



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:24 AM UTC

PDB ID : 5CBQ / pdb_00005cbq
Title : Crystal structure of a T1-like thiolase from Mycobacterium smegmatis
Authors : Janardan, N.; Murthy, M.R.N.
Deposited on : 2015-07-01
Resolution : 2.45 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

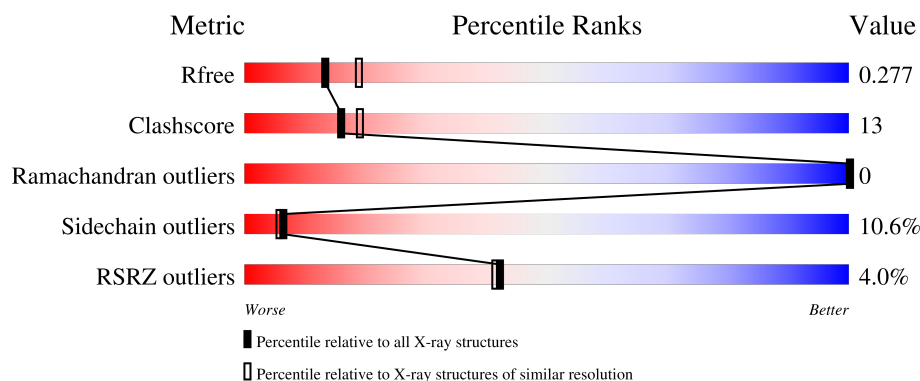
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	413	8% 59% 30% 8% .
1	B	413	50% 36% 10% . .
1	C	413	4% 57% 31% 7% .
1	D	413	57% 33% 6% .
1	E	413	2% 63% 29% . . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	413	8% 58% 31% 6% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17727 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 Beta-ketothiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			2868	1770	525	557	16			
1	B	398	Total	C	N	O	S	0	2	0
			2943	1823	538	566	16			
1	C	397	Total	C	N	O	S	0	0	0
			2882	1786	522	558	16			
1	D	398	Total	C	N	O	S	0	1	0
			2927	1813	535	563	16			
1	E	400	Total	C	N	O	S	0	0	0
			2925	1811	538	560	16			
1	F	393	Total	C	N	O	S	0	0	0
			2846	1763	523	544	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP A0QUH3
A	-4	HIS	-	expression tag	UNP A0QUH3
A	-3	HIS	-	expression tag	UNP A0QUH3
A	-2	HIS	-	expression tag	UNP A0QUH3
A	-1	HIS	-	expression tag	UNP A0QUH3
A	0	HIS	-	expression tag	UNP A0QUH3
B	-5	HIS	-	expression tag	UNP A0QUH3
B	-4	HIS	-	expression tag	UNP A0QUH3
B	-3	HIS	-	expression tag	UNP A0QUH3
B	-2	HIS	-	expression tag	UNP A0QUH3
B	-1	HIS	-	expression tag	UNP A0QUH3
B	0	HIS	-	expression tag	UNP A0QUH3
C	-5	HIS	-	expression tag	UNP A0QUH3
C	-4	HIS	-	expression tag	UNP A0QUH3
C	-3	HIS	-	expression tag	UNP A0QUH3
C	-2	HIS	-	expression tag	UNP A0QUH3
C	-1	HIS	-	expression tag	UNP A0QUH3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0QUH3
D	-5	HIS	-	expression tag	UNP A0QUH3
D	-4	HIS	-	expression tag	UNP A0QUH3
D	-3	HIS	-	expression tag	UNP A0QUH3
D	-2	HIS	-	expression tag	UNP A0QUH3
D	-1	HIS	-	expression tag	UNP A0QUH3
D	0	HIS	-	expression tag	UNP A0QUH3
E	-5	HIS	-	expression tag	UNP A0QUH3
E	-4	HIS	-	expression tag	UNP A0QUH3
E	-3	HIS	-	expression tag	UNP A0QUH3
E	-2	HIS	-	expression tag	UNP A0QUH3
E	-1	HIS	-	expression tag	UNP A0QUH3
E	0	HIS	-	expression tag	UNP A0QUH3
F	-5	HIS	-	expression tag	UNP A0QUH3
F	-4	HIS	-	expression tag	UNP A0QUH3
F	-3	HIS	-	expression tag	UNP A0QUH3
F	-2	HIS	-	expression tag	UNP A0QUH3
F	-1	HIS	-	expression tag	UNP A0QUH3
F	0	HIS	-	expression tag	UNP A0QUH3

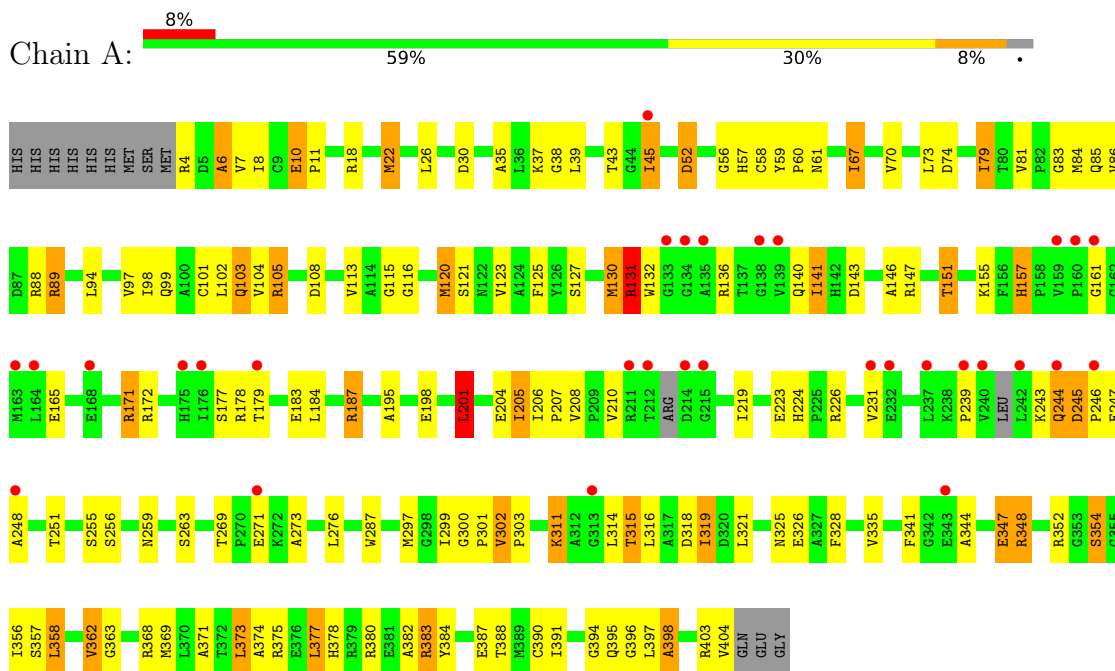
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	51	Total O 51 51	0	0
2	B	66	Total O 66 66	0	0
2	C	55	Total O 55 55	0	0
2	D	69	Total O 69 69	0	0
2	E	49	Total O 49 49	0	0
2	F	46	Total O 46 46	0	0

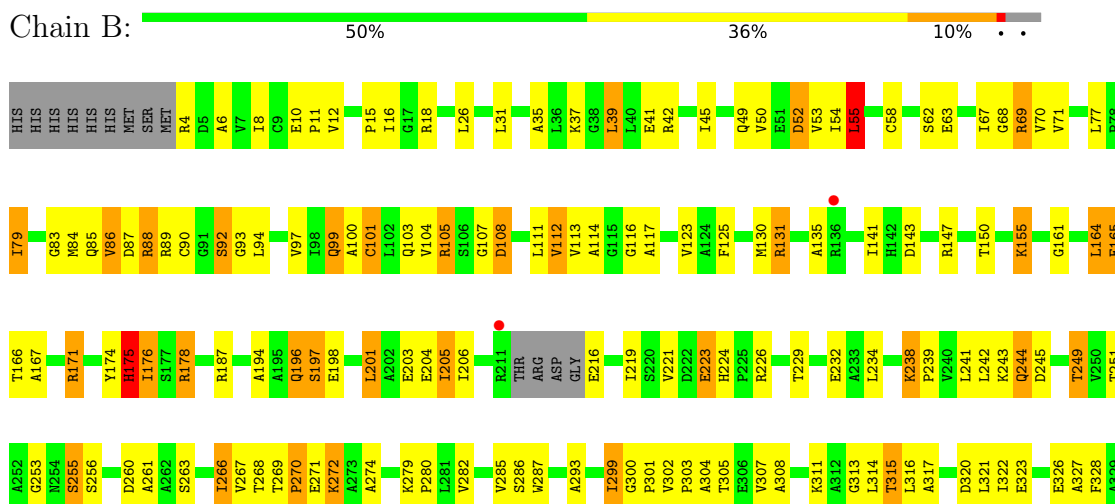
3 Residue-property plots

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 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: Beta-ketothiolase

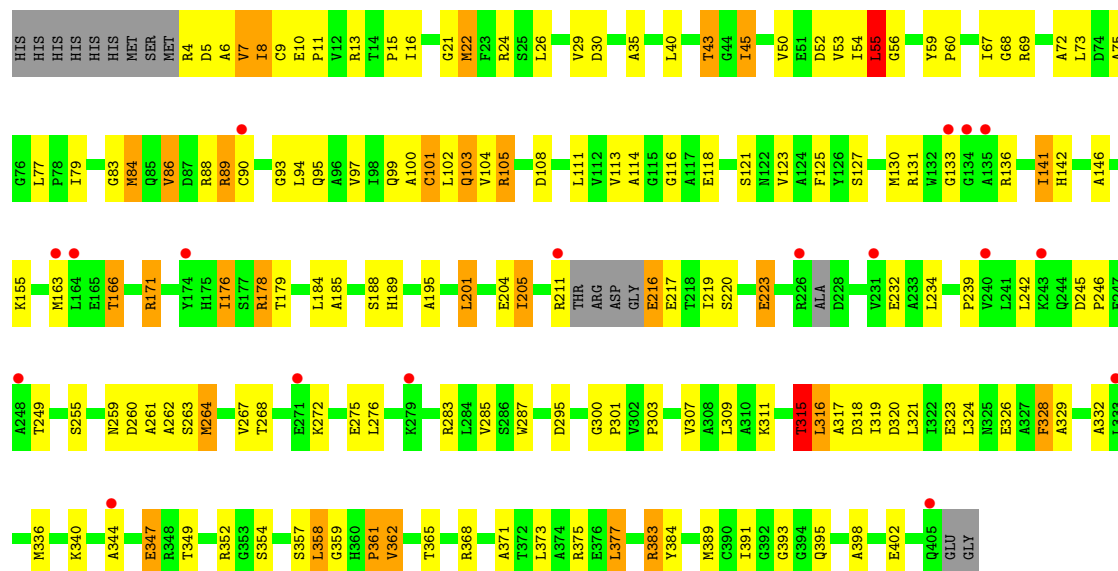


• Molecule 1: Beta-ketothiolase

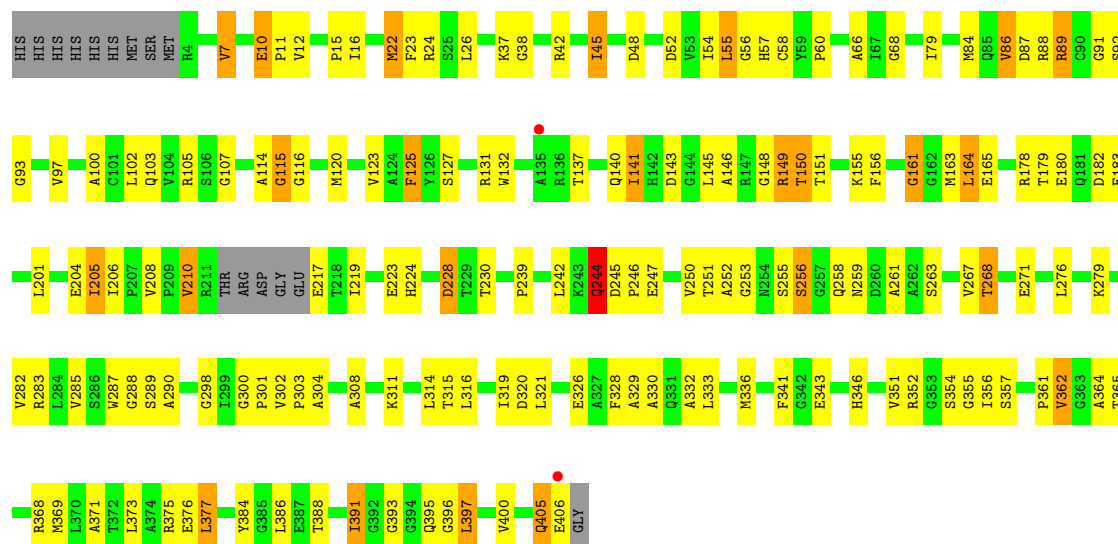




• Molecule 1: Beta-ketothiolase

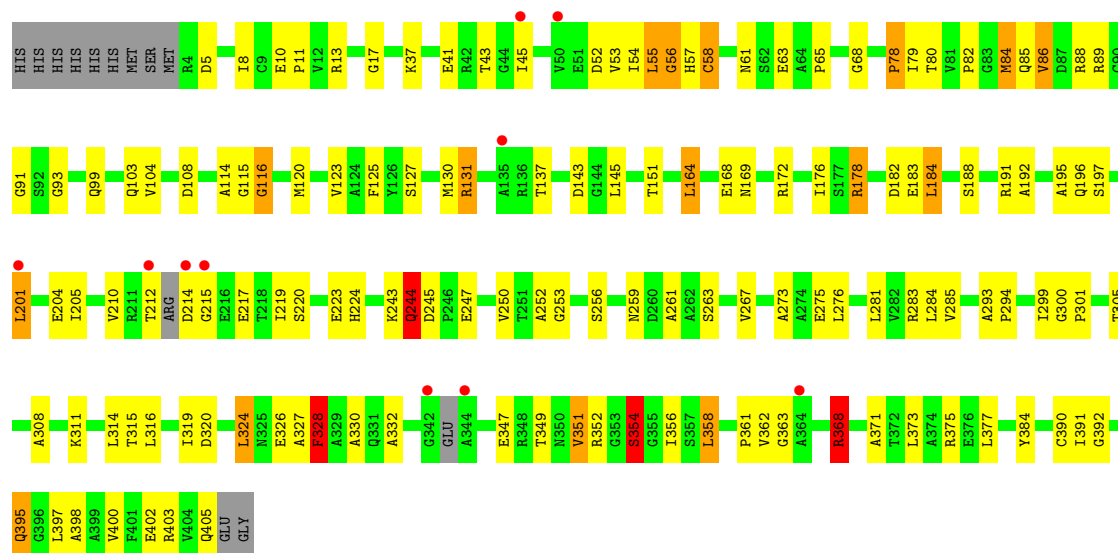


• Molecule 1: Beta-ketothiolase

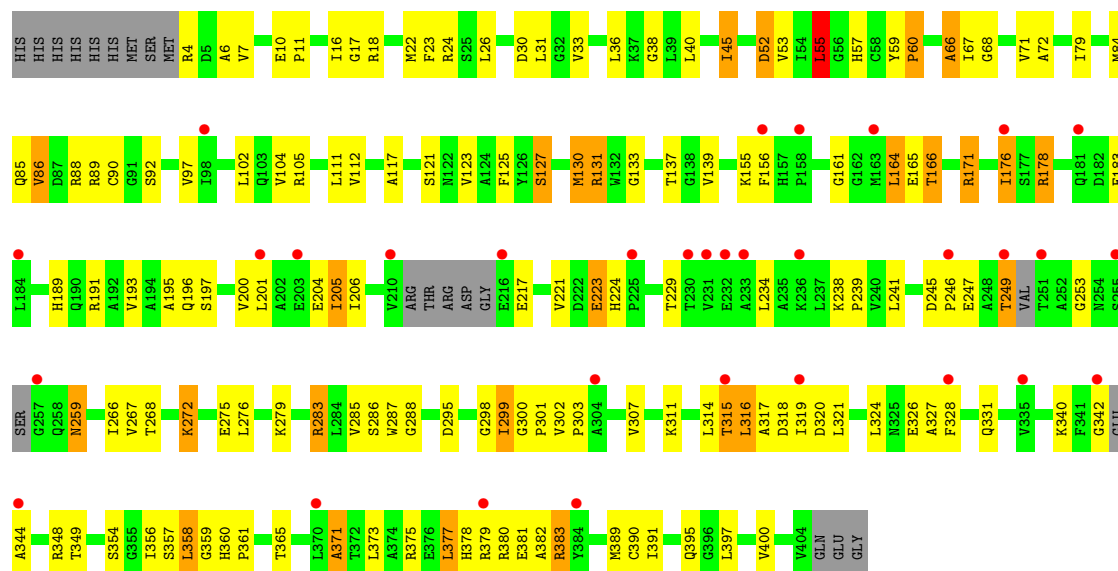


• Molecule 1: Beta-ketothiolase





• Molecule 1: Beta-ketothiolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.46Å 181.47Å 271.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	135.87 – 2.45 135.87 – 2.45	Depositor EDS
% Data completeness (in resolution range)	89.1 (135.87-2.45) 89.1 (135.87-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.226 , 0.268 0.225 , 0.277	Depositor DCC
R_{free} test set	4603 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17727	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 ⓘ

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	1.99	49/2911 (1.7%)	1.33	32/3957 (0.8%)
1	B	2.18	97/2991 (3.2%)	1.44	33/4058 (0.8%)
1	C	1.96	58/2925 (2.0%)	1.28	26/3974 (0.7%)
1	D	2.07	62/2971 (2.1%)	1.41	27/4033 (0.7%)
1	E	1.91	34/2968 (1.1%)	1.30	29/4028 (0.7%)
1	F	1.74	25/2886 (0.9%)	1.30	26/3915 (0.7%)
All	All	1.98	325/17652 (1.8%)	1.35	173/23965 (0.7%)

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	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
All	All	0	7

All (325) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	SER	C-O	-11.39	1.15	1.24
1	E	91	GLY	C-O	-9.55	1.17	1.24
1	B	10	GLU	C-O	-8.39	1.19	1.23
1	B	175[A]	HIS	N-CA	7.91	1.58	1.46
1	B	175[B]	HIS	N-CA	7.91	1.58	1.46
1	B	83	GLY	C-O	-7.63	1.15	1.24
1	D	10	GLU	C-O	-7.57	1.20	1.23
1	A	116	GLY	C-O	-7.41	1.15	1.24
1	F	10	GLU	C-O	-7.28	1.20	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	354	SER	C-O	-7.20	1.18	1.24
1	A	10	GLU	C-O	-7.17	1.20	1.23
1	C	54	ILE	C-O	-7.09	1.16	1.24
1	C	113	VAL	C-O	-7.07	1.16	1.24
1	B	54	ILE	C-O	-7.06	1.16	1.24
1	D	86	VAL	C-O	-7.00	1.17	1.24
1	E	56	GLY	C-O	-6.93	1.17	1.24
1	B	304	ALA	C-O	-6.92	1.15	1.24
1	D	333	LEU	C-O	-6.92	1.16	1.24
1	B	322	ILE	C-O	-6.90	1.16	1.24
1	E	125	PHE	C-O	-6.90	1.15	1.23
1	A	70	VAL	C-O	-6.89	1.16	1.24
1	B	97	VAL	C-O	-6.89	1.16	1.24
1	B	112	VAL	C-O	-6.86	1.15	1.23
1	A	83	GLY	C-O	-6.77	1.16	1.24
1	B	393	GLY	C-O	-6.75	1.14	1.24
1	A	102	LEU	C-O	-6.71	1.16	1.24
1	C	10	GLU	C-O	-6.69	1.20	1.23
1	B	84	MET	C-O	-6.67	1.16	1.23
1	B	113	VAL	C-O	-6.65	1.16	1.24
1	C	272	LYS	C-O	-6.62	1.16	1.24
1	B	282	VAL	C-O	-6.59	1.16	1.23
1	D	141	ILE	C-O	-6.59	1.17	1.24
1	A	99	GLN	C-O	-6.57	1.16	1.24
1	D	388	THR	C-O	-6.57	1.16	1.23
1	E	116	GLY	C-O	-6.49	1.16	1.24
1	A	97	VAL	C-O	-6.46	1.16	1.24
1	D	89	ARG	C-O	-6.43	1.18	1.24
1	B	267	VAL	C-O	-6.42	1.17	1.24
1	A	56	GLY	C-O	-6.41	1.15	1.23
1	D	56	GLY	C-O	-6.36	1.17	1.24
1	B	388	THR	C-O	-6.36	1.16	1.23
1	E	188	SER	C-O	-6.36	1.16	1.24
1	A	61	ASN	C-O	-6.35	1.17	1.23
1	A	57	HIS	C-O	-6.35	1.16	1.23
1	B	302	VAL	C-O	-6.34	1.19	1.24
1	B	400	VAL	C-O	-6.34	1.17	1.24
1	D	397	LEU	C-O	-6.34	1.16	1.23
1	A	141	ILE	C-O	-6.33	1.17	1.24
1	E	219	ILE	C-O	-6.32	1.17	1.24
1	F	97	VAL	C-O	-6.31	1.16	1.24
1	C	103	GLN	C-O	-6.31	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	VAL	C-O	-6.27	1.17	1.24
1	F	139	VAL	C-O	-6.26	1.17	1.24
1	F	299	ILE	C-O	-6.25	1.17	1.24
1	C	84	MET	C-O	-6.23	1.16	1.23
1	B	305	THR	C-O	-6.21	1.16	1.24
1	D	54	ILE	C-O	-6.20	1.17	1.24
1	C	100	ALA	C-O	-6.19	1.17	1.24
1	E	332	ALA	C-O	-6.19	1.17	1.24
1	E	400	VAL	C-O	-6.18	1.17	1.24
1	B	101	CYS	C-O	-6.17	1.17	1.24
1	D	282	VAL	C-O	-6.16	1.17	1.23
1	C	116	GLY	C-O	-6.14	1.17	1.24
1	A	52	ASP	C-O	-6.14	1.16	1.23
1	B	150	THR	C-O	-6.13	1.16	1.24
1	B	130	MET	C-O	-6.13	1.16	1.24
1	B	221	VAL	C-O	-6.09	1.17	1.24
1	F	266	ILE	C-O	-6.06	1.17	1.24
1	B	383	ARG	C-O	-6.04	1.16	1.23
1	C	30	ASP	C-O	-6.03	1.17	1.24
1	D	116	GLY	C-O	-6.01	1.17	1.24
1	B	268	THR	C-O	-6.00	1.17	1.23
1	C	56	GLY	C-O	-5.99	1.18	1.24
1	B	6	ALA	C-O	-5.98	1.16	1.24
1	A	7	VAL	C-O	-5.97	1.18	1.24
1	B	205	ILE	C-O	-5.96	1.17	1.24
1	A	115	GLY	C-O	-5.96	1.17	1.23
1	D	100	ALA	C-O	-5.96	1.17	1.24
1	B	93	GLY	C-O	-5.95	1.16	1.23
1	C	50	VAL	C-O	-5.94	1.17	1.24
1	D	319	ILE	C-O	-5.94	1.17	1.24
1	B	50	VAL	C-O	-5.94	1.17	1.24
1	B	271	GLU	C-O	-5.92	1.17	1.24
1	C	146	ALA	C-O	-5.92	1.17	1.24
1	D	393	GLY	C-O	-5.92	1.15	1.24
1	D	369	MET	C-O	-5.91	1.17	1.24
1	A	263	SER	C-O	-5.90	1.16	1.23
1	F	268	THR	C-O	-5.90	1.17	1.23
1	E	392	GLY	C-O	-5.89	1.17	1.23
1	C	141	ILE	C-O	-5.88	1.17	1.24
1	A	85	GLN	C-O	-5.87	1.16	1.24
1	E	328	PHE	C-O	-5.87	1.16	1.23
1	D	384	TYR	C-O	-5.86	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	VAL	C-O	-5.85	1.18	1.24
1	D	114	ALA	C-O	-5.82	1.16	1.24
1	C	264	MET	C-O	-5.81	1.17	1.23
1	B	116	GLY	C-O	-5.81	1.18	1.24
1	D	87	ASP	C-O	-5.80	1.17	1.24
1	B	165	GLU	C-O	-5.80	1.17	1.24
1	B	299	ILE	C-O	-5.79	1.17	1.24
1	C	99	GLN	C-O	-5.78	1.17	1.24
1	B	94	LEU	C-O	-5.78	1.17	1.24
1	D	267	VAL	C-O	-5.78	1.17	1.24
1	E	319	ILE	C-O	-5.78	1.18	1.24
1	B	42	ARG	C-O	-5.76	1.17	1.24
1	B	365	THR	C-O	-5.76	1.17	1.24
1	D	365	THR	C-O	-5.76	1.17	1.24
1	B	70	VAL	C-O	-5.75	1.17	1.24
1	B	111	LEU	C-O	-5.75	1.17	1.23
1	B	114	ALA	C-O	-5.75	1.17	1.23
1	E	261	ALA	C-O	-5.74	1.17	1.23
1	A	98	ILE	C-O	-5.74	1.17	1.24
1	B	321	LEU	C-O	-5.73	1.17	1.23
1	A	35	ALA	C-O	-5.72	1.17	1.24
1	B	397	LEU	C-O	-5.72	1.17	1.23
1	A	67	ILE	C-O	-5.70	1.16	1.24
1	B	323	GLU	C-O	-5.69	1.17	1.24
1	C	94	LEU	C-O	-5.68	1.17	1.24
1	C	89	ARG	C-O	-5.68	1.19	1.24
1	D	102	LEU	C-O	-5.66	1.17	1.24
1	D	288	GLY	C-O	-5.66	1.17	1.24
1	C	262	ALA	C-O	-5.65	1.17	1.23
1	D	400	VAL	C-O	-5.65	1.18	1.24
1	A	104	VAL	C-O	-5.64	1.17	1.24
1	B	35	ALA	C-O	-5.64	1.17	1.24
1	C	6	ALA	C-O	-5.64	1.17	1.24
1	D	253	GLY	C-O	-5.64	1.17	1.23
1	F	221	VAL	C-O	-5.63	1.18	1.24
1	C	104	VAL	C-O	-5.63	1.17	1.24
1	C	69	ARG	C-O	-5.63	1.17	1.24
1	B	333	LEU	C-O	-5.61	1.17	1.24
1	F	397	LEU	C-O	-5.61	1.17	1.23
1	A	205	ILE	C-O	-5.60	1.17	1.24
1	A	89	ARG	C-O	-5.59	1.19	1.24
1	E	330	ALA	C-O	-5.59	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	SER	C-O	-5.58	1.17	1.23
1	F	53	VAL	C-O	-5.58	1.17	1.24
1	C	111	LEU	C-O	-5.58	1.17	1.23
1	D	16	ILE	C-O	-5.57	1.18	1.24
1	C	29	VAL	C-O	-5.57	1.17	1.24
1	D	97	VAL	C-O	-5.57	1.17	1.24
1	D	105	ARG	C-O	-5.55	1.17	1.24
1	A	81	VAL	C-O	-5.55	1.17	1.24
1	B	396	GLY	C-O	-5.55	1.17	1.23
1	D	12	VAL	C-O	-5.54	1.17	1.23
1	A	302	VAL	C-O	-5.54	1.19	1.24
1	F	400	VAL	C-O	-5.54	1.17	1.24
1	B	87	ASP	C-O	-5.53	1.17	1.24
1	C	35	ALA	C-O	-5.53	1.17	1.24
1	C	263	SER	C-O	-5.53	1.17	1.24
1	B	335	VAL	C-O	-5.52	1.17	1.24
1	D	298	GLY	C-O	-5.52	1.16	1.24
1	B	99	GLN	C-O	-5.51	1.17	1.24
1	E	17	GLY	C-O	-5.51	1.16	1.23
1	E	363	GLY	C-O	-5.50	1.17	1.23
1	B	384	TYR	C-O	-5.50	1.17	1.24
1	B	260	ASP	C-O	-5.50	1.17	1.24
1	C	11	PRO	C-O	-5.50	1.17	1.23
1	C	55	LEU	C-O	-5.50	1.17	1.24
1	C	101	CYS	C-O	-5.49	1.17	1.24
1	F	72	ALA	C-O	-5.49	1.17	1.24
1	E	86	VAL	C-O	-5.48	1.18	1.24
1	B	8	ILE	C-O	-5.48	1.17	1.24
1	F	30	ASP	C-O	-5.48	1.17	1.24
1	B	39	LEU	C-O	-5.47	1.17	1.24
1	C	9	CYS	C-O	-5.47	1.17	1.23
1	B	391	ILE	C-O	-5.47	1.18	1.24
1	B	52	ASP	C-O	-5.46	1.17	1.23
1	D	261	ALA	C-O	-5.46	1.17	1.23
1	C	95	GLN	C-O	-5.45	1.17	1.24
1	B	187	ARG	C-O	-5.45	1.17	1.24
1	A	357	SER	C-O	-5.44	1.17	1.24
1	B	377	LEU	C-O	-5.44	1.17	1.24
1	B	108	ASP	C-O	-5.43	1.17	1.24
1	A	143	ASP	C-O	-5.43	1.17	1.23
1	D	223	GLU	C-O	-5.43	1.17	1.24
1	A	335	VAL	C-O	-5.42	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	VAL	C-O	-5.42	1.17	1.23
1	B	353	GLY	C-O	-5.42	1.18	1.23
1	B	398	ALA	C-O	-5.42	1.17	1.23
1	B	245	ASP	C-O	-5.41	1.20	1.25
1	E	308	ALA	C-O	-5.40	1.17	1.24
1	C	108	ASP	C-O	-5.40	1.17	1.24
1	E	164	LEU	C-O	-5.40	1.17	1.24
1	A	396	GLY	C-O	-5.39	1.17	1.23
1	C	75	ALA	C-O	-5.39	1.17	1.24
1	D	57	HIS	N-CA	-5.39	1.40	1.46
1	B	399	ALA	C-O	-5.38	1.17	1.23
1	B	104	VAL	C-O	-5.38	1.18	1.24
1	A	101	CYS	C-O	-5.37	1.17	1.24
1	C	114	ALA	C-O	-5.37	1.17	1.24
1	C	349	THR	C-O	-5.37	1.17	1.24
1	A	125	PHE	C-O	-5.36	1.17	1.23
1	B	166	THR	C-O	-5.36	1.18	1.24
1	E	127	SER	C-O	-5.36	1.17	1.23
1	A	103	GLN	C-O	-5.34	1.17	1.24
1	D	93	GLY	C-O	-5.34	1.17	1.23
1	B	117	ALA	C-O	-5.33	1.17	1.23
1	C	261	ALA	C-O	-5.33	1.18	1.23
1	D	259	ASN	C-O	-5.33	1.17	1.23
1	E	78	PRO	C-O	-5.32	1.17	1.23
1	E	58	CYS	C-O	-5.32	1.17	1.24
1	B	203	GLU	C-O	-5.32	1.17	1.24
1	B	11	PRO	C-O	-5.31	1.17	1.23
1	B	327	ALA	C-O	-5.31	1.18	1.24
1	E	114	ALA	C-O	-5.30	1.17	1.24
1	D	103	GLN	C-O	-5.30	1.17	1.24
1	A	79	ILE	C-O	-5.29	1.17	1.24
1	B	31	LEU	C-O	-5.29	1.18	1.24
1	D	285	VAL	C-O	-5.29	1.17	1.23
1	D	329	ALA	C-O	-5.29	1.18	1.24
1	B	69	ARG	C-O	-5.28	1.17	1.24
1	F	267	VAL	C-O	-5.28	1.18	1.24
1	E	273	ALA	C-O	-5.27	1.18	1.24
1	A	84	MET	C-O	-5.27	1.17	1.23
1	B	206	ILE	C-O	-5.26	1.18	1.24
1	A	108	ASP	C-O	-5.26	1.17	1.24
1	E	311	LYS	C-O	-5.26	1.17	1.24
1	F	125	PHE	C-O	-5.26	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	288	GLY	C-O	-5.25	1.17	1.23
1	B	303	PRO	C-O	-5.25	1.18	1.24
1	A	30	ASP	C-O	-5.24	1.18	1.24
1	A	146	ALA	C-O	-5.24	1.18	1.24
1	D	210	VAL	C-O	-5.24	1.18	1.24
1	D	263	SER	C-O	-5.24	1.17	1.23
1	C	319	ILE	C-O	-5.23	1.18	1.24
1	E	93	GLY	C-O	-5.23	1.17	1.23
1	E	349	THR	C-O	-5.23	1.17	1.24
1	B	125	PHE	C-O	-5.23	1.17	1.23
1	E	320	ASP	C-O	-5.23	1.17	1.24
1	D	250	VAL	C-O	-5.23	1.18	1.24
1	C	73	LEU	C-O	-5.22	1.18	1.24
1	D	396	GLY	C-O	-5.22	1.17	1.23
1	D	308	ALA	C-O	-5.22	1.18	1.24
1	A	273	ALA	C-O	-5.22	1.18	1.24
1	D	304	ALA	C-O	-5.21	1.18	1.24
1	A	6	ALA	C-O	-5.21	1.17	1.24
1	B	147	ARG	C-O	-5.21	1.18	1.24
1	A	39	LEU	C-O	-5.21	1.18	1.24
1	B	63	GLU	C-O	-5.21	1.18	1.24
1	C	97	VAL	C-O	-5.21	1.18	1.24
1	B	176	ILE	C-O	-5.21	1.18	1.24
1	B	372	THR	C-O	-5.20	1.18	1.24
1	A	74	ASP	C-O	-5.20	1.17	1.24
1	F	60	PRO	C-O	-5.20	1.18	1.23
1	A	113	VAL	C-O	-5.19	1.18	1.24
1	B	293	ALA	C-O	-5.19	1.17	1.24
1	B	359	GLY	C-O	-5.19	1.18	1.23
1	F	31	LEU	C-O	-5.19	1.18	1.24
1	D	362	VAL	C-O	-5.18	1.18	1.24
1	A	204	GLU	C-O	-5.17	1.18	1.24
1	F	123	VAL	C-O	-5.17	1.18	1.24
1	D	386	LEU	C-O	-5.17	1.17	1.24
1	B	308	ALA	C-O	-5.17	1.18	1.24
1	C	393	GLY	C-O	-5.16	1.17	1.24
1	D	391	ILE	C-O	-5.16	1.18	1.24
1	C	142	HIS	C-O	-5.16	1.17	1.24
1	B	270	PRO	C-O	-5.15	1.17	1.24
1	F	131	ARG	C-O	-5.15	1.18	1.24
1	C	125	PHE	C-O	-5.15	1.17	1.24
1	E	324	LEU	C-O	-5.14	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	371	ALA	C-O	-5.14	1.18	1.24
1	D	268	THR	C-O	-5.14	1.17	1.23
1	B	53	VAL	C-O	-5.14	1.18	1.24
1	B	313	GLY	C-O	-5.14	1.18	1.24
1	B	378	HIS	C-O	-5.13	1.18	1.24
1	C	13	ARG	C-O	-5.13	1.17	1.23
1	B	392	GLY	C-O	-5.13	1.18	1.23
1	A	94	LEU	C-O	-5.13	1.18	1.24
1	D	84	MET	C-O	-5.13	1.17	1.23
1	C	239	PRO	CA-C	-5.13	1.46	1.52
1	C	260	ASP	C-O	-5.12	1.17	1.24
1	D	164	LEU	C-O	-5.12	1.18	1.24
1	D	290	ALA	C-O	-5.12	1.17	1.23
1	A	8	ILE	C-O	-5.12	1.18	1.24
1	C	398	ALA	C-O	-5.12	1.17	1.23
1	C	328	PHE	C-O	-5.12	1.17	1.23
1	B	16	ILE	C-O	-5.11	1.18	1.24
1	E	305	THR	C-O	-5.11	1.18	1.24
1	C	72	ALA	C-O	-5.11	1.18	1.24
1	B	330	ALA	C-O	-5.10	1.18	1.24
1	D	161	GLY	C-O	-5.10	1.18	1.24
1	E	390	CYS	C-O	-5.10	1.17	1.23
1	C	324	LEU	C-O	-5.10	1.18	1.24
1	D	127	SER	C-O	-5.10	1.17	1.23
1	B	204	GLU	C-O	-5.09	1.18	1.24
1	C	93	GLY	C-O	-5.09	1.17	1.23
1	D	377	LEU	C-O	-5.08	1.18	1.24
1	B	86	VAL	C-O	-5.08	1.19	1.24
1	F	52	ASP	C-O	-5.07	1.17	1.23
1	B	280	PRO	C-O	-5.07	1.18	1.23
1	B	88	ARG	C-O	-5.06	1.17	1.23
1	D	91	GLY	C-O	-5.06	1.17	1.24
1	C	83	GLY	C-O	-5.06	1.18	1.24
1	B	55	LEU	C-O	-5.06	1.18	1.24
1	D	330	ALA	C-O	-5.06	1.18	1.24
1	B	71	VAL	C-O	-5.06	1.18	1.24
1	C	24	ARG	C-O	-5.05	1.17	1.24
1	D	115	GLY	C-O	-5.05	1.17	1.23
1	C	7	VAL	C-O	-5.05	1.19	1.24
1	A	120	MET	C-O	-5.04	1.17	1.24
1	C	8	ILE	C-O	-5.04	1.18	1.24
1	C	357	SER	C-O	-5.04	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	289	SER	C-O	-5.04	1.17	1.23
1	F	253	GLY	C-O	-5.04	1.18	1.24
1	A	201	LEU	C-O	-5.03	1.17	1.24
1	F	16	ILE	C-O	-5.03	1.18	1.24
1	F	102	LEU	C-O	-5.03	1.18	1.24
1	C	86	VAL	C-O	-5.03	1.19	1.24
1	B	274	ALA	C-O	-5.03	1.18	1.24
1	A	73	LEU	C-O	-5.03	1.18	1.24
1	A	363	GLY	C-O	-5.03	1.17	1.23
1	D	24	ARG	C-O	-5.03	1.17	1.24
1	F	365	THR	C-O	-5.02	1.18	1.24
1	B	286	SER	C-O	-5.01	1.18	1.23
1	A	398	ALA	C-O	-5.01	1.17	1.23
1	C	275	GLU	C-O	-5.01	1.17	1.24
1	E	395	GLN	C-O	-5.01	1.17	1.23
1	B	351	VAL	C-O	-5.01	1.18	1.24
1	E	368	ARG	C-O	-5.01	1.18	1.24
1	D	107	GLY	C-O	-5.01	1.17	1.24
1	D	252	ALA	C-O	-5.01	1.17	1.24
1	C	118	GLU	C-O	-5.00	1.18	1.23
1	D	125	PHE	C-O	-5.00	1.18	1.23
1	E	398	ALA	C-O	-5.00	1.17	1.23

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197[A]	SER	CA-C-N	15.42	146.48	120.72
1	B	197[A]	SER	C-N-CA	15.42	146.48	120.72
1	B	197[B]	SER	CA-C-N	15.42	146.48	120.72
1	B	197[B]	SER	C-N-CA	15.42	146.48	120.72
1	D	149[A]	ARG	CA-C-N	13.43	139.37	120.29
1	D	149[A]	ARG	C-N-CA	13.43	139.37	120.29
1	D	149[B]	ARG	CA-C-N	13.43	139.37	120.29
1	D	149[B]	ARG	C-N-CA	13.43	139.37	120.29
1	B	174	TYR	CA-C-N	11.72	139.01	122.36
1	B	174	TYR	C-N-CA	11.72	139.01	122.36
1	C	383	ARG	N-CA-C	11.01	123.26	111.03
1	A	130	MET	N-CA-C	10.62	124.14	111.82
1	D	150	THR	N-CA-C	9.99	122.25	111.36
1	E	131	ARG	N-CA-C	9.77	121.69	111.14
1	D	223	GLU	N-CA-C	9.63	121.54	111.14
1	B	285	VAL	N-CA-C	9.50	119.46	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	GLY	O-C-N	-9.46	112.21	122.24
1	D	244	GLN	N-CA-C	8.82	120.97	111.36
1	E	223	GLU	N-CA-C	8.64	120.48	111.14
1	B	175[A]	HIS	CA-C-O	-8.61	111.96	122.03
1	B	175[B]	HIS	CA-C-O	-8.61	111.96	122.03
1	A	208	VAL	N-CA-C	8.32	116.96	107.89
1	B	223	GLU	N-CA-C	8.26	120.06	111.14
1	D	204	GLU	N-CA-C	8.16	120.25	111.36
1	B	104	VAL	N-CA-C	8.01	118.06	110.53
1	C	205	ILE	N-CA-C	7.95	119.72	108.36
1	E	43	THR	N-CA-C	7.92	121.01	111.82
1	B	204	GLU	N-CA-C	7.86	119.93	111.36
1	F	86	VAL	N-CA-C	7.75	119.64	108.48
1	B	357	SER	N-CA-C	7.70	119.46	111.14
1	D	155	LYS	N-CA-C	7.62	120.66	111.82
1	A	136	ARG	N-CA-C	7.54	119.58	111.36
1	F	137	THR	N-CA-C	7.40	120.40	111.82
1	D	92	SER	N-CA-C	7.36	119.30	111.28
1	F	131	ARG	N-CA-C	7.31	119.14	111.03
1	C	358	LEU	N-CA-C	7.25	118.97	111.14
1	D	146	ALA	N-CA-C	7.24	118.81	111.07
1	C	315	THR	N-CA-C	-7.22	98.33	109.52
1	C	133	GLY	N-CA-C	7.15	121.13	112.48
1	C	320	ASP	N-CA-C	7.10	119.10	111.36
1	B	58	CYS	N-CA-C	6.99	121.89	113.23
1	F	223	GLU	N-CA-C	6.97	118.67	111.14
1	F	92	SER	N-CA-C	6.97	118.88	111.28
1	C	204	GLU	N-CA-C	6.93	118.92	111.36
1	D	48	ASP	CA-C-N	6.92	130.24	120.28
1	D	48	ASP	C-N-CA	6.92	130.24	120.28
1	B	105	ARG	CA-C-N	6.87	130.17	120.28
1	B	105	ARG	C-N-CA	6.87	130.17	120.28
1	E	281	LEU	N-CA-C	6.87	118.56	111.14
1	E	285	VAL	N-CA-C	6.83	116.95	110.53
1	C	104	VAL	N-CA-C	6.74	116.87	110.53
1	C	362	VAL	N-CA-C	6.74	116.89	110.42
1	C	146	ALA	N-CA-C	6.72	118.40	111.14
1	A	362	VAL	CB-CA-C	-6.66	103.44	111.97
1	E	204	GLU	N-CA-C	6.63	118.59	111.36
1	F	389	MET	N-CA-C	6.61	119.36	108.99
1	C	357	SER	N-CA-C	6.55	118.21	111.14
1	D	205	ILE	N-CA-C	6.44	117.85	108.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	MET	N-CA-C	6.43	117.98	108.60
1	D	320	ASP	N-CA-C	6.43	118.36	111.36
1	C	43	THR	N-CA-C	6.34	119.18	111.82
1	B	205	ILE	N-CA-C	6.34	117.71	108.58
1	A	43	THR	N-CA-C	6.32	119.15	111.82
1	B	320	ASP	N-CA-C	6.28	118.20	111.36
1	E	125	PHE	N-CA-C	-6.27	99.98	109.95
1	B	130	MET	N-CA-C	6.27	118.19	111.36
1	E	320	ASP	N-CA-C	6.24	118.17	111.36
1	A	155	LYS	N-CA-C	6.23	118.07	111.28
1	C	125	PHE	N-CA-C	-6.23	99.57	109.59
1	D	148	GLY	CA-C-N	6.22	128.62	120.28
1	D	148	GLY	C-N-CA	6.22	128.62	120.28
1	F	156	PHE	N-CA-C	6.10	119.98	112.54
1	A	204	GLU	N-CA-C	6.06	117.97	111.36
1	E	253	GLY	N-CA-C	6.04	120.50	112.77
1	D	362	VAL	N-CA-C	6.02	116.19	110.42
1	F	133	GLY	N-CA-C	6.01	119.02	112.29
1	B	261	ALA	N-CA-C	5.97	117.22	108.14
1	D	261	ALA	N-CA-C	5.95	117.19	108.14
1	A	131	ARG	N-CA-C	5.95	117.56	111.14
1	E	205	ILE	N-CA-C	5.95	116.86	108.36
1	F	55	LEU	N-CA-C	5.92	118.56	108.90
1	A	58	CYS	N-CA-C	5.91	120.49	113.28
1	B	253	GLY	N-CA-C	5.86	120.27	112.77
1	A	374	ALA	N-CA-C	5.86	117.34	111.07
1	B	358	LEU	N-CA-C	5.84	117.73	111.36
1	D	357	SER	N-CA-C	5.84	117.45	111.14
1	D	208	VAL	N-CA-C	5.82	114.36	107.73
1	E	252	ALA	CA-C-N	5.81	126.39	120.00
1	E	252	ALA	C-N-CA	5.81	126.39	120.00
1	B	84	MET	N-CA-C	5.78	116.19	108.38
1	A	244	GLN	N-CA-C	5.78	117.45	111.03
1	E	41	GLU	N-CA-C	5.77	117.38	111.14
1	C	171	ARG	N-CA-C	-5.76	105.00	111.28
1	C	102	LEU	CA-C-N	5.76	128.00	120.28
1	C	102	LEU	C-N-CA	5.76	128.00	120.28
1	E	86	VAL	N-CA-C	5.75	117.03	108.46
1	F	84	MET	N-CA-C	5.75	117.00	108.60
1	E	259	ASN	N-CA-C	5.75	117.92	109.24
1	F	285	VAL	N-CA-C	5.74	115.92	110.53
1	B	196	GLN	O-C-N	-5.74	116.04	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	HIS	N-CA-C	5.73	122.47	109.81
1	F	358	LEU	N-CA-C	5.72	117.60	111.36
1	E	351	VAL	N-CA-C	5.71	120.03	112.04
1	A	132	TRP	N-CA-C	5.69	120.22	112.88
1	A	201	LEU	N-CA-C	5.66	118.39	111.82
1	F	196	GLN	N-CA-C	5.66	117.25	111.14
1	D	224	HIS	N-CA-C	5.65	122.30	109.81
1	B	93	GLY	N-CA-C	5.62	119.47	112.73
1	B	92	SER	N-CA-C	5.61	117.39	111.28
1	C	285	VAL	N-CA-C	5.56	115.76	110.53
1	A	147	ARG	CA-C-N	5.56	127.09	120.14
1	A	147	ARG	C-N-CA	5.56	127.09	120.14
1	A	205	ILE	N-CA-C	5.54	116.56	108.58
1	E	217	GLU	N-CA-C	5.54	118.10	109.52
1	C	155	LYS	N-CA-C	5.54	117.39	111.36
1	A	81	VAL	N-CA-C	5.53	113.96	107.77
1	D	341	PHE	N-CA-C	5.53	117.83	110.53
1	A	319	ILE	N-CA-C	5.52	116.34	107.73
1	A	105	ARG	N-CA-C	5.52	118.05	111.71
1	F	259	ASN	N-CA-C	5.51	117.45	109.07
1	A	259	ASN	N-CA-C	5.51	117.17	108.96
1	E	93	GLY	N-CA-C	5.49	119.31	112.73
1	A	151	THR	N-CA-C	5.47	119.22	112.54
1	A	35	ALA	N-CA-C	5.43	117.27	111.36
1	E	104	VAL	N-CA-C	5.43	115.63	110.53
1	F	40	LEU	N-CA-C	5.43	117.27	111.36
1	E	130	MET	N-CA-C	5.42	118.11	111.82
1	F	359	GLY	N-CA-C	-5.42	106.80	111.95
1	B	224	HIS	N-CA-C	5.38	121.69	109.81
1	F	224	HIS	N-CA-C	5.36	121.65	109.81
1	C	89	ARG	N-CA-C	5.34	117.10	108.08
1	B	90	CYS	CB-CA-C	5.33	121.05	110.17
1	D	137	THR	N-CA-C	5.32	117.16	111.36
1	A	84	MET	N-CA-C	5.31	116.87	108.96
1	E	197	SER	N-CA-C	5.31	117.06	111.28
1	E	244	GLN	N-CA-C	5.30	117.14	111.36
1	E	356	ILE	N-CA-C	5.29	115.50	110.42
1	A	243	LYS	N-CA-C	-5.29	105.41	111.07
1	D	148	GLY	CA-C-O	-5.29	114.69	120.40
1	F	127	SER	N-CA-C	5.28	117.79	108.75
1	E	191	ARG	N-CA-C	5.27	117.11	111.36
1	B	219	ILE	N-CA-C	5.27	115.55	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261	ALA	N-CA-C	5.27	116.15	108.14
1	F	275	GLU	N-CA-C	5.25	117.01	111.28
1	C	21	GLY	CA-C-N	5.25	127.31	120.28
1	C	21	GLY	C-N-CA	5.25	127.31	120.28
1	F	85	GLN	N-CA-C	5.23	117.59	108.76
1	A	362	VAL	N-CA-C	5.22	115.43	110.42
1	E	5	ASP	N-CA-C	5.20	117.98	110.28
1	E	151	THR	N-CA-C	5.18	119.60	113.28
1	A	297	MET	N-CA-C	5.17	117.65	111.71
1	B	362	VAL	N-CA-C	5.17	115.38	110.42
1	F	357	SER	N-CA-C	5.16	116.71	111.14
1	F	205	ILE	N-CA-C	5.16	116.01	108.58
1	A	380	ARG	N-CA-C	5.16	117.80	111.82
1	A	358	LEU	N-CA-C	5.13	117.77	111.82
1	B	155	LYS	N-CA-C	5.12	118.79	112.54
1	B	131	ARG	N-CA-C	5.12	116.94	111.36
1	E	224	HIS	N-CA-C	5.11	121.11	109.81
1	A	357	SER	N-CA-C	5.11	116.66	111.14
1	F	217	GLU	N-CA-C	5.11	116.83	109.07
1	A	245	ASP	N-CA-C	-5.08	101.28	109.40
1	A	104	VAL	N-CA-C	5.07	115.29	110.53
1	B	367	GLY	N-CA-C	5.06	118.80	112.73
1	E	384	TYR	N-CA-C	5.06	117.14	108.90
1	C	223	GLU	N-CA-C	5.05	116.79	111.28
1	D	151	THR	N-CA-C	5.04	119.58	113.38
1	F	36	LEU	N-CA-C	5.04	116.77	111.28
1	C	389	MET	N-CA-C	5.04	116.72	109.07
1	E	358	LEU	N-CA-C	5.02	116.84	111.36
1	F	130	MET	N-CA-C	5.02	117.64	111.82
1	F	104	VAL	N-CA-C	5.02	115.25	110.53
1	C	5	ASP	N-CA-C	5.00	117.56	110.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	PRO	Peptide
1	C	361	PRO	Peptide
1	D	361	PRO	Peptide
1	D	66	ALA	Peptide
1	E	361	PRO	Peptide
1	F	361	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	F	66	ALA	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	2868	0	2782	92	0
1	B	2943	0	2941	85	0
1	C	2882	0	2840	96	0
1	D	2927	0	2917	75	0
1	E	2925	0	2912	75	0
1	F	2846	0	2799	80	0
2	A	51	0	0	3	0
2	B	66	0	0	6	0
2	C	55	0	0	2	0
2	D	69	0	0	4	0
2	E	49	0	0	1	0
2	F	46	0	0	2	0
All	All	17727	0	17191	457	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (457) 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:131:ARG:NH2	1:B:143:ASP:OD1	1.60	1.35
1:E:108:ASP:OD1	1:F:311:LYS:NZ	1.75	1.18
1:A:131:ARG:NH1	1:B:123:VAL:O	1.78	1.15
1:A:141:ILE:HD11	1:D:141:ILE:HD11	1.27	1.08
1:B:326:GLU:OE1	1:B:354:SER:HB3	1.56	1.05
1:E:86:VAL:HG12	1:F:86:VAL:HG12	1.39	1.03
1:D:326:GLU:OE1	1:D:354:SER:HB3	1.57	1.02
1:A:344:ALA:O	1:A:347:GLU:HB2	1.59	1.02
1:B:49:GLN:OE1	1:B:272:LYS:NZ	1.93	1.00
1:C:326:GLU:OE1	1:C:354:SER:HB3	1.61	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:ILE:HD12	1:F:176:ILE:H	1.28	0.98
1:E:212:THR:C	1:E:215:GLY:O	2.08	0.96
1:B:141:ILE:HD11	1:C:141:ILE:CD1	1.94	0.96
1:B:141:ILE:HD11	1:C:141:ILE:HD11	1.46	0.96
1:F:11:PRO:O	1:F:375:ARG:NH1	1.97	0.96
1:B:251:THR:O	1:B:255:SER:OG	1.81	0.96
1:E:358:LEU:HD13	1:E:368:ARG:NH1	1.82	0.94
1:E:212:THR:C	1:E:214:ASP:N	2.28	0.92
1:C:131:ARG:NH2	1:D:143:ASP:OD1	2.02	0.92
1:E:358:LEU:CD1	1:E:368:ARG:NH1	2.33	0.91
1:A:86:VAL:HG12	1:B:86:VAL:HG12	1.52	0.91
1:A:141:ILE:HD11	1:D:141:ILE:CD1	2.01	0.89
1:B:18:ARG:HG3	1:B:223:GLU:HG2	1.53	0.88
1:C:245:ASP:OD1	1:C:246:PRO:HD2	1.75	0.87
1:C:45:ILE:CD1	1:C:276:LEU:HD13	2.06	0.86
1:E:88:ARG:NH2	1:F:52:ASP:OD1	2.09	0.86
1:B:39:LEU:HD11	1:B:266:ILE:HD12	1.58	0.85
1:F:326:GLU:CD	1:F:354:SER:HB3	2.02	0.85
1:F:189:HIS:O	1:F:193:VAL:HG23	1.77	0.84
1:C:163:MET:O	1:C:166:THR:OG1	1.96	0.82
1:F:171:ARG:CG	1:F:176:ILE:HD13	1.97	0.82
1:F:315:THR:O	1:F:318:ASP:HB2	1.79	0.82
1:A:88:ARG:NH2	1:B:52:ASP:OD1	2.13	0.82
1:A:383:ARG:HD3	1:A:384:TYR:CE2	2.15	0.81
1:F:171:ARG:HG2	1:F:176:ILE:HD13	1.61	0.81
1:E:123:VAL:O	1:F:131:ARG:NH1	2.14	0.81
1:D:55:LEU:HD22	1:D:68:GLY:HA2	1.62	0.81
1:A:184:LEU:HA	1:A:187:ARG:NH1	1.97	0.79
1:B:141:ILE:CD1	1:C:141:ILE:HD11	2.12	0.79
1:C:55:LEU:HD22	1:C:68:GLY:HA2	1.65	0.79
1:E:55:LEU:HD22	1:E:68:GLY:HA2	1.64	0.79
1:B:344:ALA:O	1:B:347:GLU:HB2	1.83	0.78
1:C:45:ILE:HD11	1:C:276:LEU:HD13	1.66	0.78
1:E:212:THR:O	1:E:215:GLY:O	2.00	0.78
1:E:245:ASP:OD1	1:E:247:GLU:N	2.17	0.78
1:B:141:ILE:CD1	1:C:141:ILE:CD1	2.63	0.77
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.50	0.77
1:C:344:ALA:O	1:C:347:GLU:HB2	1.85	0.76
1:A:171:ARG:HD2	1:A:171:ARG:C	2.10	0.76
1:B:171:ARG:HA	1:B:176:ILE:HD12	1.65	0.76
1:C:391:ILE:HB	1:C:395:GLN:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HH22	1:D:143:ASP:CG	1.93	0.76
1:C:245:ASP:OD1	1:C:246:PRO:CD	2.34	0.76
1:B:178:ARG:HB2	1:B:249:THR:HG22	1.67	0.75
1:E:143:ASP:OD1	1:F:131:ARG:NH2	2.20	0.75
1:F:326:GLU:OE1	1:F:354:SER:HB3	1.87	0.75
1:C:22:MET:SD	1:C:223:GLU:HB2	2.27	0.74
1:B:326:GLU:CD	1:B:354:SER:HB3	2.12	0.74
1:E:358:LEU:HD13	1:E:368:ARG:HH11	1.51	0.74
1:A:171:ARG:NH1	1:A:247:GLU:O	2.21	0.74
1:F:55:LEU:HD22	1:F:68:GLY:HA2	1.68	0.74
1:B:55:LEU:HD22	1:B:68:GLY:HA2	1.68	0.74
1:A:171:ARG:HD2	1:A:172:ARG:N	2.04	0.72
1:C:131:ARG:NH2	1:D:143:ASP:CG	2.47	0.71
1:B:337:ARG:HG2	1:B:337:ARG:HH11	1.57	0.70
1:D:15:PRO:HD3	1:D:205:ILE:HG23	1.72	0.70
1:C:131:ARG:NH1	1:D:123:VAL:O	2.25	0.70
1:F:164:LEU:HD22	1:F:328:PHE:HE2	1.56	0.70
1:C:45:ILE:HD12	1:C:276:LEU:HD13	1.74	0.69
1:B:141:ILE:HD11	1:C:141:ILE:HD12	1.73	0.69
1:C:89:ARG:HB2	1:C:391:ILE:HG23	1.74	0.69
1:F:176:ILE:H	1:F:176:ILE:CD1	2.02	0.69
1:B:391:ILE:HB	1:B:395:GLN:HB2	1.75	0.69
1:F:326:GLU:HB3	1:F:356:ILE:HD12	1.74	0.69
1:B:326:GLU:HB3	1:B:356:ILE:HD12	1.74	0.68
1:A:45:ILE:HD11	1:A:276:LEU:HB3	1.75	0.68
1:E:184:LEU:HD11	1:E:326:GLU:OE2	1.93	0.68
1:C:255:SER:HB2	1:C:328:PHE:CD1	2.29	0.68
1:A:187:ARG:NH1	1:A:187:ARG:HG3	2.06	0.67
1:E:212:THR:CA	1:E:215:GLY:O	2.42	0.67
1:A:371:ALA:O	1:A:375:ARG:HG3	1.93	0.67
1:A:127:SER:OG	1:A:140:GLN:O	2.10	0.67
1:C:287:TRP:O	1:C:311:LYS:CE	2.42	0.67
1:F:321:LEU:HD12	1:F:377:LEU:CD1	2.25	0.67
1:B:337:ARG:HH11	1:B:337:ARG:CG	2.07	0.67
1:D:256:SER:HB3	1:D:355:GLY:O	1.94	0.67
1:E:123:VAL:HG21	1:E:145:LEU:HD21	1.75	0.67
1:E:168:GLU:OE2	1:E:250:VAL:HG23	1.94	0.67
1:C:315:THR:HG22	1:C:317:ALA:H	1.59	0.67
1:D:245:ASP:OD1	1:D:247:GLU:N	2.25	0.67
1:B:135:ALA:HB2	1:D:131:ARG:O	1.95	0.66
1:D:45:ILE:HD11	1:D:276:LEU:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:HD2	2:B:514:HOH:O	1.95	0.66
1:D:163:MET:HA	1:D:163:MET:HE2	1.77	0.66
1:A:89:ARG:HB2	1:A:391:ILE:HG23	1.76	0.66
1:C:321:LEU:HD12	1:C:377:LEU:CD1	2.26	0.66
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.59	0.65
1:A:201:LEU:O	1:A:205:ILE:HG12	1.95	0.65
1:E:371:ALA:O	1:E:375:ARG:HG3	1.96	0.65
1:B:287:TRP:O	1:B:311:LYS:HE3	1.96	0.65
1:F:176:ILE:HD12	1:F:176:ILE:N	2.07	0.65
1:F:45:ILE:HD11	1:F:276:LEU:HB3	1.77	0.65
1:C:326:GLU:CD	1:C:354:SER:HB3	2.21	0.65
1:B:196:GLN:HG3	1:B:201:LEU:HD23	1.77	0.65
1:D:326:GLU:OE1	1:D:354:SER:CB	2.39	0.65
1:F:315:THR:HG22	1:F:317:ALA:H	1.59	0.65
1:A:161:GLY:HA3	1:A:165:GLU:OE1	1.96	0.65
1:E:326:GLU:OE1	1:E:354:SER:HB3	1.97	0.65
1:A:88:ARG:HH22	1:B:52:ASP:CG	2.04	0.65
1:C:22:MET:HG2	1:C:219:ILE:HD13	1.79	0.64
1:A:52:ASP:OD1	1:B:88:ARG:NH2	2.31	0.64
1:F:178:ARG:HB2	1:F:249:THR:HG22	1.80	0.64
1:B:88:ARG:N	1:B:92:SER:OG	2.27	0.63
1:A:358:LEU:HD13	1:A:368:ARG:NH1	2.13	0.63
1:A:187:ARG:HH11	1:A:187:ARG:CG	2.11	0.63
1:A:319:ILE:O	1:A:348:ARG:NH1	2.31	0.63
1:A:131:ARG:NH2	1:B:143:ASP:CG	2.52	0.62
1:C:121:SER:O	1:D:131:ARG:HD3	1.99	0.62
1:F:298:GLY:HA3	1:F:331:GLN:HG2	1.81	0.62
1:C:383:ARG:HD3	1:C:384:TYR:CE2	2.35	0.62
1:E:89:ARG:HB2	1:E:391:ILE:HG23	1.81	0.62
1:E:192:ALA:O	1:E:196:GLN:HG3	2.00	0.62
1:B:4:ARG:N	2:B:505:HOH:O	2.32	0.62
1:C:88:ARG:NH2	1:D:52:ASP:OD1	2.33	0.61
1:A:358:LEU:CD1	1:A:368:ARG:NH1	2.64	0.61
1:C:84:MET:HE2	1:C:86:VAL:HG13	1.82	0.61
1:E:13:ARG:HD3	1:E:368:ARG:HG3	1.81	0.61
1:A:255:SER:HB2	1:A:328:PHE:CD1	2.35	0.61
1:A:300:GLY:N	1:A:301:PRO:HD2	2.14	0.61
1:E:391:ILE:HB	1:E:395:GLN:HB2	1.81	0.61
1:D:7:VAL:HG12	1:D:283:ARG:HB3	1.81	0.61
1:C:127:SER:HB3	1:C:130:MET:HG3	1.83	0.61
1:D:149[A]:ARG:NH2	1:D:258:GLN:OE1	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:THR:N	1:E:215:GLY:O	2.33	0.61
1:C:88:ARG:HH22	1:D:52:ASP:CG	2.08	0.60
1:B:232:GLU:H	1:B:232:GLU:CD	2.09	0.60
1:F:45:ILE:HD11	1:F:276:LEU:CB	2.31	0.60
1:B:255:SER:HB3	1:B:328:PHE:HD1	1.66	0.60
1:D:58:CYS:SG	1:D:362:VAL:HG12	2.42	0.60
1:A:377:LEU:HD12	1:A:382:ALA:HB3	1.84	0.59
1:A:38:GLY:HA3	1:A:206:ILE:HD12	1.83	0.59
1:E:88:ARG:HH22	1:F:52:ASP:CG	2.09	0.59
1:E:99:GLN:O	1:E:103:GLN:HG3	2.02	0.59
1:A:161:GLY:HA3	1:A:165:GLU:HB2	1.84	0.59
1:B:377:LEU:HD12	1:B:382:ALA:HB3	1.85	0.59
1:C:127:SER:HB2	1:C:130:MET:HE3	1.85	0.59
1:C:178:ARG:NH1	1:C:234:LEU:O	2.36	0.59
1:F:391:ILE:HB	1:F:395:GLN:HB2	1.85	0.59
1:E:168:GLU:CD	1:E:250:VAL:HG23	2.28	0.58
1:C:178:ARG:HB2	1:C:249:THR:HG22	1.85	0.58
1:F:342:GLY:O	1:F:344:ALA:N	2.37	0.58
1:A:287:TRP:O	1:A:311:LYS:HE2	2.03	0.58
1:F:321:LEU:HD12	1:F:377:LEU:HD12	1.84	0.58
1:E:184:LEU:C	1:E:184:LEU:HD12	2.28	0.58
1:C:287:TRP:O	1:C:311:LYS:HE3	2.04	0.58
1:F:298:GLY:CA	1:F:331:GLN:HG2	2.33	0.58
1:D:391:ILE:HB	1:D:395:GLN:HB2	1.85	0.57
1:C:55:LEU:HD11	1:C:264:MET:HE1	1.87	0.57
1:D:405:GLN:HA	1:D:405:GLN:NE2	2.20	0.57
1:C:255:SER:HB2	1:C:328:PHE:HD1	1.68	0.57
1:C:171:ARG:HA	1:C:176:ILE:HG13	1.85	0.57
1:B:89:ARG:HB2	1:B:391:ILE:HG23	1.86	0.57
1:C:184:LEU:HD23	1:C:329:ALA:HB1	1.87	0.57
1:B:161:GLY:HA3	1:B:165:GLU:OE1	2.05	0.56
1:C:123:VAL:O	1:D:131:ARG:NH1	2.37	0.56
1:D:89:ARG:HB2	1:D:391:ILE:HG23	1.86	0.56
1:E:327:ALA:C	1:E:328:PHE:CD1	2.84	0.56
1:F:383:ARG:NH1	1:F:383:ARG:HG3	2.18	0.56
1:C:242:LEU:HA	1:C:245:ASP:O	2.06	0.56
1:C:315:THR:HG22	1:C:317:ALA:N	2.21	0.56
1:F:67:ILE:O	1:F:71:VAL:HG23	2.04	0.56
1:F:178:ARG:NH2	1:F:239:PRO:HD3	2.20	0.56
1:D:11:PRO:O	1:D:375:ARG:NH1	2.39	0.56
1:D:332:ALA:O	1:D:336:MET:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:SER:CB	1:F:130:MET:HE3	2.36	0.56
1:D:364:ALA:HA	2:D:525:HOH:O	2.06	0.55
1:F:300:GLY:N	1:F:301:PRO:CD	2.68	0.55
1:A:179:THR:O	1:A:183:GLU:HG3	2.06	0.55
1:C:232:GLU:OE1	1:C:232:GLU:N	2.38	0.55
1:D:123:VAL:HG21	1:D:145:LEU:HD21	1.89	0.55
1:C:195:ALA:HB2	1:C:352:ARG:HD2	1.88	0.55
1:A:121:SER:O	1:B:131:ARG:HD3	2.07	0.55
1:A:321:LEU:HD12	1:A:377:LEU:HD13	1.89	0.55
1:A:207:PRO:HD2	2:A:544:HOH:O	2.07	0.54
1:A:391:ILE:HB	1:A:395:GLN:HB2	1.88	0.54
1:C:211:ARG:HA	1:C:216:GLU:HG2	1.89	0.54
1:C:163:MET:N	2:C:503:HOH:O	2.39	0.54
1:A:171:ARG:NH1	1:A:171:ARG:HG3	2.22	0.54
1:B:18:ARG:CG	1:B:223:GLU:HG2	2.34	0.54
1:B:178:ARG:NH2	1:B:239:PRO:HD3	2.21	0.54
1:C:321:LEU:HD12	1:C:377:LEU:HD13	1.87	0.54
1:E:8:ILE:HD12	1:E:267:VAL:HG22	1.88	0.54
1:E:13:ARG:HD3	1:E:368:ARG:CG	2.37	0.54
1:E:13:ARG:CD	1:E:368:ARG:HG3	2.37	0.54
1:D:287:TRP:O	1:D:311:LYS:HE3	2.07	0.54
1:E:52:ASP:OD1	1:F:88:ARG:NH2	2.40	0.54
1:A:4:ARG:O	1:A:105:ARG:HG2	2.08	0.54
1:A:245:ASP:OD1	1:A:247:GLU:N	2.30	0.54
1:E:212:THR:O	1:E:214:ASP:N	2.40	0.54
1:D:271:GLU:CD	1:D:271:GLU:H	2.15	0.54
1:B:15:PRO:HD3	1:B:205:ILE:HG23	1.91	0.53
1:A:120:MET:HA	1:A:123:VAL:HG23	1.89	0.53
1:A:383:ARG:HD3	1:A:384:TYR:CZ	2.42	0.53
1:E:328:PHE:CD1	1:E:328:PHE:N	2.77	0.53
1:A:239:PRO:HG2	1:A:248:ALA:O	2.08	0.53
1:A:344:ALA:O	1:A:347:GLU:CB	2.44	0.53
1:A:326:GLU:OE1	1:A:354:SER:HB3	2.09	0.53
1:A:172:ARG:NH1	1:A:245:ASP:OD2	2.41	0.53
1:F:7:VAL:HG12	1:F:283:ARG:HB2	1.90	0.53
1:A:315:THR:O	1:A:318:ASP:HB2	2.09	0.53
1:B:315:THR:HG23	1:B:317:ALA:H	1.73	0.53
1:C:242:LEU:O	1:C:245:ASP:O	2.27	0.53
1:E:120:MET:HA	1:E:123:VAL:HG23	1.91	0.53
1:C:315:THR:O	1:C:318:ASP:HB2	2.09	0.53
1:C:371:ALA:O	1:C:375:ARG:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ARG:HH21	1:D:239:PRO:HG3	1.74	0.53
1:B:175[B]:HIS:ND1	2:B:501:HOH:O	2.37	0.52
1:D:163:MET:HE2	1:D:163:MET:CA	2.40	0.52
1:C:332:ALA:O	1:C:336:MET:HG3	2.09	0.52
1:D:255:SER:HB2	1:D:328:PHE:CD1	2.44	0.52
1:D:23:PHE:HB2	2:D:516:HOH:O	2.09	0.52
1:A:311:LYS:NZ	1:B:108:ASP:OD1	2.41	0.52
1:B:269:THR:HB	1:B:270:PRO:CD	2.40	0.52
1:E:58:CYS:SG	1:E:362:VAL:HG12	2.48	0.52
1:E:86:VAL:HG12	1:F:86:VAL:CG1	2.26	0.52
1:B:161:GLY:HA3	1:B:165:GLU:HB2	1.91	0.52
1:C:300:GLY:N	1:C:301:PRO:CD	2.73	0.52
1:D:10:GLU:OE2	1:D:42:ARG:NH1	2.41	0.52
1:A:302:VAL:HB	1:A:303:PRO:CD	2.41	0.51
1:C:52:ASP:OD1	1:D:88:ARG:NH2	2.43	0.51
1:E:131:ARG:HD3	1:F:121:SER:O	2.09	0.51
1:F:127:SER:HB3	1:F:130:MET:HE3	1.93	0.51
1:B:99:GLN:O	1:B:103:GLN:HG3	2.10	0.51
1:B:141:ILE:CD1	1:C:141:ILE:HD12	2.34	0.51
1:C:344:ALA:O	1:C:347:GLU:N	2.37	0.51
1:D:22:MET:HE3	1:D:219:ILE:HG21	1.92	0.51
1:D:179:THR:O	1:D:183:GLU:HB2	2.10	0.51
1:B:373:LEU:O	1:B:377:LEU:HB2	2.10	0.51
1:F:204:GLU:HG2	1:F:371:ALA:HB1	1.93	0.51
1:E:65:PRO:HB3	1:F:89:ARG:NH1	2.26	0.51
1:E:300:GLY:N	1:E:301:PRO:CD	2.74	0.51
1:B:194:ALA:O	1:B:198:GLU:HB2	2.10	0.50
1:D:178:ARG:HD2	1:D:182:ASP:OD2	2.12	0.50
1:F:321:LEU:HD12	1:F:377:LEU:HD13	1.93	0.50
1:A:161:GLY:CA	1:A:165:GLU:OE1	2.59	0.50
1:B:238:LYS:HG2	1:B:238:LYS:O	2.12	0.50
1:D:228:ASP:O	1:D:230:THR:HG23	2.11	0.50
1:D:245:ASP:OD1	1:D:247:GLU:HB2	2.12	0.50
1:E:184:LEU:C	1:E:184:LEU:CD1	2.85	0.50
1:E:184:LEU:HD12	1:E:184:LEU:O	2.12	0.50
1:F:57:HIS:ND1	1:F:117:ALA:O	2.37	0.50
1:A:127:SER:HB3	1:A:130:MET:HG3	1.94	0.49
1:C:391:ILE:HB	1:C:395:GLN:CB	2.40	0.49
1:E:326:GLU:OE1	1:E:354:SER:CB	2.59	0.49
1:B:239:PRO:HA	1:B:251:THR:HG22	1.93	0.49
1:B:354:SER:OG	1:B:355:GLY:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ALA:HB2	1:A:352:ARG:HD2	1.94	0.49
1:E:354:SER:O	1:E:358:LEU:HB2	2.12	0.49
1:C:101:CYS:O	1:C:105:ARG:HG3	2.13	0.49
1:D:38:GLY:HA3	1:D:206:ILE:HD12	1.95	0.49
1:F:279:LYS:O	1:F:279:LYS:HG2	2.12	0.49
1:A:171:ARG:HH21	1:A:172:ARG:NH1	2.10	0.49
1:A:89:ARG:HB2	1:A:391:ILE:CG2	2.42	0.49
1:C:16:ILE:HG23	1:C:361:PRO:HG3	1.93	0.49
1:C:166:THR:HG22	1:C:295:ASP:O	2.12	0.49
1:A:358:LEU:HD13	1:A:368:ARG:HH11	1.78	0.49
1:A:383:ARG:CD	1:A:384:TYR:CE2	2.93	0.49
1:C:358:LEU:HD13	1:C:368:ARG:HD2	1.94	0.49
1:F:383:ARG:HG3	1:F:383:ARG:HH11	1.78	0.49
1:C:321:LEU:HD12	1:C:377:LEU:HD12	1.93	0.48
1:E:195:ALA:HB2	1:E:352:ARG:HD2	1.94	0.48
1:F:320:ASP:CB	1:F:382:ALA:HB1	2.43	0.48
1:A:161:GLY:HA3	1:A:165:GLU:CB	2.43	0.48
1:D:149[B]:ARG:HG2	1:D:163:MET:HG2	1.94	0.48
1:C:287:TRP:O	1:C:311:LYS:NZ	2.46	0.48
1:A:18:ARG:HD2	2:A:533:HOH:O	2.13	0.48
1:C:89:ARG:HB2	1:C:391:ILE:CG2	2.44	0.48
1:B:337:ARG:CD	2:B:514:HOH:O	2.57	0.48
1:C:315:THR:CG2	1:C:317:ALA:H	2.26	0.48
1:B:100:ALA:HB1	1:B:112:VAL:CG2	2.44	0.48
1:C:131:ARG:NH2	1:D:143:ASP:OD2	2.47	0.48
1:E:178:ARG:HD2	1:E:182:ASP:OD2	2.13	0.48
1:F:327:ALA:C	1:F:328:PHE:CD1	2.92	0.48
1:A:161:GLY:N	1:A:165:GLU:OE1	2.47	0.47
1:C:22:MET:HE3	1:C:219:ILE:HG21	1.97	0.47
1:A:300:GLY:N	1:A:301:PRO:CD	2.77	0.47
1:B:242:LEU:HD12	1:B:242:LEU:O	2.15	0.47
1:F:38:GLY:HA3	1:F:206:ILE:HD12	1.96	0.47
1:B:337:ARG:CG	1:B:337:ARG:NH1	2.72	0.47
1:D:271:GLU:CD	1:D:271:GLU:N	2.73	0.47
1:A:301:PRO:HD3	1:A:390:CYS:HA	1.96	0.47
1:C:15:PRO:HD3	1:C:205:ILE:HG23	1.96	0.47
1:C:323:GLU:OE1	1:C:368:ARG:NH2	2.47	0.47
1:F:18:ARG:HG3	1:F:223:GLU:HB3	1.97	0.47
1:E:358:LEU:CD1	1:E:368:ARG:HH12	2.22	0.47
1:F:354:SER:O	1:F:358:LEU:HB2	2.15	0.47
1:D:60:PRO:HD2	2:D:546:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ALA:HB2	1:B:328:PHE:CD2	2.50	0.47
1:A:302:VAL:HB	1:A:303:PRO:HD2	1.97	0.46
1:C:67:ILE:HG12	1:C:67:ILE:O	2.14	0.46
1:D:326:GLU:HB3	1:D:356:ILE:HG13	1.97	0.46
1:E:55:LEU:HA	1:E:115:GLY:O	2.15	0.46
1:F:302:VAL:HB	1:F:303:PRO:CD	2.45	0.46
1:B:269:THR:HB	1:B:270:PRO:HD2	1.96	0.46
1:D:88:ARG:HG2	1:D:391:ILE:HD13	1.96	0.46
1:B:244:GLN:H	1:B:244:GLN:HG2	1.51	0.46
1:F:259:ASN:OD1	1:F:360:HIS:N	2.47	0.46
1:D:58:CYS:C	1:D:60:PRO:HD3	2.40	0.46
1:F:166:THR:HB	1:F:295:ASP:O	2.16	0.46
1:F:286:SER:HA	2:F:517:HOH:O	2.14	0.46
1:F:191:ARG:NH1	1:F:349:THR:O	2.48	0.46
1:A:245:ASP:OD1	1:A:246:PRO:HD2	2.16	0.46
1:D:120:MET:HA	1:D:123:VAL:HG23	1.97	0.46
1:F:195:ALA:HB1	1:F:200:VAL:CG2	2.45	0.46
1:C:391:ILE:CB	1:C:395:GLN:HB2	2.41	0.45
1:D:371:ALA:O	1:D:375:ARG:HG3	2.16	0.45
1:C:86:VAL:HG12	1:D:86:VAL:HG12	1.98	0.45
1:E:99:GLN:NE2	1:E:103:GLN:OE1	2.42	0.45
1:A:403:ARG:HD2	2:A:513:HOH:O	2.16	0.45
1:B:255:SER:HB3	1:B:328:PHE:CD1	2.49	0.45
1:C:7:VAL:HG22	1:C:268:THR:O	2.16	0.45
1:C:127:SER:CB	1:C:130:MET:HE3	2.46	0.45
1:E:61:ASN:OD1	1:E:63:GLU:HB2	2.16	0.45
1:F:319:ILE:O	1:F:348:ARG:NH1	2.50	0.45
1:B:171:ARG:HD2	1:B:171:ARG:C	2.42	0.45
1:C:84:MET:HE2	1:C:86:VAL:CG1	2.46	0.45
1:F:171:ARG:HD2	1:F:249:THR:OG1	2.17	0.45
1:A:373:LEU:O	1:A:377:LEU:HB2	2.17	0.45
1:A:171:ARG:HD2	1:A:172:ARG:CA	2.47	0.45
1:E:10:GLU:N	1:E:11:PRO:HD3	2.32	0.45
1:A:45:ILE:CD1	1:A:276:LEU:HB3	2.45	0.44
1:C:255:SER:CB	1:C:328:PHE:HD1	2.28	0.44
1:E:45:ILE:HD11	1:E:276:LEU:HB3	1.99	0.44
1:C:166:THR:HG22	1:C:295:ASP:C	2.42	0.44
1:E:45:ILE:CD1	1:E:276:LEU:HB3	2.47	0.44
1:A:18:ARG:HG3	1:A:223:GLU:HB3	1.99	0.44
1:A:326:GLU:HB3	1:A:356:ILE:CD1	2.47	0.44
1:D:405:GLN:HA	1:D:405:GLN:HE21	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:HG2	1:D:132:TRP:CD1	2.52	0.44
1:E:169:ASN:OD1	1:E:172:ARG:NH2	2.51	0.44
1:E:293:ALA:HA	1:E:294:PRO:HD3	1.89	0.44
1:F:279:LYS:HE2	1:F:378:HIS:CE1	2.53	0.44
1:A:255:SER:CB	1:A:328:PHE:HD1	2.31	0.44
1:B:67:ILE:HG22	1:B:85:GLN:HB2	2.00	0.44
1:F:59:TYR:N	1:F:60:PRO:CD	2.81	0.44
1:F:298:GLY:O	1:F:331:GLN:NE2	2.30	0.44
1:B:79:ILE:H	1:B:79:ILE:HG13	1.58	0.43
1:B:101:CYS:O	1:B:105:ARG:HG3	2.18	0.43
1:D:300:GLY:N	1:D:301:PRO:CD	2.80	0.43
1:E:212:THR:CB	1:E:215:GLY:O	2.65	0.43
1:F:331:GLN:C	1:F:331:GLN:CD	2.86	0.43
1:F:371:ALA:O	1:F:375:ARG:HG3	2.17	0.43
1:A:11:PRO:O	1:A:375:ARG:NH1	2.50	0.43
1:A:157:HIS:CD2	1:A:157:HIS:N	2.85	0.43
1:B:164:LEU:HD12	1:B:241:LEU:HG	2.00	0.43
1:D:89:ARG:HB2	1:D:391:ILE:CG2	2.49	0.43
1:D:242:LEU:HD12	1:D:246:PRO:HA	2.00	0.43
1:E:57:HIS:HB3	1:E:85:GLN:CG	2.48	0.43
1:E:80:THR:O	1:E:82:PRO:HD3	2.18	0.43
1:B:343:GLU:O	1:B:343:GLU:HG2	2.18	0.43
1:D:131:ARG:HG2	1:D:132:TRP:NE1	2.34	0.43
1:E:84:MET:HE3	1:E:84:MET:HB2	1.76	0.43
1:A:131:ARG:HH21	1:B:143:ASP:CG	2.20	0.43
1:B:307:VAL:HG12	1:B:311:LYS:HE2	2.00	0.43
1:F:23:PHE:HB2	2:F:503:HOH:O	2.19	0.43
1:A:10:GLU:N	1:A:11:PRO:CD	2.81	0.43
1:A:151:THR:OG1	1:B:62:SER:O	2.29	0.43
1:B:300:GLY:N	1:B:301:PRO:CD	2.81	0.43
1:D:368:ARG:O	1:D:368:ARG:HG2	2.18	0.43
1:F:272:LYS:O	1:F:276:LEU:HG	2.19	0.43
1:B:141:ILE:CG1	1:C:141:ILE:HD12	2.47	0.43
1:D:244:GLN:H	1:D:244:GLN:HG2	1.63	0.43
1:E:88:ARG:HG2	1:E:391:ILE:HD13	2.01	0.43
1:A:6:ALA:HB2	1:A:105:ARG:HG3	2.01	0.42
1:E:78:PRO:C	1:E:80:THR:H	2.27	0.42
1:A:388:THR:HA	1:A:397:LEU:O	2.19	0.42
1:C:303:PRO:O	1:C:307:VAL:HG23	2.18	0.42
1:D:161:GLY:HA3	1:D:165:GLU:HB2	2.00	0.42
1:D:321:LEU:HD11	1:D:376:GLU:CG	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:OG1	1:A:271:GLU:HG2	2.19	0.42
1:C:8:ILE:CD1	1:C:267:VAL:HG22	2.49	0.42
1:C:184:LEU:HD23	1:C:329:ALA:CB	2.48	0.42
1:C:283:ARG:NH2	1:C:402:GLU:OE1	2.52	0.42
1:D:7:VAL:HG22	1:D:268:THR:O	2.19	0.42
1:E:55:LEU:HD22	1:E:68:GLY:CA	2.43	0.42
1:F:205:ILE:HD13	1:F:205:ILE:HA	1.77	0.42
1:F:315:THR:CG2	1:F:316:LEU:N	2.81	0.42
1:F:328:PHE:CD1	1:F:328:PHE:N	2.85	0.42
1:A:352:ARG:HD3	1:A:352:ARG:HA	1.73	0.42
1:B:77:LEU:O	2:B:503:HOH:O	2.22	0.42
1:C:40:LEU:HD11	1:C:77:LEU:HD11	2.02	0.42
1:A:123:VAL:O	1:B:131:ARG:NH1	2.53	0.42
1:E:53:VAL:HG12	1:E:55:LEU:HD13	2.00	0.42
1:E:397:LEU:HA	1:E:397:LEU:HD12	1.84	0.42
1:A:387:GLU:O	1:A:398:ALA:HA	2.19	0.42
1:E:56:GLY:O	1:E:116:GLY:HA2	2.19	0.42
1:A:255:SER:HB2	1:A:328:PHE:HD1	1.80	0.42
1:A:326:GLU:HB3	1:A:356:ILE:HD12	2.02	0.42
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.90	0.42
1:A:369:MET:HE2	1:A:387:GLU:HG3	2.02	0.42
1:B:299:ILE:HD12	1:B:299:ILE:HA	1.95	0.42
1:E:300:GLY:N	1:E:301:PRO:HD2	2.35	0.42
1:F:17:GLY:HA2	1:F:22:MET:HE2	2.02	0.42
1:C:105:ARG:HE	1:C:105:ARG:HB3	1.80	0.42
1:D:239:PRO:HA	1:D:251:THR:HG22	2.01	0.42
1:D:302:VAL:HB	1:D:303:PRO:CD	2.50	0.42
1:E:201:LEU:HD12	1:E:201:LEU:HA	1.76	0.42
1:E:244:GLN:H	1:E:244:GLN:HG2	1.58	0.42
1:B:326:GLU:CD	1:B:354:SER:CB	2.89	0.42
1:B:256:SER:HB3	1:B:355:GLY:O	2.20	0.41
1:D:55:LEU:HA	1:D:115:GLY:O	2.19	0.41
1:C:201:LEU:HD12	1:C:201:LEU:HA	1.80	0.41
1:D:45:ILE:HD12	1:D:45:ILE:HA	1.90	0.41
1:D:140:GLN:HA	2:D:551:HOH:O	2.20	0.41
1:E:299:ILE:C	1:E:301:PRO:HD2	2.44	0.41
1:C:59:TYR:N	1:C:60:PRO:CD	2.83	0.41
1:C:259:ASN:OD1	1:C:359:GLY:CA	2.68	0.41
1:D:55:LEU:CD2	1:D:68:GLY:HA2	2.44	0.41
1:E:65:PRO:HB3	1:F:89:ARG:CZ	2.50	0.41
1:B:4:ARG:NH2	1:B:107:GLY:HA2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:HB2	1:B:391:ILE:CG2	2.50	0.41
1:B:287:TRP:O	1:B:311:LYS:CE	2.66	0.41
1:C:352:ARG:HD3	1:C:352:ARG:HA	1.82	0.41
1:B:358:LEU:HD13	1:B:368:ARG:HD2	2.02	0.41
1:C:45:ILE:HD11	1:C:276:LEU:CD1	2.44	0.41
1:D:397:LEU:HD12	1:D:397:LEU:HA	1.86	0.41
1:E:403:ARG:HD2	2:E:521:HOH:O	2.20	0.41
1:F:287:TRP:O	1:F:311:LYS:HE3	2.20	0.41
1:D:343:GLU:O	1:D:346:HIS:HB2	2.21	0.41
1:E:57:HIS:HB3	1:E:85:GLN:HG2	2.02	0.41
1:B:45:ILE:HA	1:B:45:ILE:HD13	1.88	0.41
1:B:300:GLY:N	1:B:301:PRO:HD2	2.36	0.41
1:B:364:ALA:HA	2:B:542:HOH:O	2.21	0.41
1:C:43:THR:HG22	2:C:542:HOH:O	2.20	0.41
1:C:309:LEU:HD11	1:C:316:LEU:HD23	2.02	0.41
1:D:178:ARG:NH2	1:D:239:PRO:HG3	2.36	0.41
1:F:6:ALA:HB2	1:F:105:ARG:HG3	2.03	0.41
1:F:380:ARG:O	1:F:381:GLU:HB2	2.21	0.41
1:A:22:MET:HE3	1:A:219:ILE:HG21	2.02	0.41
1:A:59:TYR:N	1:A:60:PRO:CD	2.84	0.41
1:C:8:ILE:HD12	1:C:267:VAL:HG22	2.03	0.41
1:D:125:PHE:CZ	1:D:143:ASP:HB2	2.56	0.41
1:C:90:CYS:HA	1:C:362:VAL:CG1	2.51	0.40
1:A:184:LEU:CA	1:A:187:ARG:NH1	2.79	0.40
1:F:79:ILE:H	1:F:79:ILE:HG13	1.73	0.40
1:F:307:VAL:O	1:F:311:LYS:HG3	2.21	0.40
1:F:390:CYS:C	1:F:391:ILE:HG13	2.45	0.40
1:C:45:ILE:HD13	1:C:45:ILE:HA	1.69	0.40
1:C:185:ALA:O	1:C:189:HIS:HD2	2.05	0.40
1:D:156:PHE:HA	1:E:275:GLU:O	2.22	0.40
1:E:283:ARG:NH2	1:E:402:GLU:OE1	2.55	0.40
1:F:111:LEU:O	1:F:112:VAL:CG1	2.69	0.40
1:F:161:GLY:N	1:F:165:GLU:OE1	2.53	0.40
1:F:245:ASP:HA	1:F:246:PRO:HD3	1.92	0.40
1:A:299:ILE:O	1:A:303:PRO:HD2	2.21	0.40
1:A:394:GLY:O	1:B:69:ARG:NH2	2.55	0.40
1:F:66:ALA:O	1:F:68:GLY:N	2.54	0.40

There are no symmetry-related clashes.

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	393/413 (95%)	388 (99%)	5 (1%)	0	100	100
1	B	396/413 (96%)	391 (99%)	5 (1%)	0	100	100
1	C	391/413 (95%)	385 (98%)	6 (2%)	0	100	100
1	D	395/413 (96%)	393 (100%)	2 (0%)	0	100	100
1	E	394/413 (95%)	392 (100%)	2 (0%)	0	100	100
1	F	383/413 (93%)	380 (99%)	3 (1%)	0	100	100
All	All	2352/2478 (95%)	2329 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	282/315 (90%)	246 (87%)	36 (13%)	4	3
1	B	302/315 (96%)	266 (88%)	36 (12%)	5	4
1	C	290/315 (92%)	265 (91%)	25 (9%)	10	11
1	D	298/315 (95%)	273 (92%)	25 (8%)	10	12
1	E	296/315 (94%)	265 (90%)	31 (10%)	6	6
1	F	281/315 (89%)	247 (88%)	34 (12%)	5	4
All	All	1749/1890 (92%)	1562 (89%)	187 (11%)	6	6

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	26	LEU
1	A	37	LYS
1	A	45	ILE
1	A	67	ILE
1	A	79	ILE
1	A	103	GLN
1	A	131	ARG
1	A	157	HIS
1	A	171	ARG
1	A	177	SER
1	A	178	ARG
1	A	187	ARG
1	A	198	GLU
1	A	201	LEU
1	A	210	VAL
1	A	226	ARG
1	A	231	VAL
1	A	244	GLN
1	A	251	THR
1	A	256	SER
1	A	311	LYS
1	A	314	LEU
1	A	315	THR
1	A	316	LEU
1	A	325	ASN
1	A	341	PHE
1	A	347	GLU
1	A	348	ARG
1	A	354	SER
1	A	362	VAL
1	A	373	LEU
1	A	377	LEU
1	A	378	HIS
1	A	383	ARG
1	A	404	VAL
1	B	26	LEU
1	B	37	LYS
1	B	41	GLU
1	B	55	LEU
1	B	79	ILE
1	B	155	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	164	LEU
1	B	171	ARG
1	B	175[A]	HIS
1	B	175[B]	HIS
1	B	178	ARG
1	B	197[A]	SER
1	B	197[B]	SER
1	B	201	LEU
1	B	216	GLU
1	B	226	ARG
1	B	229	THR
1	B	234	LEU
1	B	238	LYS
1	B	243	LYS
1	B	244	GLN
1	B	249	THR
1	B	255	SER
1	B	266	ILE
1	B	272	LYS
1	B	279	LYS
1	B	314	LEU
1	B	315	THR
1	B	316	LEU
1	B	337	ARG
1	B	343	GLU
1	B	348	ARG
1	B	352	ARG
1	B	365	THR
1	B	373	LEU
1	B	377	LEU
1	C	4	ARG
1	C	22	MET
1	C	26	LEU
1	C	45	ILE
1	C	55	LEU
1	C	79	ILE
1	C	103	GLN
1	C	105	ARG
1	C	136	ARG
1	C	166	THR
1	C	176	ILE
1	C	178	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	179	THR
1	C	188	SER
1	C	201	LEU
1	C	216	GLU
1	C	217	GLU
1	C	220	SER
1	C	315	THR
1	C	316	LEU
1	C	340	LYS
1	C	347	GLU
1	C	365	THR
1	C	373	LEU
1	C	377	LEU
1	D	22	MET
1	D	26	LEU
1	D	37	LYS
1	D	45	ILE
1	D	55	LEU
1	D	79	ILE
1	D	150	THR
1	D	164	LEU
1	D	180	GLU
1	D	201	LEU
1	D	210	VAL
1	D	217	GLU
1	D	228	ASP
1	D	244	GLN
1	D	256	SER
1	D	279	LYS
1	D	314	LEU
1	D	315	THR
1	D	316	LEU
1	D	351	VAL
1	D	352	ARG
1	D	373	LEU
1	D	377	LEU
1	D	405	GLN
1	D	406	GLU
1	E	37	LYS
1	E	54	ILE
1	E	55	LEU
1	E	79	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	84	MET
1	E	137	THR
1	E	164	LEU
1	E	176	ILE
1	E	178	ARG
1	E	183	GLU
1	E	184	LEU
1	E	201	LEU
1	E	210	VAL
1	E	220	SER
1	E	243	LYS
1	E	244	GLN
1	E	256	SER
1	E	263	SER
1	E	284	LEU
1	E	314	LEU
1	E	315	THR
1	E	316	LEU
1	E	324	LEU
1	E	328	PHE
1	E	347	GLU
1	E	351	VAL
1	E	354	SER
1	E	368	ARG
1	E	373	LEU
1	E	377	LEU
1	E	405	GLN
1	F	4	ARG
1	F	24	ARG
1	F	26	LEU
1	F	33	VAL
1	F	45	ILE
1	F	55	LEU
1	F	90	CYS
1	F	155	LYS
1	F	164	LEU
1	F	166	THR
1	F	171	ARG
1	F	176	ILE
1	F	178	ARG
1	F	183	GLU
1	F	197	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	201	LEU
1	F	229	THR
1	F	234	LEU
1	F	238	LYS
1	F	241	LEU
1	F	247	GLU
1	F	249	THR
1	F	272	LYS
1	F	283	ARG
1	F	299	ILE
1	F	314	LEU
1	F	315	THR
1	F	316	LEU
1	F	324	LEU
1	F	340	LYS
1	F	373	LEU
1	F	377	LEU
1	F	379	ARG
1	F	383	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	157	HIS
1	A	244	GLN
1	A	258	GLN
1	A	325	ASN
1	A	360	HIS
1	A	378	HIS
1	B	378	HIS
1	C	122	ASN
1	C	189	HIS
1	C	346	HIS
1	D	122	ASN
1	D	157	HIS
1	D	181	GLN
1	D	405	GLN
1	F	122	ASN
1	F	142	HIS
1	F	224	HIS
1	F	378	HIS

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](#)

There are no ligands in this entry.

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	399/413 (96%)	0.50	31 (7%) 19 16	17, 37, 69, 89	0
1	B	398/413 (96%)	-0.01	2 (0%) 87 88	16, 31, 52, 75	2 (0%)
1	C	397/413 (96%)	0.34	18 (4%) 38 37	17, 38, 67, 84	0
1	D	398/413 (96%)	0.03	2 (0%) 87 88	16, 32, 51, 74	1 (0%)
1	E	400/413 (96%)	0.43	10 (2%) 58 61	22, 36, 61, 78	0
1	F	393/413 (95%)	0.81	32 (8%) 18 16	24, 43, 68, 84	0
All	All	2385/2478 (96%)	0.35	95 (3%) 42 41	16, 36, 65, 89	3 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	THR	5.4
1	C	135	ALA	5.2
1	F	257	GLY	5.2
1	A	240	VAL	5.1
1	E	344	ALA	4.7
1	A	176	ILE	4.6
1	A	214	ASP	4.6
1	A	242	LEU	4.5
1	A	248	ALA	4.3
1	E	342	GLY	4.2
1	F	216	GLU	4.2
1	A	135	ALA	4.2
1	F	230	THR	4.0
1	C	134	GLY	3.9
1	E	212	THR	3.7
1	A	271	GLU	3.6
1	C	211	ARG	3.6
1	A	164	LEU	3.6
1	A	179	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	244	GLN	3.6
1	C	226	ARG	3.6
1	A	133	GLY	3.6
1	A	237	LEU	3.6
1	B	211	ARG	3.5
1	F	342	GLY	3.4
1	F	184	LEU	3.4
1	C	164	LEU	3.3
1	F	231	VAL	3.3
1	D	135	ALA	3.2
1	F	344	ALA	3.2
1	F	315	THR	3.2
1	A	138	GLY	3.0
1	F	210	VAL	2.9
1	F	158	PRO	2.9
1	A	163	MET	2.9
1	F	249	THR	2.9
1	A	246	PRO	2.9
1	A	313	GLY	2.9
1	A	232	GLU	2.8
1	E	215	GLY	2.8
1	E	201	LEU	2.8
1	C	243	LYS	2.8
1	A	45	ILE	2.7
1	F	328	PHE	2.7
1	A	175	HIS	2.7
1	A	231	VAL	2.6
1	F	203	GLU	2.6
1	A	134	GLY	2.6
1	F	319	ILE	2.6
1	F	176	ILE	2.6
1	C	90	CYS	2.5
1	C	133	GLY	2.5
1	A	215	GLY	2.5
1	F	236	LYS	2.5
1	C	405	GLN	2.5
1	C	174	TYR	2.4
1	F	98	ILE	2.4
1	A	343	GLU	2.4
1	F	232	GLU	2.4
1	F	163	MET	2.4
1	C	163	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	231	VAL	2.4
1	A	239	PRO	2.3
1	E	214	ASP	2.3
1	A	139	VAL	2.3
1	D	406	GLU	2.3
1	E	135	ALA	2.3
1	E	364	ALA	2.3
1	A	159	VAL	2.3
1	C	279	LYS	2.3
1	A	160	PRO	2.3
1	F	246	PRO	2.3
1	C	248	ALA	2.2
1	F	304	ALA	2.2
1	F	251	THR	2.2
1	F	379	ARG	2.2
1	F	370	LEU	2.2
1	C	240	VAL	2.2
1	C	344	ALA	2.2
1	F	233	ALA	2.2
1	F	255	SER	2.2
1	F	181	GLN	2.1
1	A	161	GLY	2.1
1	F	201	LEU	2.1
1	A	168	GLU	2.1
1	C	271	GLU	2.1
1	F	156	PHE	2.1
1	B	136	ARG	2.1
1	C	333	LEU	2.1
1	E	45	ILE	2.1
1	F	384	TYR	2.1
1	E	50	VAL	2.0
1	A	211	ARG	2.0
1	F	335	VAL	2.0
1	F	225	PRO	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.