5	ASN	CA-C-N	5.09	127.81	120.38
1	B	5	ASN	C-N-CA	5.09	127.81	120.38
1	A	139	SER	O-C-N	5.08	129.57	122.36
1	B	183	PRO	CA-C-N	5.06	127.06	120.28
1	B	183	PRO	C-N-CA	5.06	127.06	120.28
1	A	9	ILE	N-CA-CB	-5.05	103.00	110.58
1	B	236	SER	O-C-N	5.05	128.13	122.32
1	B	267	ASN	O-C-N	5.05	128.59	122.48
1	A	344	ASP	CA-C-N	5.05	126.15	119.84
1	A	344	ASP	C-N-CA	5.05	126.15	119.84
1	B	332	CYS	CB-CA-C	-5.05	102.89	110.92
1	B	109	TRP	N-CA-C	-5.04	105.06	111.11
1	A	96	LEU	N-CA-CB	5.04	117.53	110.12
1	B	14	ILE	N-CA-C	5.04	119.76	108.88
1	B	401	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	B	431	ILE	CA-C-O	-5.03	115.72	120.95
1	B	64	ILE	CA-C-O	5.03	126.94	120.76
1	B	23	THR	N-CA-CB	-5.02	102.72	110.20
1	A	185	VAL	CA-CB-CG1	5.01	118.92	110.40
1	A	351	ALA	CA-C-O	5.01	125.42	119.56
1	A	136	HIS	CA-C-N	5.01	126.10	119.84
1	A	136	HIS	C-N-CA	5.01	126.10	119.84
1	B	308	THR	N-CA-CB	-5.01	103.16	110.47
1	B	318	TYR	O-C-N	5.01	129.40	123.24
1	B	309	LEU	O-C-N	5.00	127.29	122.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	37	THR	CB
1	B	37	THR	CB
1	B	307	ASN	CA

All (209) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLN	Mainchain
1	A	102	PRO	Mainchain
1	A	106	GLN	Mainchain,Peptide
1	A	11	ALA	Mainchain
1	A	113	GLU	Sidechain
1	A	134	ASN	Mainchain
1	A	135	LEU	Mainchain
1	A	140	GLN	Sidechain
1	A	143	ALA	Mainchain
1	A	144	ALA	Mainchain
1	A	160	GLU	Sidechain
1	A	161	GLY	Mainchain
1	A	165	THR	Mainchain
1	A	167	TYR	Sidechain
1	A	18	GLN	Sidechain
1	A	191	ARG	Sidechain
1	A	194	TYR	Sidechain
1	A	195	ARG	Mainchain
1	A	202	ALA	Mainchain,Peptide
1	A	204	ASP	Sidechain
1	A	206	LYS	Mainchain
1	A	213	PHE	Mainchain
1	A	219	TYR	Mainchain
1	A	223	GLN	Sidechain
1	A	237	ASP	Sidechain
1	A	25	ARG	Sidechain
1	A	251	VAL	Mainchain
1	A	254	ALA	Mainchain
1	A	256	SER	Mainchain
1	A	26	GLN	Sidechain
1	A	267	ASN	Sidechain
1	A	280	GLU	Mainchain,Peptide,Sidechain
1	A	283	VAL	Mainchain
1	A	284	TRP	Mainchain
1	A	285	LEU	Mainchain
1	A	287	GLN	Mainchain,Sidechain
1	A	289	GLN	Mainchain
1	A	290	LYS	Mainchain,Peptide
1	A	292	VAL	Mainchain
1	A	300	LYS	Mainchain
1	A	304	TYR	Mainchain
1	A	308	THR	Mainchain
1	A	310	ASN	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	315	VAL	Mainchain
1	A	32	VAL	Mainchain
1	A	324	ARG	Sidechain
1	A	326	THR	Mainchain
1	A	333	GLN	Sidechain
1	A	335	GLU	Sidechain
1	A	342	PRO	Mainchain
1	A	344	ASP	Mainchain
1	A	346	MET	Mainchain
1	A	347	PHE	Mainchain
1	A	348	LYS	Mainchain
1	A	35	GLN	Sidechain
1	A	350	VAL	Mainchain
1	A	352	GLN	Mainchain
1	A	354	TYR	Mainchain
1	A	365	GLY	Mainchain
1	A	366	LYS	Mainchain,Peptide
1	A	373	ASN	Mainchain,Sidechain
1	A	375	ASP	Sidechain
1	A	376	ALA	Mainchain
1	A	384	TYR	Mainchain,Sidechain
1	A	385	TYR	Mainchain
1	A	39	ASP	Sidechain
1	A	390	MET	Mainchain
1	A	394	THR	Mainchain
1	A	399	VAL	Mainchain
1	A	401	ARG	Mainchain
1	A	406	LEU	Mainchain
1	A	410	ILE	Mainchain
1	A	411	TRP	Mainchain
1	A	420	GLU	Sidechain
1	A	428	ASP	Mainchain,Sidechain
1	A	431	ILE	Mainchain
1	A	433	LEU	Mainchain
1	A	52	VAL	Mainchain
1	A	54	GLU	Sidechain
1	A	59	ASP	Sidechain
1	A	61	ASP	Sidechain
1	A	62	GLU	Sidechain
1	A	64	ILE	Mainchain
1	A	66	PHE	Mainchain,Peptide
1	A	67	ARG	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	68	GLY	Mainchain
1	A	73	GLU	Mainchain
1	A	75	GLN	Sidechain
1	A	81	ALA	Mainchain
1	A	84	GLY	Mainchain
1	A	85	GLU	Mainchain
1	A	88	LEU	Mainchain
1	A	90	GLU	Sidechain
1	A	93	PHE	Mainchain
1	B	100	GLN	Sidechain
1	B	101	ILE	Mainchain,Peptide
1	B	102	PRO	Mainchain
1	B	115	ALA	Mainchain,Peptide
1	B	117	ARG	Mainchain
1	B	130	ASN	Sidechain
1	B	139	SER	Mainchain
1	B	140	GLN	Sidechain
1	B	153	ASN	Sidechain
1	B	158	TYR	Sidechain
1	B	160	GLU	Sidechain
1	B	166	LYS	Mainchain
1	B	169	GLU	Mainchain
1	B	17	GLU	Sidechain
1	B	177	ASP	Mainchain
1	B	18	GLN	Sidechain
1	B	184	CYS	Mainchain
1	B	188	LYS	Mainchain
1	B	191	ARG	Sidechain
1	B	192	ASN	Sidechain
1	B	195	ARG	Mainchain
1	B	200	ILE	Mainchain
1	B	206	LYS	Mainchain
1	B	207	LEU	Mainchain
1	B	208	ASP	Mainchain
1	B	221	ASP	Sidechain
1	B	223	GLN	Sidechain
1	B	231	TYR	Sidechain
1	B	232	LEU	Mainchain
1	B	235	HIS	Mainchain
1	B	237	ASP	Sidechain
1	B	238	HIS	Mainchain
1	B	239	GLU	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	251	VAL	Mainchain
1	B	267	ASN	Mainchain
1	B	278	ASN	Mainchain
1	B	280	GLU	Sidechain
1	B	284	TRP	Mainchain
1	B	287	GLN	Sidechain
1	B	290	LYS	Mainchain
1	B	291	GLU	Mainchain
1	B	298	ASP	Sidechain
1	B	299	GLU	Mainchain
1	B	30	ASN	Mainchain
1	B	303	ASP	Sidechain
1	B	305	ILE	Mainchain
1	B	311	SER	Mainchain
1	B	312	GLY	Mainchain
1	B	32	VAL	Mainchain
1	B	321	ALA	Mainchain
1	B	327	ASP	Sidechain
1	B	329	ARG	Mainchain
1	B	330	TYR	Sidechain
1	B	335	GLU	Sidechain
1	B	349	LEU	Mainchain
1	B	350	VAL	Mainchain
1	B	358	PRO	Mainchain
1	B	359	ASN	Mainchain
1	B	362	LEU	Mainchain
1	B	363	GLU	Sidechain
1	B	366	LYS	Mainchain
1	B	367	ALA	Mainchain,Peptide
1	B	370	PRO	Mainchain
1	B	373	ASN	Mainchain,Sidechain
1	B	374	VAL	Mainchain
1	B	376	ALA	Mainchain,Peptide
1	B	383	GLN	Sidechain
1	B	385	TYR	Mainchain
1	B	386	GLY	Mainchain,Peptide
1	B	389	GLU	Sidechain
1	B	390	MET	Mainchain
1	B	391	ASN	Sidechain
1	B	394	THR	Mainchain
1	B	399	VAL	Mainchain
1	B	404	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	405	VAL	Mainchain
1	B	420	GLU	Sidechain
1	B	422	PRO	Mainchain,Peptide
1	B	425	MET	Mainchain
1	B	431	ILE	Mainchain
1	B	433	LEU	Mainchain
1	B	46	ARG	Sidechain
1	B	51	LEU	Mainchain,Peptide
1	B	54	GLU	Sidechain
1	B	55	THR	Mainchain
1	B	61	ASP	Sidechain
1	B	63	GLY	Mainchain
1	B	66	PHE	Mainchain,Peptide
1	B	67	ARG	Mainchain
1	B	73	GLU	Mainchain
1	B	80	LYS	Mainchain,Peptide
1	B	84	GLY	Mainchain
1	B	86	GLU	Mainchain
1	B	93	PHE	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3444	0	3436	297	17
1	B	3444	0	3436	297	27
2	A	9	0	2	0	0
2	B	9	0	2	0	0
3	A	49	0	0	4	0
3	B	47	0	0	0	2
All	All	7002	0	6876	518	38

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 40.

All (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:MET:HE3	1:B:127:MET:HE3	1.41	0.99
1:A:268:GLY:HA2	1:B:251:VAL:HG13	1.47	0.96
1:A:419:LEU:HD11	1:B:243:VAL:HG22	1.51	0.92
1:B:58:LEU:HD12	1:B:63:GLY:HA2	1.53	0.90
1:A:280:GLU:HA	1:A:283:VAL:HB	1.54	0.90
1:A:75:GLN:HA	1:A:87:PRO:HG3	1.56	0.88
1:B:188:LYS:HB2	1:B:200:ILE:HD13	1.54	0.88
1:A:55:THR:HG21	1:A:407:ALA:HB1	1.57	0.86
1:B:272:PRO:HA	1:B:276:LEU:HB2	1.56	0.86
1:A:288:LEU:HD22	1:A:301:LEU:HD11	1.57	0.86
1:A:81:ALA:HB2	1:A:88:LEU:HD13	1.59	0.85
1:A:434:VAL:HG23	1:B:31:THR:HG21	1.57	0.84
1:A:273:LEU:HD22	1:B:255:LEU:HG	1.60	0.84
1:A:6:LEU:HD21	1:A:97:VAL:HG11	1.58	0.84
1:B:75:GLN:HA	1:B:87:PRO:HG3	1.59	0.83
1:B:298:ASP:HA	1:B:301:LEU:HB3	1.61	0.83
1:B:127:MET:HE2	1:B:131:PHE:HZ	1.44	0.82
1:B:359:ASN:HA	1:B:362:LEU:HD12	1.60	0.82
1:A:434:VAL:CG2	1:B:31:THR:HG21	2.10	0.81
1:A:168:TRP:HB3	1:A:414:ALA:HB2	1.64	0.80
1:B:282:LEU:HD12	1:B:285:LEU:HB3	1.64	0.80
1:A:167:TYR:HB3	1:A:413:ARG:HG3	1.62	0.79
1:A:281:VAL:HG12	1:A:285:LEU:HD22	1.63	0.79
1:A:359:ASN:HA	1:A:362:LEU:HB2	1.64	0.78
1:A:138:MET:HG2	1:A:395:VAL:HG22	1.66	0.78
1:B:86:GLU:HG2	1:B:230:LEU:HB2	1.65	0.78
1:A:137:PRO:HB2	1:A:395:VAL:HG21	1.64	0.77
1:B:250:LEU:HD13	1:B:420:GLU:HB3	1.66	0.77
1:A:267:ASN:HB3	1:B:260:LEU:HG	1.67	0.76
1:A:41:MET:HE1	1:B:33:VAL:HG11	1.68	0.76
1:A:81:ALA:HB2	1:A:88:LEU:CD1	2.16	0.76
1:A:127:MET:CE	1:B:127:MET:HE3	2.15	0.76
1:A:200:ILE:O	1:A:216:MET:HG2	1.86	0.76
1:A:162:ILE:HD13	1:A:170:LEU:HD12	1.68	0.75
1:A:422:PRO:HB3	1:B:45:MET:HE2	1.68	0.75
1:B:120:LEU:HD21	1:B:185:VAL:HG22	1.69	0.74
1:B:282:LEU:HA	1:B:285:LEU:HB2	1.68	0.74
1:A:137:PRO:HB3	1:A:189:ILE:CG2	2.17	0.74
1:A:419:LEU:HD11	1:B:243:VAL:CG2	2.18	0.73
1:B:17:GLU:HA	1:B:20:ARG:HB2	1.70	0.73
1:B:90:GLU:HB2	1:B:107:VAL:HG13	1.69	0.73
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:CD2	1:B:101:ILE:HD13	2.20	0.72
1:B:282:LEU:HD12	1:B:285:LEU:CB	2.20	0.71
1:B:425:MET:HG2	1:B:430:LEU:HG	1.71	0.71
1:B:300:LYS:HA	1:B:303:ASP:HB2	1.72	0.71
1:B:145:ILE:HG22	1:B:263:ALA:HB2	1.72	0.71
1:A:57:VAL:HG21	1:B:426:SER:HB3	1.71	0.70
1:A:298:ASP:OD2	1:A:301:LEU:HD23	1.92	0.69
1:A:171:ILE:HD11	1:A:410:ILE:HA	1.74	0.69
1:B:86:GLU:HG3	1:B:87:PRO:HD2	1.73	0.69
1:B:250:LEU:CD1	1:B:420:GLU:HB3	2.21	0.69
1:B:298:ASP:O	1:B:302:ARG:HB2	1.93	0.69
1:A:424:SER:CB	1:B:51:LEU:HB2	2.23	0.69
1:A:49:LYS:HA	1:B:423:LYS:HB3	1.75	0.69
1:B:342:PRO:HA	1:B:347:PHE:CE1	2.28	0.68
1:A:273:LEU:HB2	1:B:254:ALA:O	1.94	0.68
1:B:37:THR:HG22	1:B:40:MET:HE3	1.73	0.68
1:B:148:LEU:HB3	1:B:259:TYR:CD1	2.28	0.68
1:B:103:THR:H	1:B:106:GLN:HG2	1.57	0.68
1:A:14:ILE:HG21	1:A:414:ALA:HB1	1.75	0.68
1:B:243:VAL:HB	1:B:274:HIS:CD2	2.28	0.67
1:B:67:ARG:HB3	1:B:69:TYR:CD1	2.30	0.67
1:B:276:LEU:C	1:B:280:GLU:HG2	2.20	0.67
1:A:298:ASP:HA	1:A:301:LEU:HB3	1.77	0.67
1:A:45:MET:HE2	1:B:422:PRO:HB3	1.77	0.67
1:B:81:ALA:HB2	1:B:88:LEU:HD13	1.76	0.66
1:B:190:TYR:HB2	1:B:392:TYR:CE1	2.31	0.66
1:A:171:ILE:HG21	1:A:413:ARG:HG2	1.76	0.66
1:A:120:LEU:HD23	1:A:125:VAL:HG22	1.77	0.66
1:B:78:LEU:HD23	1:B:101:ILE:HD13	1.78	0.66
1:B:272:PRO:HA	1:B:276:LEU:CB	2.26	0.66
1:B:324:ARG:HE	1:B:368:LYS:HD3	1.61	0.66
1:B:276:LEU:O	1:B:280:GLU:HG2	1.96	0.66
1:B:344:ASP:HB3	1:B:347:PHE:HB3	1.79	0.65
1:A:51:LEU:HB2	1:B:424:SER:CB	2.27	0.65
1:A:67:ARG:HB3	1:A:69:TYR:CD1	2.32	0.64
1:B:228:MET:CE	1:B:228:MET:HA	2.26	0.64
1:B:127:MET:HE2	1:B:131:PHE:CZ	2.29	0.64
1:B:59:ASP:HB3	1:B:63:GLY:N	2.12	0.64
1:B:425:MET:CG	1:B:430:LEU:HG	2.27	0.64
1:A:146:THR:HG23	1:A:260:LEU:HD12	1.79	0.64
1:B:45:MET:HG2	1:B:48:MET:CE	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLU:HG3	1:B:114:TRP:CZ3	2.33	0.64
1:A:52:VAL:HG22	1:B:430:LEU:CD1	2.28	0.64
1:B:371:TRP:HB3	1:B:372:PRO:HD2	1.79	0.64
1:A:138:MET:HA	1:A:141:LEU:HB3	1.79	0.64
1:A:282:LEU:HB3	1:A:390:MET:SD	2.37	0.63
1:A:168:TRP:CB	1:A:414:ALA:HB2	2.27	0.63
1:A:398:GLY:HA2	1:A:401:ARG:HB3	1.80	0.63
1:B:169:GLU:O	1:B:172:TYR:HB3	1.98	0.63
1:A:41:MET:HG2	1:B:52:VAL:HG23	1.79	0.63
1:A:300:LYS:HA	1:A:303:ASP:HB2	1.80	0.63
1:A:312:GLY:O	1:B:164:ARG:HD2	1.99	0.63
1:B:162:ILE:HD11	1:B:167:TYR:HD1	1.64	0.63
1:A:52:VAL:HA	1:B:425:MET:O	1.99	0.62
1:A:247:THR:HG21	1:A:265:ALA:HA	1.80	0.62
1:A:178:LEU:HG	1:A:182:LEU:HD12	1.81	0.62
1:A:420:GLU:HG2	1:A:422:PRO:HD3	1.82	0.62
1:A:421:ARG:HH22	1:B:239:GLU:CG	2.12	0.62
1:B:135:LEU:HD22	1:B:139:SER:HB2	1.81	0.62
1:A:41:MET:SD	1:A:430:LEU:HD11	2.40	0.62
1:B:22:LYS:O	1:B:26:GLN:HG3	2.00	0.62
1:A:103:THR:HG22	1:A:105:GLU:HB3	1.82	0.61
1:A:284:TRP:CH2	1:A:305:ILE:HG12	2.36	0.61
1:A:31:THR:HG21	1:B:434:VAL:HB	1.81	0.61
1:A:276:LEU:O	1:A:279:GLN:HB3	2.01	0.61
1:B:344:ASP:HB3	1:B:347:PHE:CB	2.31	0.61
1:B:281:VAL:HG12	1:B:285:LEU:HD22	1.81	0.61
1:B:55:THR:HG23	1:B:408:GLN:OE1	2.01	0.60
1:B:166:LYS:O	1:B:169:GLU:HB2	2.00	0.60
1:B:430:LEU:O	1:B:434:VAL:HG12	2.02	0.60
1:A:341:LEU:HD13	1:A:384:TYR:CG	2.36	0.60
1:B:157:ALA:HB1	1:B:162:ILE:HG21	1.84	0.60
1:A:52:VAL:HG23	1:B:41:MET:HG2	1.83	0.60
1:B:276:LEU:O	1:B:279:GLN:HB3	2.00	0.60
1:A:4:THR:HG21	1:A:106:GLN:CB	2.32	0.60
1:A:209:TRP:HZ3	1:A:232:LEU:HD23	1.67	0.60
1:A:6:LEU:O	1:A:9:ILE:HB	2.02	0.60
1:A:231:TYR:HD1	1:A:232:LEU:HD12	1.67	0.59
1:A:341:LEU:HD22	1:A:384:TYR:CD2	2.37	0.59
1:B:133:THR:HG23	1:B:193:LEU:HD12	1.84	0.59
1:A:55:THR:HG22	1:A:96:LEU:HB3	1.83	0.59
1:B:279:GLN:O	1:B:283:VAL:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HB2	1:B:424:SER:HA	1.84	0.59
1:B:59:ASP:HB3	1:B:63:GLY:H	1.65	0.58
1:A:90:GLU:HB2	1:A:107:VAL:HG13	1.85	0.58
1:A:163:HIS:O	1:A:166:LYS:HB2	2.03	0.58
1:A:288:LEU:CD2	1:A:301:LEU:HD11	2.31	0.58
1:A:350:VAL:CG2	1:A:380:VAL:HG21	2.32	0.58
1:A:425:MET:O	1:B:52:VAL:HA	2.03	0.58
1:A:425:MET:HG2	1:A:430:LEU:HG	1.83	0.58
1:A:127:MET:HE3	1:B:127:MET:CE	2.26	0.58
1:A:55:THR:O	1:A:96:LEU:HD22	2.02	0.58
1:A:189:ILE:O	1:A:193:LEU:HB2	2.04	0.58
1:A:52:VAL:HG23	1:B:41:MET:O	2.04	0.58
1:A:86:GLU:HG2	1:A:230:LEU:HB2	1.86	0.57
1:B:167:TYR:HB3	1:B:413:ARG:HG3	1.86	0.57
1:B:354:TYR:O	1:B:355:LYS:HD3	2.04	0.57
1:A:207:LEU:HD12	1:A:212:ASN:ND2	2.19	0.57
1:B:324:ARG:HA	1:B:369:ASN:HB2	1.86	0.57
1:B:190:TYR:HB2	1:B:392:TYR:CZ	2.39	0.57
1:A:103:THR:CG2	1:A:105:GLU:HB3	2.35	0.57
1:A:255:LEU:HD12	1:B:273:LEU:HD13	1.87	0.57
1:B:78:LEU:HD21	1:B:101:ILE:HD13	1.87	0.57
1:A:57:VAL:CG2	1:B:426:SER:HB3	2.35	0.56
1:A:354:TYR:C	1:A:355:LYS:HD3	2.30	0.56
1:B:103:THR:CG2	1:B:105:GLU:HB3	2.35	0.56
1:B:162:ILE:HD11	1:B:167:TYR:CD1	2.39	0.56
1:B:157:ALA:HB1	1:B:162:ILE:CG2	2.35	0.56
1:B:171:ILE:HD11	1:B:409:LEU:O	2.06	0.56
1:A:154:PHE:HD1	1:A:170:LEU:HB2	1.70	0.56
1:A:282:LEU:HA	1:A:285:LEU:HB2	1.87	0.56
1:A:284:TRP:CZ2	1:A:305:ILE:HG12	2.41	0.56
1:A:267:ASN:N	1:A:267:ASN:HD22	2.04	0.55
1:B:228:MET:HA	1:B:228:MET:HE3	1.87	0.55
1:A:280:GLU:CA	1:A:283:VAL:HB	2.33	0.55
1:A:37:THR:CG2	1:A:40:MET:HG3	2.37	0.55
1:A:204:ASP:H	1:A:212:ASN:HD21	1.54	0.55
1:A:240:GLY:O	1:A:246:HIS:HB2	2.06	0.55
1:B:262:PHE:CE1	1:B:266:MET:HE3	2.42	0.55
1:B:231:TYR:HD1	1:B:232:LEU:HD12	1.72	0.55
1:A:52:VAL:HG22	1:B:430:LEU:HD11	1.89	0.55
1:B:103:THR:HG22	1:B:105:GLU:H	1.72	0.55
1:B:236:SER:O	1:B:401:ARG:HD3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD13	1:A:259:TYR:CE1	2.41	0.55
1:A:209:TRP:CZ3	1:A:232:LEU:HD23	2.42	0.55
1:A:321:ALA:HB1	1:A:322:VAL:HG23	1.89	0.55
1:A:54:GLU:H	1:A:408:GLN:CD	2.15	0.55
1:A:182:LEU:HD21	1:A:262:PHE:HE2	1.70	0.55
1:B:72:PRO:HA	1:B:75:GLN:HB2	1.88	0.55
1:A:371:TRP:HB3	1:A:372:PRO:HD2	1.89	0.55
1:B:103:THR:HB	1:B:106:GLN:H	1.72	0.55
1:A:266:MET:HA	1:A:266:MET:HE2	1.89	0.54
1:B:37:THR:HG22	1:B:40:MET:HG3	1.89	0.54
1:A:156:ARG:HD2	3:A:467:HOH:O	2.07	0.54
1:A:257:ASP:HB2	1:A:258:PRO:HD2	1.88	0.54
1:B:65:ARG:HB3	1:B:68:GLY:C	2.32	0.54
1:B:93:PHE:O	1:B:97:VAL:HG23	2.06	0.54
1:B:284:TRP:HA	1:B:287:GLN:HB2	1.89	0.54
1:A:238:HIS:HE1	1:A:320:HIS:CE1	2.24	0.54
1:A:255:LEU:HG	1:B:273:LEU:HD22	1.90	0.54
1:B:257:ASP:HB2	1:B:258:PRO:HD2	1.90	0.54
1:B:427:THR:HG22	1:B:431:ILE:HD12	1.89	0.54
1:A:248:SER:OG	1:A:405:VAL:HG22	2.08	0.54
1:A:164:ARG:HA	1:A:167:TYR:CE1	2.43	0.53
1:A:427:THR:HG22	1:A:431:ILE:HD12	1.90	0.53
1:B:5:ASN:HD22	1:B:5:ASN:C	2.16	0.53
1:B:319:GLY:HA2	1:B:369:ASN:O	2.09	0.53
1:A:42:TYR:CE1	1:B:52:VAL:HG11	2.43	0.53
1:A:423:LYS:HB3	1:B:49:LYS:HA	1.90	0.53
1:B:154:PHE:O	1:B:157:ALA:HB3	2.08	0.53
1:B:227:LEU:HB2	1:B:336:PHE:CZ	2.43	0.53
1:B:300:LYS:O	1:B:304:TYR:HB2	2.09	0.53
1:B:92:LEU:HD12	1:B:95:LEU:HD23	1.91	0.53
1:B:148:LEU:C	1:B:150:SER:H	2.17	0.53
1:B:279:GLN:HG2	1:B:280:GLU:OE2	2.09	0.53
1:B:124:VAL:O	1:B:127:MET:HB3	2.08	0.53
1:B:354:TYR:C	1:B:355:LYS:HD3	2.34	0.53
1:A:273:LEU:HD22	1:B:255:LEU:CG	2.36	0.52
1:A:128:LEU:HD11	1:A:185:VAL:HG13	1.92	0.52
1:A:129:ASP:HA	1:A:192:ASN:HD21	1.75	0.52
1:B:67:ARG:H	1:B:69:TYR:H	1.56	0.52
1:A:285:LEU:O	1:A:289:GLN:HB2	2.09	0.52
1:A:268:GLY:CA	1:B:251:VAL:HG13	2.31	0.52
1:A:425:MET:HG2	1:A:430:LEU:CD2	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TYR:O	1:B:171:ILE:HG23	2.09	0.52
1:B:277:ALA:HA	1:B:280:GLU:HB2	1.91	0.52
1:A:37:THR:HA	1:B:31:THR:O	2.09	0.52
1:A:37:THR:HG22	1:A:40:MET:HG3	1.92	0.52
1:A:137:PRO:HB2	1:A:395:VAL:CG2	2.37	0.52
1:A:309:LEU:HD21	1:A:315:VAL:HG21	1.92	0.52
1:B:10:LEU:O	1:B:14:ILE:HG13	2.10	0.52
1:A:273:LEU:HB3	1:B:419:LEU:HD22	1.92	0.52
1:B:181:LYS:C	1:B:183:PRO:HD2	2.35	0.52
1:A:86:GLU:CG	1:A:230:LEU:HB2	2.41	0.51
1:B:333:GLN:OE1	1:B:378:SER:HB3	2.10	0.51
1:B:319:GLY:O	1:B:320:HIS:HB2	2.10	0.51
1:A:38:VAL:HG22	1:B:33:VAL:HG23	1.91	0.51
1:A:90:GLU:HG3	1:A:114:TRP:CZ3	2.45	0.51
1:B:69:TYR:CD1	1:B:95:LEU:HD11	2.45	0.51
1:A:136:HIS:HE1	1:A:279:GLN:HE22	1.56	0.51
1:A:359:ASN:HA	1:A:362:LEU:CB	2.38	0.51
1:B:132:PRO:HB2	1:B:134:ASN:OD1	2.11	0.51
1:A:29:GLY:HA3	1:B:39:ASP:OD2	2.11	0.51
1:A:344:ASP:O	1:A:348:LYS:HG3	2.10	0.51
1:A:277:ALA:HA	1:A:280:GLU:HG2	1.91	0.51
1:A:130:ASN:HD21	1:B:130:ASN:ND2	2.09	0.51
1:A:137:PRO:HB3	1:A:189:ILE:HG22	1.92	0.51
1:B:224:PHE:CE1	1:B:227:LEU:HD23	2.45	0.51
1:B:425:MET:HG2	1:B:430:LEU:CG	2.40	0.51
1:A:155:ALA:HB1	3:A:487:HOH:O	2.10	0.51
1:A:157:ALA:CB	1:A:170:LEU:HD13	2.40	0.51
1:A:330:TYR:HE1	1:A:334:ARG:HH11	1.59	0.51
1:B:157:ALA:CB	1:B:170:LEU:HD13	2.41	0.51
1:A:108:SER:O	1:A:112:LYS:HB3	2.11	0.50
1:A:424:SER:HA	1:B:51:LEU:HB2	1.93	0.50
1:A:434:VAL:HG23	1:B:31:THR:CG2	2.36	0.50
1:A:280:GLU:HB3	1:A:283:VAL:HB	1.92	0.50
1:B:266:MET:O	1:B:270:ALA:HB2	2.11	0.50
1:A:354:TYR:O	1:A:355:LYS:HD3	2.10	0.50
1:B:242:ASN:ND2	1:B:245:ALA:HB3	2.26	0.50
1:B:288:LEU:HD21	1:B:301:LEU:HD11	1.93	0.50
1:A:51:LEU:HB2	1:B:424:SER:HB2	1.93	0.50
1:A:251:VAL:HG13	1:B:267:ASN:C	2.36	0.50
1:A:69:TYR:HD1	1:A:95:LEU:HD11	1.77	0.50
1:B:324:ARG:HD3	1:B:369:ASN:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ASP:O	1:B:431:ILE:HG22	2.12	0.50
1:A:319:GLY:O	1:A:320:HIS:HB2	2.08	0.50
1:A:349:LEU:C	1:A:352:GLN:H	2.20	0.50
1:A:153:ASN:HB2	1:A:174:ASP:OD1	2.12	0.50
1:B:74:CYS:HA	1:B:78:LEU:HG	1.93	0.50
1:B:350:VAL:HG21	1:B:380:VAL:HG21	1.93	0.50
1:A:38:VAL:HG22	1:B:33:VAL:CG2	2.41	0.49
1:A:51:LEU:HB2	1:B:424:SER:CA	2.42	0.49
1:A:51:LEU:HD12	1:B:424:SER:HB3	1.93	0.49
1:B:103:THR:HG22	1:B:105:GLU:HB3	1.93	0.49
1:B:127:MET:CE	1:B:143:ALA:HB1	2.42	0.49
1:A:5:ASN:C	1:A:5:ASN:HD22	2.20	0.49
1:B:65:ARG:HB3	1:B:68:GLY:HA2	1.95	0.49
1:B:171:ILE:HD12	1:B:409:LEU:HG	1.95	0.49
1:B:285:LEU:O	1:B:289:GLN:HB2	2.12	0.49
1:B:371:TRP:HA	1:B:371:TRP:CE3	2.46	0.49
1:A:428:ASP:O	1:A:431:ILE:HB	2.13	0.49
1:A:214:THR:HG21	1:A:225:THR:CG2	2.43	0.49
1:A:4:THR:HG21	1:A:106:GLN:HB2	1.95	0.49
1:A:113:GLU:O	1:A:117:ARG:HG3	2.13	0.49
1:A:145:ILE:O	1:A:148:LEU:HB2	2.12	0.49
1:B:37:THR:HG22	1:B:40:MET:CE	2.42	0.49
1:B:342:PRO:HA	1:B:347:PHE:HE1	1.71	0.49
1:B:347:PHE:HA	1:B:380:VAL:HG11	1.94	0.49
1:B:71:ILE:HB	1:B:72:PRO:HD3	1.94	0.49
1:B:317:GLY:O	1:B:373:ASN:HB2	2.12	0.49
1:A:387:MET:HG2	1:A:393:TYR:HE1	1.77	0.49
1:B:92:LEU:O	1:B:95:LEU:HB3	2.12	0.49
1:B:320:HIS:ND1	1:B:323:LEU:HB2	2.27	0.49
1:B:342:PRO:HA	1:B:347:PHE:CD1	2.47	0.49
1:A:334:ARG:O	1:A:338:LEU:HG	2.13	0.48
1:B:98:THR:C	1:B:100:GLN:H	2.21	0.48
1:A:137:PRO:HB3	1:A:189:ILE:HG21	1.92	0.48
1:A:148:LEU:HB3	1:A:259:TYR:CD1	2.48	0.48
1:A:121:PRO:HG3	1:A:151:GLU:HG3	1.95	0.48
1:B:188:LYS:HB2	1:B:200:ILE:CD1	2.36	0.48
1:A:421:ARG:HH12	1:B:239:GLU:CD	2.21	0.48
1:A:174:ASP:CB	1:A:258:PRO:HG2	2.43	0.48
1:A:342:PRO:HA	1:A:347:PHE:CE1	2.48	0.48
1:A:103:THR:HB	1:A:106:GLN:HG2	1.95	0.48
1:B:359:ASN:HA	1:B:362:LEU:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:CG2	1:B:414:ALA:HB1	2.43	0.48
1:A:17:GLU:O	1:A:21:ILE:HG13	2.14	0.48
1:A:45:MET:HE2	1:B:422:PRO:CB	2.42	0.48
1:A:210:SER:O	1:A:213:PHE:HB3	2.14	0.48
1:A:280:GLU:CB	1:A:283:VAL:HB	2.44	0.48
1:B:148:LEU:HB3	1:B:259:TYR:CE1	2.49	0.47
1:B:182:LEU:HD23	1:B:399:VAL:HG22	1.96	0.47
1:A:86:GLU:HG3	1:A:230:LEU:HD13	1.97	0.47
1:A:328:PRO:O	1:A:332:CYS:HB2	2.14	0.47
1:B:281:VAL:O	1:B:285:LEU:HB2	2.14	0.47
1:B:359:ASN:CA	1:B:362:LEU:HD12	2.38	0.47
1:A:39:ASP:OD2	1:B:29:GLY:HA3	2.14	0.47
1:B:277:ALA:HA	1:B:280:GLU:CG	2.45	0.47
1:B:304:TYR:O	1:B:307:ASN:HA	2.15	0.47
1:A:25:ARG:HD2	1:B:42:TYR:CD2	2.49	0.47
1:A:31:THR:HB	1:B:38:VAL:HG23	1.95	0.47
1:A:419:LEU:O	1:B:46:ARG:NH1	2.48	0.47
1:B:92:LEU:CD1	1:B:95:LEU:HD23	2.45	0.47
1:A:25:ARG:HH21	1:B:39:ASP:HA	1.79	0.47
1:A:238:HIS:HE1	1:A:320:HIS:HE1	1.62	0.47
1:A:323:LEU:HD22	1:A:325:LYS:O	2.15	0.47
1:A:371:TRP:CE3	1:A:371:TRP:HA	2.49	0.47
1:A:90:GLU:CB	1:A:107:VAL:HG13	2.44	0.47
1:A:137:PRO:O	1:A:141:LEU:HB2	2.14	0.47
1:A:188:LYS:HB2	1:A:200:ILE:HD13	1.97	0.47
1:B:14:ILE:HG21	1:B:414:ALA:HB1	1.97	0.47
1:B:209:TRP:CZ3	1:B:232:LEU:HD23	2.50	0.47
1:B:425:MET:HG2	1:B:430:LEU:CD2	2.44	0.47
1:A:21:ILE:O	1:A:25:ARG:HG3	2.15	0.47
1:A:52:VAL:CG2	1:B:41:MET:HG2	2.45	0.47
1:A:267:ASN:CB	1:B:260:LEU:HG	2.39	0.47
1:A:421:ARG:HH22	1:B:239:GLU:HG2	1.80	0.47
1:A:33:VAL:HG13	1:B:433:LEU:HD23	1.97	0.47
1:A:86:GLU:HB2	1:A:226:GLU:OE1	2.15	0.47
1:A:228:MET:O	1:A:232:LEU:HB2	2.15	0.46
1:B:227:LEU:HD13	1:B:381:LEU:HD23	1.96	0.46
1:B:320:HIS:CG	1:B:323:LEU:HB2	2.50	0.46
1:A:308:THR:HG22	1:A:313:ARG:HB2	1.96	0.46
1:A:227:LEU:O	1:A:230:LEU:HB3	2.16	0.46
1:A:346:MET:O	1:A:350:VAL:HB	2.15	0.46
1:A:177:ASP:O	1:A:181:LYS:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASP:CG	1:B:206:LYS:H	2.24	0.46
1:B:359:ASN:HA	1:B:362:LEU:CD1	2.38	0.46
1:A:359:ASN:CA	1:A:362:LEU:HB2	2.39	0.46
1:B:383:GLN:HA	1:B:387:MET:O	2.15	0.46
1:A:217:LEU:HB3	1:A:219:TYR:HD2	1.81	0.46
1:B:162:ILE:HD13	1:B:170:LEU:CD1	2.46	0.46
1:B:194:TYR:CD2	1:B:389:GLU:HG3	2.51	0.46
1:A:284:TRP:HH2	1:A:305:ILE:HG12	1.80	0.46
1:B:182:LEU:N	1:B:183:PRO:HD2	2.31	0.46
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.67	0.46
1:A:172:TYR:CE2	1:A:176:MET:HG3	2.50	0.46
1:A:39:ASP:OD1	1:B:25:ARG:NH2	2.48	0.45
1:A:213:PHE:CE2	1:A:399:VAL:HG11	2.51	0.45
1:B:37:THR:HG22	1:B:40:MET:SD	2.57	0.45
1:B:37:THR:CG2	1:B:40:MET:HE3	2.42	0.45
1:B:253:SER:HB2	1:B:418:PRO:O	2.14	0.45
1:B:377:HIS:O	1:B:381:LEU:HD13	2.16	0.45
1:A:135:LEU:HB3	1:A:140:GLN:HG3	1.98	0.45
1:A:425:MET:HG2	1:A:430:LEU:CG	2.47	0.45
1:B:178:LEU:HG	1:B:182:LEU:HD12	1.97	0.45
1:A:420:GLU:HA	1:B:44:GLY:O	2.17	0.45
1:B:125:VAL:HG13	1:B:188:LYS:HE2	1.97	0.45
1:B:190:TYR:CE1	1:B:387:MET:HE2	2.52	0.45
1:B:298:ASP:OD2	1:B:301:LEU:HD23	2.15	0.45
1:A:175:CYS:O	1:A:179:ILE:HG13	2.16	0.45
1:A:247:THR:CG2	1:A:265:ALA:HA	2.46	0.45
1:A:92:LEU:HD22	1:A:233:THR:HG23	1.99	0.45
1:A:137:PRO:HG3	1:A:193:LEU:HD23	1.99	0.45
1:A:168:TRP:HA	1:A:413:ARG:HB3	1.98	0.45
1:A:347:PHE:C	1:A:350:VAL:H	2.24	0.45
1:B:86:GLU:CG	1:B:230:LEU:HB2	2.43	0.45
1:A:151:GLU:HB3	3:A:465:HOH:O	2.17	0.45
1:B:329:ARG:O	1:B:374:VAL:HG23	2.16	0.45
1:A:14:ILE:CG2	1:A:414:ALA:HB1	2.43	0.45
1:A:187:ALA:O	1:A:191:ARG:HB2	2.17	0.45
1:A:329:ARG:HB3	1:A:374:VAL:CG2	2.47	0.45
1:A:128:LEU:HD23	1:A:131:PHE:CD2	2.52	0.45
1:B:210:SER:O	1:B:213:PHE:HB3	2.16	0.45
1:B:276:LEU:HD23	1:B:280:GLU:OE1	2.17	0.45
1:B:65:ARG:HB3	1:B:68:GLY:CA	2.47	0.44
1:B:277:ALA:HB3	1:B:375:ASP:OD1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:HA	1:A:410:ILE:CD1	2.47	0.44
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.61	0.44
1:B:6:LEU:HB2	1:B:94:TRP:CH2	2.52	0.44
1:A:136:HIS:CE1	1:A:279:GLN:HE22	2.34	0.44
1:A:272:PRO:CB	1:B:158:TYR:CE1	3.00	0.44
1:B:6:LEU:HB2	1:B:94:TRP:CZ3	2.52	0.44
1:B:260:LEU:HA	1:B:260:LEU:HD12	1.72	0.44
1:B:337:ALA:C	1:B:339:LYS:H	2.25	0.44
1:A:109:TRP:CZ3	1:A:110:LEU:HD12	2.53	0.44
1:A:204:ASP:OD2	1:A:206:LYS:HG3	2.18	0.44
1:A:266:MET:HE1	1:A:269:LEU:HD23	1.99	0.44
1:B:421:ARG:HA	1:B:422:PRO:HD2	1.89	0.44
1:A:9:ILE:CG2	1:A:13:LEU:HD13	2.48	0.44
1:A:228:MET:HA	1:A:228:MET:CE	2.48	0.44
1:B:59:ASP:H	1:B:63:GLY:HA2	1.82	0.44
1:B:67:ARG:HB3	1:B:69:TYR:HD1	1.77	0.44
1:B:117:ARG:HH11	1:B:117:ARG:HD3	1.56	0.44
1:B:133:THR:HA	1:B:193:LEU:HD11	2.00	0.44
1:B:366:LYS:HB3	1:B:367:ALA:H	1.64	0.44
1:B:45:MET:HG2	1:B:48:MET:SD	2.58	0.44
1:B:171:ILE:HD11	1:B:409:LEU:C	2.42	0.44
1:B:178:LEU:CD1	1:B:182:LEU:HD12	2.48	0.44
1:B:23:THR:O	1:B:26:GLN:HB2	2.18	0.44
1:B:54:GLU:H	1:B:408:GLN:CD	2.26	0.44
1:B:168:TRP:CE2	1:B:169:GLU:HG3	2.53	0.44
1:B:200:ILE:O	1:B:216:MET:HG2	2.17	0.44
1:B:303:ASP:O	1:B:307:ASN:HB2	2.18	0.44
1:A:69:TYR:CD1	1:A:95:LEU:HD11	2.53	0.44
1:A:86:GLU:HG3	1:A:87:PRO:HD2	2.00	0.44
1:A:281:VAL:O	1:A:285:LEU:HB2	2.18	0.44
1:B:204:ASP:OD2	1:B:206:LYS:HG3	2.18	0.44
1:A:66:PHE:HD1	1:A:96:LEU:HD21	1.83	0.43
1:A:422:PRO:HG3	1:B:45:MET:CE	2.48	0.43
1:A:425:MET:CG	1:A:430:LEU:HG	2.48	0.43
1:B:288:LEU:HD12	1:B:288:LEU:O	2.18	0.43
1:A:228:MET:HA	1:A:228:MET:HE3	2.00	0.43
1:B:59:ASP:OD2	1:B:62:GLU:HG2	2.18	0.43
1:A:418:PRO:HB2	1:A:419:LEU:H	1.49	0.43
1:B:132:PRO:HD2	1:B:135:LEU:HD12	1.99	0.43
1:B:228:MET:HE1	1:B:396:LEU:HD13	2.01	0.43
1:A:35:GLN:HB3	1:B:32:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HH22	1:B:418:PRO:CB	2.32	0.43
1:A:178:LEU:HG	1:A:182:LEU:CD1	2.47	0.43
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.87	0.43
1:A:424:SER:HB2	1:B:51:LEU:HB2	1.96	0.43
1:A:9:ILE:HG22	1:A:13:LEU:HD13	2.01	0.43
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.77	0.43
1:A:101:ILE:HA	1:A:102:PRO:HD3	1.94	0.43
1:A:149:ASN:HB3	1:A:259:TYR:HB2	2.01	0.43
1:A:227:LEU:HD13	1:A:381:LEU:HD23	2.01	0.43
1:A:266:MET:CE	1:A:269:LEU:HD23	2.48	0.43
1:A:269:LEU:HA	1:A:274:HIS:CD2	2.53	0.43
1:A:298:ASP:HA	1:A:301:LEU:CB	2.47	0.43
1:B:59:ASP:CG	1:B:62:GLU:H	2.26	0.43
1:B:347:PHE:O	1:B:350:VAL:HB	2.19	0.43
1:B:300:LYS:HA	1:B:303:ASP:CB	2.46	0.43
1:B:313:ARG:HE	1:B:313:ARG:HB2	1.65	0.43
1:A:155:ALA:HB2	1:A:257:ASP:OD2	2.19	0.43
1:A:272:PRO:CB	1:B:158:TYR:HE1	2.32	0.43
1:B:173:GLU:OE2	1:B:173:GLU:HA	2.18	0.43
1:B:324:ARG:HG3	1:B:368:LYS:HE2	2.00	0.43
1:A:6:LEU:HB3	1:A:172:TYR:OH	2.18	0.42
1:A:17:GLU:HA	1:A:20:ARG:HB2	2.00	0.42
1:A:145:ILE:HG12	1:A:148:LEU:HD12	2.00	0.42
1:A:285:LEU:HD12	1:A:285:LEU:HA	1.81	0.42
3:A:471:HOH:O	1:B:419:LEU:HD21	2.19	0.42
1:B:101:ILE:HA	1:B:102:PRO:HD3	1.54	0.42
1:B:120:LEU:HD12	1:B:120:LEU:HA	1.78	0.42
1:A:145:ILE:HG22	1:A:263:ALA:HB2	2.01	0.42
1:A:174:ASP:HB3	1:A:258:PRO:HG2	2.01	0.42
1:A:272:PRO:HA	1:A:276:LEU:HB3	2.01	0.42
1:A:253:SER:HB2	1:A:418:PRO:O	2.19	0.42
1:B:120:LEU:HD21	1:B:185:VAL:CG2	2.45	0.42
1:A:273:LEU:HB2	1:B:254:ALA:C	2.43	0.42
1:A:278:ASN:HD21	1:A:397:PHE:HD2	1.67	0.42
1:A:404:GLY:O	1:A:407:ALA:HB3	2.19	0.42
1:A:89:PRO:HG3	1:A:229:ARG:O	2.19	0.42
1:A:131:PHE:HZ	1:A:143:ALA:HB3	1.84	0.42
1:B:157:ALA:HB2	1:B:170:LEU:HD13	2.02	0.42
1:A:284:TRP:HE3	1:A:285:LEU:HD13	1.84	0.42
1:B:127:MET:HE2	1:B:143:ALA:HB1	2.00	0.42
1:A:52:VAL:HG11	1:B:42:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TRP:CZ2	1:B:305:ILE:HG12	2.53	0.42
1:A:138:MET:HE3	1:A:270:ALA:HB2	2.01	0.42
1:B:271:GLY:HA2	1:B:272:PRO:HD3	1.90	0.42
1:A:168:TRP:HB3	1:A:414:ALA:CB	2.42	0.42
1:B:162:ILE:HD13	1:B:170:LEU:HD12	2.02	0.42
1:A:211:HIS:O	1:A:214:THR:HG22	2.20	0.42
1:A:225:THR:O	1:A:229:ARG:HG3	2.20	0.42
1:A:418:PRO:HB2	1:B:46:ARG:HH22	1.84	0.42
1:A:420:GLU:OE1	1:B:246:HIS:HE1	2.03	0.42
1:B:103:THR:HG21	1:B:105:GLU:HB3	2.02	0.42
1:B:258:PRO:HA	1:B:261:SER:OG	2.20	0.42
1:B:329:ARG:HB3	1:B:374:VAL:CG2	2.50	0.42
1:A:6:LEU:O	1:A:10:LEU:HG	2.20	0.41
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.80	0.41
1:B:148:LEU:HB3	1:B:259:TYR:HD1	1.82	0.41
1:B:204:ASP:N	1:B:212:ASN:HD21	2.18	0.41
1:B:324:ARG:HA	1:B:324:ARG:HD3	1.69	0.41
1:A:422:PRO:CB	1:B:45:MET:HE2	2.45	0.41
1:B:215:ASN:HD22	1:B:215:ASN:N	2.18	0.41
1:A:112:LYS:HE2	1:A:112:LYS:HB2	1.88	0.41
1:A:308:THR:HG23	1:A:313:ARG:HE	1.84	0.41
1:A:360:VAL:HA	1:A:363:GLU:HB2	2.01	0.41
1:A:41:MET:O	1:B:52:VAL:HG23	2.20	0.41
1:A:172:TYR:HA	1:A:410:ILE:HD13	2.03	0.41
1:A:333:GLN:NE2	1:A:377:HIS:HB3	2.35	0.41
1:B:64:ILE:CD1	1:B:238:HIS:HA	2.50	0.41
1:A:391:ASN:N	1:A:391:ASN:HD22	2.17	0.41
1:A:413:ARG:HH11	1:A:413:ARG:HD3	1.62	0.41
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.83	0.41
1:B:247:THR:HG21	1:B:265:ALA:HA	2.03	0.41
1:A:305:ILE:O	1:A:309:LEU:HD12	2.20	0.41
1:B:86:GLU:HG3	1:B:230:LEU:HD13	2.02	0.41
1:B:207:LEU:HD13	1:B:211:HIS:ND1	2.35	0.41
1:A:272:PRO:HB2	1:B:158:TYR:CE1	2.56	0.41
1:B:209:TRP:HZ3	1:B:232:LEU:HD23	1.85	0.41
1:A:127:MET:HE2	1:A:131:PHE:CZ	2.56	0.41
1:A:178:LEU:HD13	1:A:259:TYR:CD1	2.55	0.41
1:A:214:THR:HG21	1:A:225:THR:OG1	2.21	0.41
1:A:273:LEU:HA	1:A:273:LEU:HD12	1.82	0.41
1:A:404:GLY:HA2	1:A:407:ALA:HB3	2.02	0.41
1:A:427:THR:HG21	1:B:20:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:H	1:B:63:GLY:CA	2.34	0.41
1:B:95:LEU:HD13	1:B:101:ILE:HG12	2.03	0.41
1:B:114:TRP:CE3	1:B:209:TRP:CD1	3.09	0.41
1:A:157:ALA:HB2	1:A:170:LEU:HD13	2.02	0.41
1:A:330:TYR:CD2	1:A:372:PRO:HB2	2.56	0.41
1:A:344:ASP:HB3	1:A:347:PHE:HB2	2.03	0.41
1:B:227:LEU:HA	1:B:336:PHE:CE2	2.56	0.41
1:A:174:ASP:HB2	1:A:258:PRO:HG2	2.02	0.40
1:A:167:TYR:HE2	1:A:255:LEU:HD11	1.86	0.40
1:B:131:PHE:HD1	1:B:131:PHE:HA	1.73	0.40
1:B:423:LYS:HD2	1:B:423:LYS:HA	1.89	0.40
1:A:5:ASN:HD22	1:A:7:LYS:H	1.69	0.40
1:A:178:LEU:O	1:A:182:LEU:HB2	2.21	0.40
1:B:81:ALA:CB	1:B:88:LEU:HD13	2.46	0.40
1:B:136:HIS:HE1	1:B:279:GLN:HE22	1.68	0.40
1:B:245:ALA:HA	1:B:405:VAL:CG2	2.52	0.40
1:A:301:LEU:O	1:A:305:ILE:HG13	2.21	0.40
1:B:337:ALA:HB1	1:B:347:PHE:CE2	2.56	0.40
1:B:344:ASP:HB3	1:B:347:PHE:HB2	2.04	0.40
1:A:51:LEU:CD1	1:B:424:SER:HB3	2.52	0.40
1:A:77:MET:CB	1:A:101:ILE:HD13	2.51	0.40
1:A:308:THR:O	1:A:313:ARG:HB2	2.21	0.40
1:A:430:LEU:O	1:A:434:VAL:HG12	2.22	0.40
1:B:171:ILE:HG21	1:B:171:ILE:HD13	1.80	0.40
1:B:178:LEU:O	1:B:178:LEU:HD12	2.21	0.40

All (38) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:O	3:B:476:HOH:O[6_455]	0.90	1.30
1:B:153:ASN:OD1	1:B:306:TRP:CH2[3_544]	0.98	1.22
1:A:206:LYS:CD	1:B:191:ARG:NH2[6_455]	1.22	0.98
1:B:156:ARG:CZ	1:B:303:ASP:CB[3_544]	1.41	0.79
1:B:153:ASN:CG	1:B:306:TRP:CH2[3_544]	1.42	0.78
1:B:153:ASN:CB	1:B:306:TRP:CZ2[3_544]	1.45	0.75
1:B:156:ARG:NH1	1:B:303:ASP:CB[3_544]	1.52	0.68
1:B:170:LEU:CD2	1:B:310:ASN:OD1[3_544]	1.52	0.68
1:A:206:LYS:CE	1:B:198:SER:OG[6_455]	1.55	0.65
1:A:203:ILE:C	3:B:476:HOH:O[6_455]	1.59	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:NH1	1:B:303:ASP:OD1[3_544]	1.59	0.61
1:A:153:ASN:CG	1:A:306:TRP:CH2[4_555]	1.66	0.54
1:A:170:LEU:CD2	1:A:310:ASN:OD1[4_555]	1.67	0.53
1:B:153:ASN:OD1	1:B:306:TRP:CZ3[3_544]	1.69	0.51
1:B:156:ARG:NH1	1:B:303:ASP:CG[3_544]	1.69	0.51
1:B:162:ILE:CG2	1:B:311:SER:OG[3_544]	1.74	0.46
1:A:166:LYS:CD	1:A:310:ASN:O[4_555]	1.77	0.43
1:B:156:ARG:NE	1:B:303:ASP:CB[3_544]	1.79	0.41
1:B:157:ALA:CA	1:B:307:ASN:OD1[3_544]	1.80	0.40
1:A:153:ASN:ND2	1:A:306:TRP:CH2[4_555]	1.82	0.38
1:B:153:ASN:CB	1:B:306:TRP:CH2[3_544]	1.82	0.38
1:B:153:ASN:CG	1:B:306:TRP:CZ2[3_544]	1.84	0.36
1:A:206:LYS:NZ	1:B:191:ARG:NE[6_455]	1.87	0.33
1:A:153:ASN:OD1	1:A:306:TRP:CZ3[4_555]	1.92	0.28
1:A:206:LYS:CE	1:B:191:ARG:NH2[6_455]	1.92	0.28
1:B:156:ARG:NH2	1:B:300:LYS:O[3_544]	1.94	0.26
1:A:156:ARG:CZ	1:A:303:ASP:CB[4_555]	1.95	0.25
1:B:157:ALA:N	1:B:307:ASN:OD1[3_544]	1.95	0.25
1:B:156:ARG:O	1:B:307:ASN:OD1[3_544]	1.96	0.24
1:A:156:ARG:O	1:A:307:ASN:OD1[4_555]	1.97	0.23
1:B:156:ARG:C	1:B:307:ASN:OD1[3_544]	2.04	0.16
1:A:287:GLN:OE1	1:B:290:LYS:NZ[3_544]	2.05	0.15
1:A:153:ASN:OD1	1:A:306:TRP:CH2[4_555]	2.06	0.14
1:A:290:LYS:NZ	1:B:287:GLN:OE1[3_544]	2.08	0.12
1:A:156:ARG:NH2	1:A:303:ASP:CB[4_555]	2.11	0.09
1:B:153:ASN:CA	1:B:306:TRP:CH2[3_544]	2.16	0.04
1:B:166:LYS:CD	1:B:310:ASN:O[3_544]	2.16	0.04
1:B:153:ASN:OD1	1:B:306:TRP:CZ2[3_544]	2.18	0.02

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	435/437 (100%)	359 (82%)	55 (13%)	21 (5%)	2	7
1	B	435/437 (100%)	357 (82%)	59 (14%)	19 (4%)	2	8
All	All	870/874 (100%)	716 (82%)	114 (13%)	40 (5%)	2	7

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
1	A	205	SER
1	A	239	GLU
1	B	166	LYS
1	B	239	GLU
1	B	278	ASN
1	B	376	ALA
1	A	5	ASN
1	A	75	GLN
1	A	148	LEU
1	A	149	ASN
1	A	196	GLU
1	A	313	ARG
1	A	418	PRO
1	B	5	ASN
1	B	196	GLU
1	B	277	ALA
1	B	279	GLN
1	B	320	HIS
1	B	338	LEU
1	B	418	PRO
1	A	164	ARG
1	A	202	ALA
1	A	294	LYS
1	A	321	ALA
1	A	420	GLU
1	B	294	LYS
1	A	137	PRO
1	A	276	LEU
1	A	278	ASN
1	A	345	PRO
1	B	149	ASN
1	A	49	LYS
1	B	87	PRO
1	B	243	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	307	ASN
1	B	137	PRO
1	A	243	VAL
1	B	14	ILE
1	B	60	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/371 (100%)	311 (84%)	60 (16%)	2	8
1	B	371/371 (100%)	315 (85%)	56 (15%)	3	10
All	All	742/742 (100%)	626 (84%)	116 (16%)	2	9

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	13	LEU
1	A	17	GLU
1	A	20	ARG
1	A	22	LYS
1	A	32	VAL
1	A	35	GLN
1	A	38	VAL
1	A	46	ARG
1	A	49	LYS
1	A	54	GLU
1	A	62	GLU
1	A	64	ILE
1	A	76	LYS
1	A	80	LYS
1	A	86	GLU
1	A	98	THR
1	A	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112	LYS
1	A	127	MET
1	A	136	HIS
1	A	149	ASN
1	A	151	GLU
1	A	169	GLU
1	A	171	ILE
1	A	182	LEU
1	A	193	LEU
1	A	203	ILE
1	A	205	SER
1	A	206	LYS
1	A	212	ASN
1	A	214	THR
1	A	217	LEU
1	A	225	THR
1	A	228	MET
1	A	237	ASP
1	A	256	SER
1	A	260	LEU
1	A	261	SER
1	A	273	LEU
1	A	274	HIS
1	A	283	VAL
1	A	285	LEU
1	A	287	GLN
1	A	288	LEU
1	A	289	GLN
1	A	292	VAL
1	A	305	ILE
1	A	313	ARG
1	A	323	LEU
1	A	339	LYS
1	A	350	VAL
1	A	355	LYS
1	A	356	ILE
1	A	363	GLU
1	A	373	ASN
1	A	389	GLU
1	A	405	VAL
1	A	413	ARG
1	A	434	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	20	ARG
1	B	32	VAL
1	B	36	ILE
1	B	46	ARG
1	B	49	LYS
1	B	75	GLN
1	B	80	LYS
1	B	86	GLU
1	B	96	LEU
1	B	98	THR
1	B	101	ILE
1	B	110	LEU
1	B	112	LYS
1	B	120	LEU
1	B	135	LEU
1	B	149	ASN
1	B	156	ARG
1	B	162	ILE
1	B	171	ILE
1	B	182	LEU
1	B	193	LEU
1	B	195	ARG
1	B	203	ILE
1	B	205	SER
1	B	210	SER
1	B	214	THR
1	B	225	THR
1	B	228	MET
1	B	267	ASN
1	B	276	LEU
1	B	283	VAL
1	B	285	LEU
1	B	287	GLN
1	B	292	VAL
1	B	296	VAL
1	B	305	ILE
1	B	307	ASN
1	B	310	ASN
1	B	313	ARG
1	B	315	VAL
1	B	323	LEU
1	B	331	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	349	LEU
1	B	355	LYS
1	B	356	ILE
1	B	373	ASN
1	B	389	GLU
1	B	391	ASN
1	B	394	THR
1	B	399	VAL
1	B	405	VAL
1	B	413	ARG
1	B	428	ASP
1	B	431	ILE
1	B	432	LYS
1	B	434	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	27	GLN
1	A	30	ASN
1	A	75	GLN
1	A	130	ASN
1	A	140	GLN
1	A	149	ASN
1	A	211	HIS
1	A	212	ASN
1	A	215	ASN
1	A	238	HIS
1	A	267	ASN
1	A	274	HIS
1	A	278	ASN
1	A	279	GLN
1	A	333	GLN
1	A	359	ASN
1	A	383	GLN
1	A	391	ASN
1	B	5	ASN
1	B	27	GLN
1	B	30	ASN
1	B	106	GLN
1	B	149	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	ASN
1	B	212	ASN
1	B	215	ASN
1	B	246	HIS
1	B	267	ASN
1	B	279	GLN
1	B	359	ASN
1	B	383	GLN
1	B	391	ASN

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OAA	B	438	-	8,8,8	3.81	2 (25%)	8,10,10	1.62	2 (25%)
2	OAA	A	438	-	8,8,8	4.12	1 (12%)	8,10,10	1.37	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OAA	B	438	-	-	1/8/8/8	-
2	OAA	A	438	-	-	2/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	438	OAA	C3-C4	-11.21	1.36	1.53
2	B	438	OAA	C3-C4	-10.08	1.38	1.53
2	B	438	OAA	O5-C4	-2.03	1.25	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	438	OAA	O5-C4-C3	2.60	120.80	113.59
2	A	438	OAA	O2-C1-O1	-2.35	117.28	123.33
2	B	438	OAA	O5-C4-O4	-2.25	118.53	123.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	438	OAA	C1-C2-C3-O3
2	A	438	OAA	C1-C2-C3-O3
2	A	438	OAA	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.