



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:33 PM UTC

PDB ID : 5YC9 / pdb_00005yc9
Title : Crystal structure of a Pseudomonas aeruginosa transcriptional regulator
Authors : Harikiran, R.; Rohan, S.
Deposited on : 2017-09-07
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
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

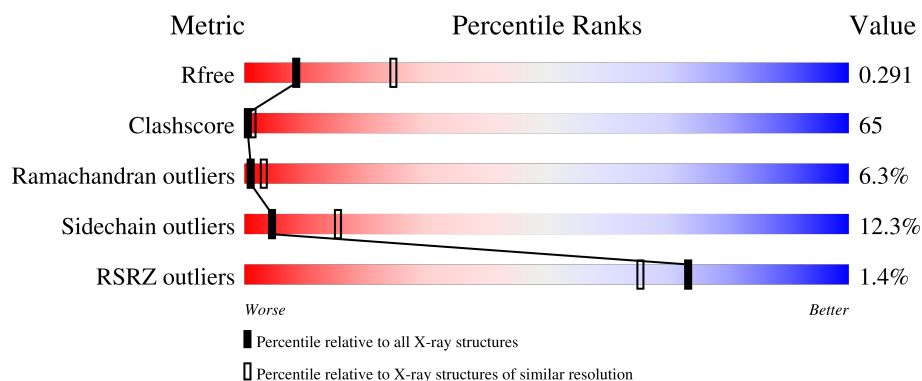
1 Overall quality at a glance

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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	291	
1	B	291	
1	C	291	
1	D	291	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8286 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 C-di-GMP-binding multidrug transporter transcriptional regulator BrIR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			2048	1305	373	366	4			
1	B	254	Total	C	N	O	S	0	0	0
			2095	1340	379	371	5			
1	C	249	Total	C	N	O	S	0	0	0
			2048	1305	373	366	4			
1	D	254	Total	C	N	O	S	0	0	0
			2095	1340	379	371	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A0A069Q416
A	-18	GLY	-	expression tag	UNP A0A069Q416
A	-17	SER	-	expression tag	UNP A0A069Q416
A	-16	SER	-	expression tag	UNP A0A069Q416
A	-15	HIS	-	expression tag	UNP A0A069Q416
A	-14	HIS	-	expression tag	UNP A0A069Q416
A	-13	HIS	-	expression tag	UNP A0A069Q416
A	-12	HIS	-	expression tag	UNP A0A069Q416
A	-11	HIS	-	expression tag	UNP A0A069Q416
A	-10	HIS	-	expression tag	UNP A0A069Q416
A	-9	SER	-	expression tag	UNP A0A069Q416
A	-8	SER	-	expression tag	UNP A0A069Q416
A	-7	GLY	-	expression tag	UNP A0A069Q416
A	-6	LEU	-	expression tag	UNP A0A069Q416
A	-5	VAL	-	expression tag	UNP A0A069Q416
A	-4	PRO	-	expression tag	UNP A0A069Q416
A	-3	ARG	-	expression tag	UNP A0A069Q416
A	-2	GLY	-	expression tag	UNP A0A069Q416
A	-1	SER	-	expression tag	UNP A0A069Q416
A	0	HIS	-	expression tag	UNP A0A069Q416

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	GLY	-	expression tag	UNP A0A069Q416
B	-19	MET	-	expression tag	UNP A0A069Q416
B	-18	GLY	-	expression tag	UNP A0A069Q416
B	-17	SER	-	expression tag	UNP A0A069Q416
B	-16	SER	-	expression tag	UNP A0A069Q416
B	-15	HIS	-	expression tag	UNP A0A069Q416
B	-14	HIS	-	expression tag	UNP A0A069Q416
B	-13	HIS	-	expression tag	UNP A0A069Q416
B	-12	HIS	-	expression tag	UNP A0A069Q416
B	-11	HIS	-	expression tag	UNP A0A069Q416
B	-10	HIS	-	expression tag	UNP A0A069Q416
B	-9	SER	-	expression tag	UNP A0A069Q416
B	-8	SER	-	expression tag	UNP A0A069Q416
B	-7	GLY	-	expression tag	UNP A0A069Q416
B	-6	LEU	-	expression tag	UNP A0A069Q416
B	-5	VAL	-	expression tag	UNP A0A069Q416
B	-4	PRO	-	expression tag	UNP A0A069Q416
B	-3	ARG	-	expression tag	UNP A0A069Q416
B	-2	GLY	-	expression tag	UNP A0A069Q416
B	-1	SER	-	expression tag	UNP A0A069Q416
B	0	HIS	-	expression tag	UNP A0A069Q416
B	271	GLY	-	expression tag	UNP A0A069Q416
C	-19	MET	-	expression tag	UNP A0A069Q416
C	-18	GLY	-	expression tag	UNP A0A069Q416
C	-17	SER	-	expression tag	UNP A0A069Q416
C	-16	SER	-	expression tag	UNP A0A069Q416
C	-15	HIS	-	expression tag	UNP A0A069Q416
C	-14	HIS	-	expression tag	UNP A0A069Q416
C	-13	HIS	-	expression tag	UNP A0A069Q416
C	-12	HIS	-	expression tag	UNP A0A069Q416
C	-11	HIS	-	expression tag	UNP A0A069Q416
C	-10	HIS	-	expression tag	UNP A0A069Q416
C	-9	SER	-	expression tag	UNP A0A069Q416
C	-8	SER	-	expression tag	UNP A0A069Q416
C	-7	GLY	-	expression tag	UNP A0A069Q416
C	-6	LEU	-	expression tag	UNP A0A069Q416
C	-5	VAL	-	expression tag	UNP A0A069Q416
C	-4	PRO	-	expression tag	UNP A0A069Q416
C	-3	ARG	-	expression tag	UNP A0A069Q416
C	-2	GLY	-	expression tag	UNP A0A069Q416
C	-1	SER	-	expression tag	UNP A0A069Q416
C	0	HIS	-	expression tag	UNP A0A069Q416

Continued on next page...

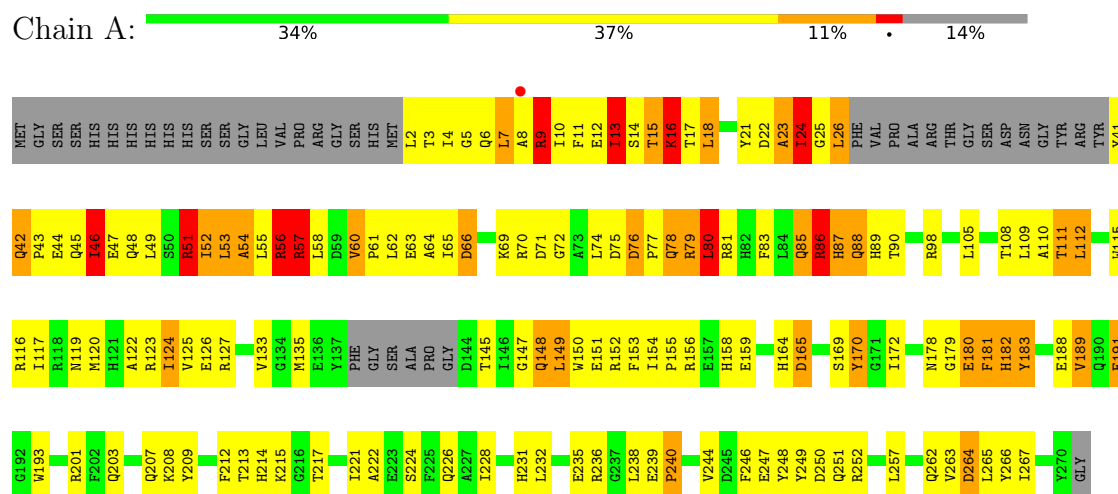
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	271	GLY	-	expression tag	UNP A0A069Q416
D	-19	MET	-	expression tag	UNP A0A069Q416
D	-18	GLY	-	expression tag	UNP A0A069Q416
D	-17	SER	-	expression tag	UNP A0A069Q416
D	-16	SER	-	expression tag	UNP A0A069Q416
D	-15	HIS	-	expression tag	UNP A0A069Q416
D	-14	HIS	-	expression tag	UNP A0A069Q416
D	-13	HIS	-	expression tag	UNP A0A069Q416
D	-12	HIS	-	expression tag	UNP A0A069Q416
D	-11	HIS	-	expression tag	UNP A0A069Q416
D	-10	HIS	-	expression tag	UNP A0A069Q416
D	-9	SER	-	expression tag	UNP A0A069Q416
D	-8	SER	-	expression tag	UNP A0A069Q416
D	-7	GLY	-	expression tag	UNP A0A069Q416
D	-6	LEU	-	expression tag	UNP A0A069Q416
D	-5	VAL	-	expression tag	UNP A0A069Q416
D	-4	PRO	-	expression tag	UNP A0A069Q416
D	-3	ARG	-	expression tag	UNP A0A069Q416
D	-2	GLY	-	expression tag	UNP A0A069Q416
D	-1	SER	-	expression tag	UNP A0A069Q416
D	0	HIS	-	expression tag	UNP A0A069Q416
D	271	GLY	-	expression tag	UNP A0A069Q416

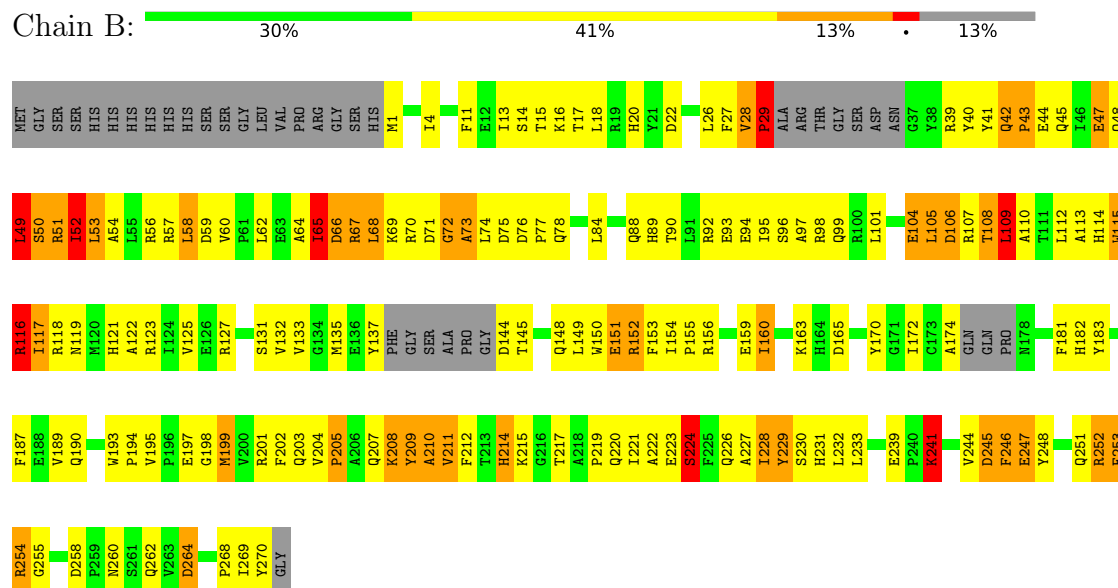
3 Residue-property plots

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.

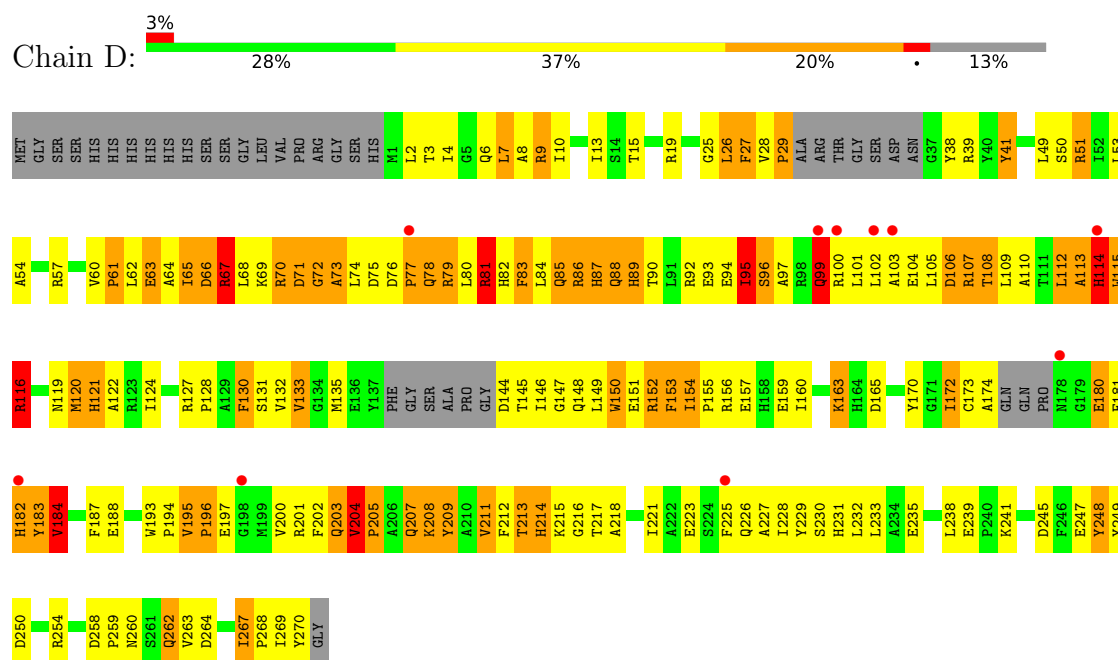
- Molecule 1: C-di-GMP-binding multidrug transporter transcriptional regulator BrlR



- Molecule 1: C-di-GMP-binding multidrug transporter transcriptional regulator BrlR



- Molecule 1: C-di-GMP-binding multidrug transporter transcriptional regulator BrlR



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	111.64Å 111.64Å 261.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.32 – 2.90 34.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	74.8 (34.32-2.90) 86.0 (34.32-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.90Å)	Xtriage
Refinement program	PHENIX (dev_2875)	Depositor
R, R_{free}	0.268 , 0.307 0.258 , 0.291	Depositor DCC
R_{free} test set	1987 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.427 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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	1.23	27/2099 (1.3%)	1.12	16/2842 (0.6%)
1	B	1.40	26/2148 (1.2%)	1.25	35/2906 (1.2%)
1	C	1.83	59/2099 (2.8%)	1.37	34/2842 (1.2%)
1	D	1.48	20/2148 (0.9%)	1.34	33/2906 (1.1%)
All	All	1.50	132/8494 (1.6%)	1.27	118/11496 (1.0%)

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	TRP	CA-C	-13.49	1.43	1.52
1	A	124	ILE	C-O	-9.13	1.14	1.24
1	C	207	GLN	CA-C	-8.81	1.41	1.52
1	C	241	LYS	C-O	-8.62	1.13	1.24
1	C	207	GLN	C-O	-8.19	1.13	1.23
1	B	204	VAL	CA-C	-8.00	1.46	1.53
1	C	249	TYR	C-O	-7.97	1.14	1.24
1	B	244	VAL	C-O	-7.93	1.15	1.24
1	A	125	VAL	C-O	-7.89	1.15	1.24
1	C	228	ILE	C-O	-7.77	1.15	1.24
1	D	60	VAL	N-CA	-7.63	1.40	1.46
1	C	124	ILE	C-O	-7.59	1.15	1.24
1	D	195	VAL	CA-C	-7.45	1.46	1.52
1	A	239	GLU	CA-C	-7.41	1.42	1.52
1	C	250	ASP	CA-C	-7.41	1.46	1.53
1	C	247	GLU	C-O	-7.27	1.15	1.24
1	C	239	GLU	CA-C	-7.12	1.44	1.52
1	C	208	LYS	CA-C	-7.07	1.44	1.52
1	A	191	GLU	CA-C	-6.97	1.44	1.52
1	B	49	LEU	C-O	-6.89	1.15	1.23
1	C	184	VAL	C-O	-6.85	1.17	1.24
1	D	89	HIS	CA-C	-6.81	1.44	1.53
1	C	231	HIS	C-O	-6.74	1.16	1.24
1	D	264	ASP	C-O	-6.71	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	76	ASP	C-N	-6.70	1.28	1.33
1	C	168	VAL	C-O	-6.67	1.16	1.24
1	C	122	ALA	C-O	-6.66	1.15	1.23
1	C	172	ILE	C-O	-6.65	1.15	1.24
1	B	211	VAL	C-O	-6.62	1.16	1.24
1	B	204	VAL	C-O	-6.61	1.16	1.24
1	A	189	VAL	C-O	-6.59	1.16	1.23
1	D	60	VAL	CA-C	-6.58	1.47	1.53
1	C	267	ILE	C-O	-6.54	1.16	1.24
1	A	170	TYR	C-O	-6.53	1.15	1.23
1	C	263	VAL	C-O	-6.52	1.17	1.24
1	C	170	TYR	C-O	-6.47	1.16	1.23
1	C	208	LYS	C-O	-6.45	1.15	1.24
1	C	213	THR	C-O	-6.43	1.16	1.24
1	D	165	ASP	CA-C	-6.39	1.46	1.53
1	A	165	ASP	CA-C	-6.34	1.47	1.52
1	A	266	TYR	C-O	-6.32	1.16	1.24
1	C	135	MET	C-O	-6.29	1.15	1.23
1	D	112	LEU	CA-C	-6.28	1.45	1.52
1	C	104	GLU	CA-C	-6.25	1.45	1.52
1	C	240	PRO	C-O	-6.25	1.15	1.24
1	B	47	GLU	C-O	-6.25	1.16	1.24
1	D	249	TYR	C-O	-6.22	1.16	1.23
1	C	104	GLU	C-O	-6.21	1.17	1.24
1	C	204	VAL	CA-C	-6.19	1.46	1.52
1	D	61	PRO	C-O	-6.15	1.16	1.23
1	C	266	TYR	C-O	-6.13	1.16	1.24
1	C	203	GLN	C-O	-6.11	1.16	1.24
1	B	76	ASP	CA-C	-6.10	1.45	1.52
1	D	83	PHE	C-O	-6.10	1.16	1.24
1	B	49	LEU	CA-C	-6.06	1.46	1.53
1	C	110	ALA	CA-C	-6.06	1.45	1.53
1	A	169	SER	C-O	-6.03	1.16	1.23
1	C	237	GLY	C-O	-5.96	1.15	1.23
1	C	209	TYR	C-O	-5.96	1.16	1.23
1	A	193	TRP	CA-C	-5.94	1.45	1.52
1	C	216	GLY	CA-C	-5.94	1.44	1.52
1	C	107	ARG	CA-C	-5.91	1.44	1.52
1	C	123	ARG	C-O	-5.90	1.16	1.23
1	B	76	ASP	C-N	5.85	1.38	1.33
1	C	123	ARG	CA-C	-5.85	1.45	1.52
1	C	245	ASP	C-O	-5.85	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	ALA	CA-C	-5.79	1.45	1.52
1	B	43	PRO	C-O	-5.78	1.16	1.24
1	A	239	GLU	C-O	-5.77	1.16	1.24
1	C	171	GLY	C-O	-5.77	1.16	1.23
1	B	47	GLU	CA-C	-5.76	1.44	1.52
1	C	193	TRP	C-O	-5.74	1.17	1.24
1	D	76	ASP	CA-C	-5.68	1.45	1.52
1	C	250	ASP	C-O	-5.66	1.18	1.24
1	D	82	HIS	N-CA	-5.65	1.39	1.46
1	A	189	VAL	CA-C	-5.63	1.46	1.52
1	C	235	GLU	CA-C	-5.62	1.44	1.52
1	D	247	GLU	C-O	-5.61	1.17	1.23
1	C	240	PRO	CA-C	-5.60	1.44	1.52
1	A	183	TYR	C-O	-5.59	1.16	1.23
1	A	240	PRO	C-O	-5.59	1.17	1.23
1	D	82	HIS	CA-C	-5.58	1.46	1.52
1	B	241	LYS	CA-C	-5.58	1.46	1.52
1	A	238	LEU	C-O	-5.58	1.17	1.23
1	D	41	TYR	CA-C	-5.58	1.45	1.52
1	B	205	PRO	CA-C	-5.56	1.46	1.53
1	B	258	ASP	CA-C	-5.55	1.46	1.53
1	C	260	ASN	CA-C	-5.54	1.45	1.52
1	A	42	GLN	CA-C	-5.51	1.45	1.52
1	C	101	LEU	C-O	-5.51	1.17	1.24
1	D	87	HIS	C-O	-5.50	1.17	1.24
1	A	123	ARG	CA-C	-5.48	1.45	1.52
1	A	213	THR	C-O	-5.46	1.17	1.24
1	A	264	ASP	C-O	-5.43	1.17	1.24
1	A	149	LEU	CA-C	-5.42	1.45	1.52
1	A	123	ARG	C-O	-5.38	1.17	1.23
1	A	170	TYR	CE1-CZ	-5.34	1.25	1.38
1	A	265	LEU	C-O	-5.33	1.17	1.24
1	C	56	ARG	CA-C	-5.33	1.47	1.53
1	C	249	TYR	CA-C	-5.33	1.46	1.52
1	C	248	TYR	C-O	-5.31	1.17	1.24
1	C	107	ARG	C-O	-5.30	1.17	1.24
1	C	265	LEU	C-O	-5.30	1.17	1.24
1	C	235	GLU	C-O	-5.29	1.17	1.24
1	C	205	PRO	C-O	-5.28	1.17	1.24
1	C	165	ASP	C-O	-5.27	1.20	1.25
1	C	246	PHE	C-O	-5.25	1.17	1.23
1	A	123	ARG	N-CA	-5.23	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	SER	C-O	-5.21	1.17	1.23
1	B	246	PHE	C-O	-5.19	1.17	1.23
1	A	170	TYR	CA-C	-5.19	1.46	1.52
1	C	234	ALA	CA-C	-5.18	1.45	1.52
1	B	210	ALA	C-O	-5.18	1.18	1.24
1	B	214	HIS	C-O	-5.18	1.17	1.23
1	C	106	ASP	CA-C	-5.15	1.46	1.52
1	B	254	ARG	C-O	-5.14	1.16	1.23
1	D	8	ALA	C-O	-5.13	1.17	1.24
1	B	208	LYS	CA-C	-5.13	1.46	1.52
1	A	80	LEU	C-O	-5.12	1.17	1.24
1	B	76	ASP	C-O	-5.11	1.17	1.24
1	C	205	PRO	CA-CB	-5.11	1.46	1.53
1	B	104	GLU	C-O	-5.10	1.17	1.24
1	B	247	GLU	C-O	-5.09	1.17	1.23
1	C	122	ALA	CA-C	-5.08	1.45	1.53
1	A	191	GLU	C-O	-5.08	1.17	1.24
1	B	115	TRP	N-CA	-5.08	1.41	1.46
1	B	262	GLN	C-O	-5.07	1.18	1.23
1	D	80	LEU	C-O	-5.04	1.17	1.24
1	C	204	VAL	C-O	-5.03	1.18	1.24
1	D	89	HIS	C-O	-5.03	1.18	1.24
1	B	264	ASP	C-O	-5.01	1.17	1.23
1	C	87	HIS	C-O	-5.01	1.17	1.24

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	LEU	N-CA-C	11.35	126.29	109.95
1	A	86	ARG	N-CA-C	-11.21	99.03	111.14
1	D	72	GLY	N-CA-C	-10.94	87.25	113.18
1	B	72	GLY	N-CA-C	-9.82	89.90	113.18
1	B	76	ASP	N-CA-C	-9.77	88.22	109.81
1	A	12	GLU	N-CA-C	-9.66	93.16	108.90
1	A	66	ASP	N-CA-C	-9.48	100.32	112.93
1	C	157	GLU	N-CA-C	9.31	121.43	111.28
1	C	159	GLU	N-CA-C	-9.21	101.19	111.14
1	B	71	ASP	N-CA-C	-9.17	100.48	112.68
1	C	91	LEU	N-CA-C	-9.02	91.58	110.80
1	D	82	HIS	N-CA-C	-9.01	99.61	111.24
1	C	60	VAL	C-N-CD	-8.60	89.75	125.00
1	B	114	HIS	CA-C-N	-8.58	112.23	122.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	HIS	C-N-CA	-8.58	112.23	122.44
1	B	49	LEU	N-CA-C	-8.36	100.18	111.96
1	B	258	ASP	N-CA-C	-8.24	99.71	109.93
1	C	5	GLY	N-CA-C	-8.17	93.81	113.18
1	D	116	ARG	N-CA-C	-8.16	100.29	112.04
1	C	57	ARG	N-CA-C	-7.93	93.90	110.80
1	C	251	GLN	CA-C-N	-7.87	106.50	121.54
1	C	251	GLN	C-N-CA	-7.87	106.50	121.54
1	C	93	GLU	N-CA-C	-7.86	102.03	111.69
1	C	250	ASP	N-CA-C	-7.86	94.11	108.65
1	B	151	GLU	N-CA-C	-7.83	103.68	113.55
1	C	55	LEU	N-CA-C	-7.83	103.33	113.12
1	C	82	HIS	N-CA-C	-7.79	102.87	111.36
1	B	205	PRO	N-CA-C	7.76	122.90	110.40
1	C	208	LYS	N-CA-C	-7.74	96.78	109.40
1	D	95	ILE	N-CA-C	-7.64	103.34	110.53
1	D	211	VAL	N-CA-C	7.45	118.61	107.51
1	A	189	VAL	CB-CA-C	-7.17	99.65	110.55
1	C	168	VAL	N-CA-C	6.95	118.13	107.99
1	B	58	LEU	N-CA-C	-6.93	102.12	110.44
1	C	123	ARG	N-CA-C	-6.92	98.56	109.50
1	C	56	ARG	N-CA-C	-6.88	100.04	110.70
1	D	81	ARG	N-CA-C	-6.85	104.92	113.28
1	D	60	VAL	CA-C-O	6.67	123.08	119.15
1	B	223	GLU	N-CA-C	-6.64	105.47	113.97
1	A	76	ASP	O-C-N	6.61	124.57	121.53
1	B	115	TRP	N-CA-C	-6.61	100.98	111.02
1	D	152	ARG	N-CA-C	-6.55	104.06	111.07
1	B	209	TYR	N-CA-C	6.55	119.67	109.52
1	B	67	ARG	N-CA-C	-6.52	105.62	113.97
1	B	65	ILE	N-CA-C	-6.45	95.93	109.34
1	D	76	ASP	C-N-CD	-6.35	98.97	125.00
1	D	51	ARG	N-CA-C	-6.27	106.22	114.31
1	A	85	GLN	N-CA-C	-6.22	105.47	114.12
1	D	207	GLN	N-CA-C	6.21	117.31	108.74
1	B	193	TRP	N-CA-C	-6.18	99.43	109.82
1	D	63	GLU	N-CA-C	-6.14	107.01	114.75
1	B	109	LEU	N-CA-C	-6.08	104.66	114.09
1	B	190	GLN	N-CA-C	-6.04	99.39	109.24
1	D	76	ASP	N-CA-C	-6.04	96.47	109.81
1	C	196	PRO	N-CA-C	6.00	124.83	112.47
1	A	111	THR	N-CA-C	-5.98	106.07	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	ARG	N-CA-C	-5.97	105.48	112.89
1	C	99	GLN	N-CA-C	-5.97	104.16	112.45
1	D	209	TYR	N-CA-C	5.95	119.26	109.85
1	B	255	GLY	CA-C-N	5.92	126.03	119.87
1	B	255	GLY	C-N-CA	5.92	126.03	119.87
1	C	251	GLN	CB-CA-C	-5.92	98.65	110.42
1	D	127	ARG	CA-C-N	-5.89	114.69	120.52
1	D	127	ARG	C-N-CA	-5.89	114.69	120.52
1	C	216	GLY	N-CA-C	-5.88	102.85	110.38
1	B	116	ARG	CB-CA-C	5.87	120.00	110.96
1	D	77	PRO	N-CA-C	5.83	120.74	114.68
1	B	51	ARG	N-CA-C	-5.81	104.82	112.72
1	D	29	PRO	CA-N-CD	-5.74	103.97	112.00
1	B	52	ILE	N-CA-C	-5.72	97.45	109.34
1	C	106	ASP	N-CA-C	-5.69	104.71	111.03
1	D	248	TYR	N-CA-C	5.67	117.77	108.52
1	B	194	PRO	CA-N-CD	-5.63	104.11	112.00
1	D	184	VAL	CB-CA-C	-5.63	102.05	111.29
1	D	205	PRO	N-CA-C	5.62	119.45	110.40
1	B	204	VAL	CA-C-N	-5.60	114.99	120.98
1	B	204	VAL	C-N-CA	-5.60	114.99	120.98
1	B	165	ASP	CA-C-N	-5.47	114.61	120.47
1	B	165	ASP	C-N-CA	-5.47	114.61	120.47
1	C	196	PRO	CA-N-CD	-5.46	104.35	112.00
1	B	77	PRO	CA-N-CD	-5.45	104.37	112.00
1	B	78	GLN	N-CA-C	-5.45	106.68	113.38
1	C	195	VAL	N-CA-C	5.41	120.56	108.88
1	A	239	GLU	CA-C-N	-5.40	115.02	120.31
1	A	239	GLU	C-N-CA	-5.40	115.02	120.31
1	C	190	GLN	N-CA-C	-5.37	101.96	109.96
1	D	204	VAL	CA-C-N	-5.36	115.25	120.98
1	D	204	VAL	C-N-CA	-5.36	115.25	120.98
1	C	184	VAL	N-CA-C	5.35	116.44	108.46
1	C	177	PRO	CA-N-CD	-5.34	104.52	112.00
1	C	167	GLU	N-CA-C	5.32	119.03	112.54
1	C	89	HIS	N-CA-C	-5.31	105.18	110.97
1	D	195	VAL	N-CA-C	-5.31	101.79	108.05
1	B	29	PRO	CA-N-CD	-5.30	104.58	112.00
1	A	193	TRP	CA-C-N	-5.29	114.47	119.76
1	A	193	TRP	C-N-CA	-5.29	114.47	119.76
1	A	51	ARG	N-CA-C	-5.29	105.43	111.14
1	C	184	VAL	CA-C-N	-5.25	115.37	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	VAL	C-N-CA	-5.25	115.37	123.14
1	D	89	HIS	N-CA-C	-5.25	103.53	111.56
1	B	224	SER	N-CA-C	-5.24	105.62	112.23
1	B	13	ILE	N-CA-C	5.18	115.14	108.82
1	C	7	LEU	N-CA-C	-5.18	106.23	113.37
1	B	68	LEU	N-CA-C	-5.16	105.35	111.69
1	A	56	ARG	N-CA-C	-5.15	99.83	110.80
1	B	57	ARG	N-CA-C	-5.13	107.08	113.19
1	D	165	ASP	N-CA-C	-5.13	92.18	107.37
1	D	121	HIS	N-CA-CB	5.11	119.37	111.24
1	D	99	GLN	N-CA-C	5.09	118.27	111.75
1	C	157	GLU	CA-C-N	-5.09	114.58	122.67
1	C	157	GLU	C-N-CA	-5.09	114.58	122.67
1	D	108	THR	N-CA-C	-5.08	106.77	113.17
1	A	45	GLN	N-CA-C	-5.05	104.54	111.81
1	C	171	GLY	N-CA-C	-5.05	101.22	113.18
1	D	78	GLN	CB-CA-C	5.04	116.99	109.13
1	D	128	PRO	N-CA-C	5.03	118.63	111.13
1	A	60	VAL	CA-C-N	-5.02	114.49	120.11
1	A	60	VAL	C-N-CA	-5.02	114.49	120.11

There are no chirality outliers.

There are no planarity outliers.

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	2048	0	2011	280	5
1	B	2095	0	2057	260	5
1	C	2048	0	2009	244	2
1	D	2095	0	2058	363	2
All	All	8286	0	8135	1074	7

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 65.

All (1074) 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:C:4:ILE:HD11	1:C:41:TYR:CZ	1.33	1.62
1:D:27:PHE:HE2	1:D:49:LEU:CD2	1.14	1.55
1:D:29:PRO:HG2	1:D:41:TYR:CE1	1.03	1.55
1:A:60:VAL:CG1	1:A:65:ILE:HD11	1.42	1.50
1:D:27:PHE:CD2	1:D:49:LEU:HD11	1.44	1.49
1:B:214:HIS:CE1	1:B:221:ILE:HG22	1.44	1.48
1:D:27:PHE:CE2	1:D:49:LEU:CD1	1.96	1.48
1:D:27:PHE:CE2	1:D:49:LEU:HD11	1.48	1.48
1:D:51:ARG:HH22	1:D:75:ASP:CG	1.23	1.46
1:D:64:ALA:O	1:D:67:ARG:CD	1.64	1.45
1:D:27:PHE:CE2	1:D:49:LEU:CD2	2.00	1.44
1:D:29:PRO:CG	1:D:41:TYR:CE1	1.99	1.43
1:D:51:ARG:NH2	1:D:75:ASP:CG	1.72	1.43
1:C:4:ILE:CD1	1:C:41:TYR:CE1	2.01	1.42
1:D:88:GLN:HE21	1:D:92:ARG:NH1	1.13	1.41
1:A:51:ARG:NH1	1:A:80:LEU:CD1	1.82	1.40
1:D:3:THR:CG2	1:D:6:GLN:HG2	1.51	1.39
1:D:27:PHE:CE2	1:D:49:LEU:HD21	1.55	1.39
1:C:4:ILE:HD12	1:C:41:TYR:CE1	1.59	1.36
1:B:254:ARG:NH2	1:B:260:ASN:O	1.59	1.33
1:A:17:THR:O	1:A:21:TYR:CD1	1.81	1.33
1:B:135:MET:HE1	1:B:152:ARG:O	1.16	1.32
1:D:88:GLN:NE2	1:D:92:ARG:NH1	1.78	1.32
1:D:108:THR:O	1:D:112:LEU:HD23	1.24	1.32
1:D:51:ARG:CZ	1:D:75:ASP:OD2	1.76	1.31
1:C:4:ILE:HD11	1:C:41:TYR:OH	1.15	1.30
1:A:51:ARG:NH1	1:A:80:LEU:HD12	1.39	1.30
1:C:133:VAL:CG2	1:C:200:VAL:O	1.80	1.28
1:D:3:THR:CG2	1:D:6:GLN:CG	2.13	1.27
1:D:104:GLU:OE1	1:D:105:LEU:CD1	1.82	1.25
1:D:64:ALA:O	1:D:67:ARG:NE	1.68	1.22
1:C:4:ILE:CD1	1:C:41:TYR:OH	1.88	1.21
1:C:4:ILE:CD1	1:C:41:TYR:CZ	2.16	1.21
1:A:52:ILE:O	1:A:54:ALA:N	1.73	1.21
1:B:104:GLU:OE2	1:B:107:ARG:CZ	1.90	1.20
1:A:214:HIS:CD2	1:A:221:ILE:HG12	1.76	1.19
1:B:214:HIS:ND1	1:B:221:ILE:HG22	1.53	1.19
1:D:104:GLU:OE1	1:D:105:LEU:HD13	1.40	1.19
1:A:47:GLU:O	1:A:51:ARG:CG	1.92	1.18
1:D:25:GLY:O	1:D:69:LYS:NZ	1.77	1.17
1:D:133:VAL:CG2	1:D:201:ARG:HA	1.73	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ALA:O	1:D:67:ARG:HD2	1.35	1.17
1:A:51:ARG:HH12	1:A:80:LEU:CD1	1.49	1.16
1:A:61:PRO:O	1:A:65:ILE:HD13	1.41	1.16
1:B:48:GLN:NE2	1:B:75:ASP:OD1	1.78	1.16
1:D:72:GLY:HA3	1:D:73:ALA:HB2	1.18	1.16
1:D:133:VAL:HG23	1:D:201:ARG:CA	1.69	1.16
1:C:196:PRO:CB	1:C:199:MET:HE2	1.76	1.16
1:D:3:THR:HG23	1:D:6:GLN:HG2	1.17	1.15
1:A:60:VAL:CG1	1:A:65:ILE:CD1	2.24	1.15
1:C:53:LEU:O	1:C:57:ARG:NH2	1.79	1.15
1:D:153:PHE:O	1:D:155:PRO:N	1.78	1.14
1:A:47:GLU:O	1:A:51:ARG:HG2	1.46	1.14
1:C:90:THR:O	1:C:91:LEU:O	1.64	1.14
1:B:228:ILE:HA	1:B:232:LEU:HB2	1.25	1.13
1:C:134:GLY:O	1:C:199:MET:CB	1.96	1.13
1:A:60:VAL:HG12	1:A:65:ILE:CD1	1.77	1.13
1:C:4:ILE:HD11	1:C:41:TYR:CE1	1.73	1.12
1:D:104:GLU:CD	1:D:105:LEU:HD12	1.74	1.12
1:D:29:PRO:HG2	1:D:41:TYR:CD1	1.83	1.12
1:D:108:THR:O	1:D:112:LEU:CD2	1.96	1.12
1:A:60:VAL:HG11	1:A:65:ILE:HD11	1.21	1.12
1:C:163:LYS:HA	1:C:189:VAL:HG13	1.13	1.11
1:D:160:ILE:O	1:D:163:LYS:NZ	1.82	1.11
1:D:172:ILE:CD1	1:D:202:PHE:CE1	2.33	1.11
1:C:196:PRO:HB2	1:C:199:MET:HE2	1.14	1.11
1:B:135:MET:CE	1:B:152:ARG:O	1.99	1.10
1:C:133:VAL:HG22	1:C:200:VAL:O	1.52	1.10
1:B:214:HIS:CE1	1:B:221:ILE:CG2	2.33	1.10
1:D:29:PRO:HG2	1:D:41:TYR:CZ	1.85	1.10
1:D:3:THR:HG22	1:D:6:GLN:HE21	1.05	1.10
1:C:133:VAL:HG23	1:C:200:VAL:C	1.77	1.10
1:D:172:ILE:HD11	1:D:202:PHE:CE1	1.86	1.09
1:C:163:LYS:CA	1:C:189:VAL:HG13	1.81	1.09
1:A:17:THR:O	1:A:21:TYR:CE1	2.03	1.09
1:A:54:ALA:HB1	1:A:57:ARG:HD3	1.32	1.09
1:C:133:VAL:HG23	1:C:200:VAL:O	1.43	1.09
1:A:85:GLN:OE1	1:A:88:GLN:CG	2.01	1.08
1:D:27:PHE:CE2	1:D:49:LEU:CG	2.36	1.08
1:B:116:ARG:O	1:B:119:ASN:N	1.87	1.07
1:D:153:PHE:O	1:D:155:PRO:CD	2.01	1.07
1:D:172:ILE:HD11	1:D:202:PHE:HE1	1.09	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:O	1:B:112:LEU:HD21	1.56	1.06
1:C:133:VAL:HG23	1:C:201:ARG:HA	1.36	1.06
1:D:3:THR:HG22	1:D:6:GLN:NE2	1.68	1.06
1:B:116:ARG:NH1	1:B:117:ILE:N	2.04	1.05
1:A:85:GLN:OE1	1:A:88:GLN:CD	1.99	1.05
1:C:9:ARG:HG3	1:C:10:ILE:N	1.62	1.05
1:A:51:ARG:HH11	1:A:80:LEU:HD12	0.95	1.05
1:A:60:VAL:HG12	1:A:65:ILE:HD11	1.33	1.05
1:B:116:ARG:O	1:B:118:ARG:N	1.88	1.05
1:C:251:GLN:OE1	1:C:251:GLN:N	1.88	1.05
1:A:51:ARG:HH12	1:A:80:LEU:HD13	1.22	1.04
1:A:115:TRP:CE2	1:D:77:PRO:HG3	1.93	1.04
1:D:172:ILE:HD13	1:D:202:PHE:CD1	1.92	1.03
1:D:4:ILE:HD12	1:D:4:ILE:H	1.23	1.03
1:D:92:ARG:O	1:D:96:SER:OG	1.75	1.03
1:C:133:VAL:HG23	1:C:201:ARG:CA	1.88	1.03
1:B:11:PHE:CE2	1:B:49:LEU:HD13	1.93	1.02
1:D:27:PHE:HE2	1:D:49:LEU:CG	1.71	1.02
1:D:122:ALA:HB2	1:D:212:PHE:CE1	1.94	1.02
1:D:214:HIS:CE1	1:D:216:GLY:HA3	1.94	1.02
1:C:133:VAL:CG2	1:C:200:VAL:C	2.33	1.01
1:A:55:LEU:O	1:A:58:LEU:N	1.93	1.01
1:D:65:ILE:O	1:D:68:LEU:N	1.92	1.01
1:B:116:ARG:HH12	1:B:117:ILE:HA	1.22	1.00
1:D:131:SER:OG	1:D:203:GLN:OE1	1.77	1.00
1:B:48:GLN:HE22	1:B:75:ASP:CG	1.70	1.00
1:C:90:THR:C	1:C:91:LEU:O	1.89	0.99
1:D:214:HIS:HE1	1:D:216:GLY:HA3	1.23	0.99
1:B:72:GLY:HA3	1:B:73:ALA:HB2	1.45	0.98
1:D:27:PHE:HE2	1:D:49:LEU:HD22	1.24	0.98
1:A:115:TRP:CD2	1:D:77:PRO:HG3	1.97	0.98
1:C:9:ARG:HG3	1:C:10:ILE:H	1.18	0.98
1:B:116:ARG:HH12	1:B:117:ILE:CA	1.77	0.98
1:A:115:TRP:CH2	1:D:77:PRO:HD3	1.99	0.97
1:A:13:ILE:HD13	1:A:13:ILE:H	1.28	0.97
1:C:53:LEU:HD13	1:C:57:ARG:HH21	1.25	0.97
1:A:41:TYR:OH	1:B:239:GLU:OE2	1.81	0.97
1:D:72:GLY:CA	1:D:73:ALA:HB2	1.93	0.97
1:D:122:ALA:HB2	1:D:212:PHE:HE1	1.24	0.97
1:A:46:ILE:HG23	1:A:47:GLU:N	1.80	0.96
1:B:29:PRO:HB3	1:B:41:TYR:CE1	2.00	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:O	1:B:152:ARG:NH2	1.98	0.96
1:D:27:PHE:CD2	1:D:49:LEU:CD1	2.32	0.96
1:C:134:GLY:O	1:C:199:MET:HB3	1.63	0.96
1:A:58:LEU:HD12	1:A:60:VAL:HG22	1.45	0.95
1:C:61:PRO:C	1:C:62:LEU:HD12	1.91	0.95
1:A:86:ARG:O	1:A:89:HIS:HB3	1.66	0.95
1:D:3:THR:HG23	1:D:6:GLN:CG	1.88	0.95
1:B:115:TRP:O	1:B:118:ARG:HG2	1.67	0.94
1:A:214:HIS:HD2	1:A:221:ILE:HG12	1.22	0.94
1:A:42:GLN:HG3	1:A:43:PRO:HD2	1.46	0.94
1:A:46:ILE:HG23	1:A:47:GLU:H	1.32	0.94
1:C:4:ILE:HD12	1:C:41:TYR:HE1	0.79	0.94
1:C:197:GLU:N	1:C:197:GLU:OE1	2.00	0.94
1:C:95:ILE:HG22	1:C:99:GLN:NE2	1.83	0.94
1:C:163:LYS:HA	1:C:189:VAL:CG1	1.98	0.94
1:C:4:ILE:CD1	1:C:41:TYR:HE1	1.57	0.93
1:D:72:GLY:HA3	1:D:73:ALA:CB	1.98	0.93
1:D:104:GLU:OE1	1:D:105:LEU:HD12	1.64	0.93
1:A:47:GLU:O	1:A:51:ARG:HG3	1.67	0.93
1:A:48:GLN:O	1:A:52:ILE:HG13	1.68	0.93
1:A:58:LEU:HD12	1:A:60:VAL:CG2	1.97	0.93
1:C:91:LEU:O	1:C:93:GLU:N	2.00	0.93
1:D:3:THR:HG21	1:D:6:GLN:HG2	1.50	0.92
1:D:29:PRO:CG	1:D:41:TYR:CD1	2.48	0.92
1:C:196:PRO:HG2	1:C:199:MET:CE	1.99	0.92
1:D:65:ILE:O	1:D:67:ARG:N	2.03	0.92
1:D:104:GLU:CD	1:D:105:LEU:CD1	2.37	0.92
1:D:149:LEU:HA	1:D:152:ARG:CD	2.00	0.92
1:B:48:GLN:NE2	1:B:75:ASP:CG	2.28	0.92
1:D:88:GLN:NE2	1:D:92:ARG:HH12	1.66	0.92
1:D:3:THR:CG2	1:D:6:GLN:HE21	1.81	0.92
1:A:87:HIS:O	1:A:90:THR:N	2.03	0.92
1:C:87:HIS:HE1	1:C:91:LEU:HD11	1.34	0.91
1:A:215:LYS:CE	1:A:262:GLN:OE1	2.19	0.91
1:B:112:LEU:HD23	1:B:112:LEU:H	1.36	0.91
1:D:106:ASP:HA	1:D:109:LEU:CD2	2.00	0.91
1:B:49:LEU:HD22	1:B:53:LEU:CD2	2.00	0.91
1:C:214:HIS:O	1:C:262:GLN:HA	1.71	0.91
1:D:104:GLU:OE2	1:D:105:LEU:HD12	1.68	0.91
1:C:87:HIS:CE1	1:C:91:LEU:HD11	2.05	0.91
1:D:3:THR:HG22	1:D:6:GLN:CG	1.99	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LEU:HA	1:B:152:ARG:HD3	1.52	0.90
1:D:27:PHE:CE2	1:D:49:LEU:HD13	2.05	0.90
1:D:153:PHE:C	1:D:155:PRO:HD2	1.96	0.90
1:A:13:ILE:HB	1:A:14:SER:HA	1.53	0.90
1:A:15:THR:C	1:A:17:THR:H	1.80	0.90
1:B:65:ILE:HD12	1:B:66:ASP:H	1.33	0.90
1:A:54:ALA:CB	1:A:57:ARG:HD3	2.01	0.89
1:A:88:GLN:OE1	1:D:106:ASP:OD1	1.89	0.89
1:A:15:THR:O	1:A:17:THR:N	2.05	0.89
1:B:65:ILE:O	1:B:67:ARG:N	2.04	0.89
1:C:73:ALA:HB2	1:C:79:ARG:HE	1.36	0.89
1:D:86:ARG:O	1:D:89:HIS:N	2.04	0.89
1:C:4:ILE:CG1	1:C:41:TYR:OH	2.20	0.89
1:D:133:VAL:HG23	1:D:201:ARG:HA	0.91	0.89
1:B:42:GLN:HG3	1:B:44:GLU:OE2	1.73	0.88
1:B:133:VAL:HG23	1:B:160:ILE:HD11	1.54	0.88
1:A:42:GLN:HE21	1:A:43:PRO:HD2	1.36	0.88
1:B:58:LEU:O	1:B:60:VAL:HG23	1.74	0.88
1:D:88:GLN:HE21	1:D:92:ARG:HH11	0.93	0.88
1:D:133:VAL:CG2	1:D:201:ARG:CA	2.40	0.88
1:A:109:LEU:HA	1:A:112:LEU:CD2	2.04	0.88
1:A:252:ARG:HE	1:A:262:GLN:HE21	1.20	0.87
1:D:214:HIS:CE1	1:D:216:GLY:CA	2.56	0.87
1:D:27:PHE:CD2	1:D:49:LEU:HD21	2.09	0.87
1:D:29:PRO:HG2	1:D:41:TYR:HE1	1.10	0.87
1:B:123:ARG:HH21	1:B:125:VAL:HG21	1.37	0.87
1:C:5:GLY:O	1:C:7:LEU:N	2.08	0.86
1:D:67:ARG:O	1:D:71:ASP:HB3	1.75	0.86
1:A:13:ILE:CB	1:A:14:SER:HA	2.05	0.86
1:C:196:PRO:CG	1:C:199:MET:HE2	2.06	0.86
1:D:3:THR:CG2	1:D:6:GLN:NE2	2.36	0.86
1:D:172:ILE:HG22	1:D:184:VAL:O	1.75	0.86
1:D:149:LEU:HA	1:D:152:ARG:HD3	1.57	0.86
1:C:55:LEU:O	1:C:58:LEU:N	2.06	0.86
1:C:133:VAL:HG23	1:C:201:ARG:N	1.91	0.86
1:A:78:GLN:OE1	1:D:259:PRO:O	1.94	0.86
1:A:191:GLU:HA	1:A:201:ARG:NH2	1.90	0.86
1:A:42:GLN:NE2	1:A:43:PRO:HD2	1.89	0.86
1:D:172:ILE:HD13	1:D:202:PHE:CE1	2.05	0.86
1:B:107:ARG:HH21	1:C:57:ARG:NH1	1.74	0.85
1:D:69:LYS:CE	1:D:70:ARG:HH11	1.89	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:O	1:A:21:TYR:HD1	1.33	0.85
1:A:80:LEU:HD23	1:A:80:LEU:H	1.41	0.85
1:A:52:ILE:C	1:A:54:ALA:H	1.83	0.85
1:B:133:VAL:CG2	1:B:160:ILE:HD11	2.07	0.85
1:D:153:PHE:O	1:D:155:PRO:HD2	1.76	0.85
1:C:4:ILE:HD11	1:C:41:TYR:HH	1.39	0.85
1:B:49:LEU:HD22	1:B:53:LEU:HD23	1.56	0.84
1:A:23:ALA:C	1:A:24:ILE:HG12	2.02	0.84
1:B:116:ARG:HH11	1:B:117:ILE:N	1.71	0.84
1:C:87:HIS:CE1	1:C:91:LEU:CD1	2.60	0.84
1:C:214:HIS:O	1:C:262:GLN:CA	2.25	0.84
1:B:116:ARG:NH1	1:B:117:ILE:CA	2.39	0.84
1:B:228:ILE:HA	1:B:232:LEU:CB	2.07	0.84
1:D:214:HIS:CE1	1:D:216:GLY:N	2.46	0.84
1:C:53:LEU:CD1	1:C:57:ARG:HH21	1.90	0.83
1:B:116:ARG:O	1:B:117:ILE:C	2.16	0.83
1:C:192:GLY:H	1:C:201:ARG:HH12	1.26	0.83
1:A:215:LYS:HE3	1:A:262:GLN:OE1	1.77	0.83
1:D:66:ASP:O	1:D:69:LYS:HB3	1.79	0.83
1:D:145:THR:HG22	1:D:148:GLN:OE1	1.78	0.83
1:B:65:ILE:CD1	1:B:66:ASP:H	1.90	0.83
1:B:104:GLU:OE2	1:B:107:ARG:NE	2.10	0.83
1:B:108:THR:O	1:B:112:LEU:CD2	2.27	0.83
1:B:116:ARG:NH1	1:B:117:ILE:HA	1.93	0.83
1:D:172:ILE:CD1	1:D:202:PHE:HE1	1.78	0.83
1:B:58:LEU:O	1:B:60:VAL:N	2.12	0.83
1:A:42:GLN:HG3	1:A:43:PRO:CD	2.08	0.82
1:D:90:THR:O	1:D:94:GLU:HG3	1.79	0.82
1:D:105:LEU:O	1:D:108:THR:HG22	1.79	0.82
1:D:214:HIS:HE1	1:D:216:GLY:CA	1.93	0.82
1:C:134:GLY:O	1:C:199:MET:HB2	1.78	0.82
1:D:69:LYS:HE3	1:D:70:ARG:HH11	1.45	0.81
1:A:109:LEU:HA	1:A:112:LEU:HD23	1.63	0.81
1:A:105:LEU:HD22	1:D:84:LEU:HD22	1.61	0.81
1:B:160:ILE:HG23	1:B:163:LYS:HD2	1.62	0.81
1:B:11:PHE:HE2	1:B:49:LEU:HD13	1.42	0.81
1:B:228:ILE:HG13	1:B:229:TYR:H	1.44	0.81
1:C:95:ILE:HG22	1:C:99:GLN:HE22	1.43	0.81
1:D:182:HIS:ND1	1:D:182:HIS:O	2.13	0.80
1:B:214:HIS:HD2	1:B:215:LYS:N	1.79	0.80
1:C:214:HIS:O	1:C:262:GLN:CB	2.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLN:HE21	1:D:92:ARG:HH12	1.14	0.80
1:D:106:ASP:HA	1:D:109:LEU:HD23	1.63	0.80
1:D:135:MET:CE	1:D:153:PHE:HD1	1.93	0.80
1:B:227:ALA:C	1:B:232:LEU:HD12	2.07	0.80
1:B:160:ILE:CG2	1:B:163:LYS:HD2	2.12	0.80
1:B:228:ILE:CA	1:B:232:LEU:HB2	2.10	0.79
1:D:95:ILE:O	1:D:99:GLN:HB2	1.82	0.79
1:B:29:PRO:CB	1:B:41:TYR:CE1	2.65	0.79
1:D:29:PRO:CB	1:D:41:TYR:CD1	2.65	0.79
1:A:215:LYS:HE2	1:A:262:GLN:OE1	1.82	0.79
1:B:214:HIS:HE1	1:B:221:ILE:HG22	1.42	0.79
1:A:60:VAL:CB	1:A:65:ILE:HD11	2.12	0.79
1:D:29:PRO:HB2	1:D:41:TYR:CD1	2.18	0.79
1:B:69:LYS:CG	1:B:74:LEU:HD23	2.13	0.79
1:A:85:GLN:OE1	1:A:88:GLN:HG2	1.83	0.79
1:A:115:TRP:CE2	1:D:77:PRO:CG	2.65	0.79
1:B:105:LEU:HD13	1:B:105:LEU:O	1.83	0.79
1:A:54:ALA:N	1:A:55:LEU:HB3	1.98	0.78
1:C:196:PRO:HB2	1:C:199:MET:CE	2.05	0.78
1:A:58:LEU:CD1	1:A:60:VAL:HG22	2.13	0.78
1:C:60:VAL:HG23	1:C:61:PRO:O	1.82	0.78
1:B:106:ASP:OD2	1:D:103:ALA:O	2.01	0.78
1:A:115:TRP:CZ2	1:D:77:PRO:HD3	2.19	0.78
1:A:85:GLN:OE1	1:A:88:GLN:CB	2.33	0.77
1:B:214:HIS:ND1	1:B:221:ILE:CG2	2.43	0.77
1:D:152:ARG:O	1:D:155:PRO:HG2	1.85	0.77
1:A:76:ASP:C	1:A:78:GLN:H	1.90	0.77
1:C:105:LEU:HD12	1:C:105:LEU:O	1.85	0.77
1:C:214:HIS:O	1:C:262:GLN:HB3	1.85	0.77
1:D:153:PHE:O	1:D:156:ARG:N	2.18	0.77
1:D:69:LYS:O	1:D:72:GLY:O	2.00	0.77
1:A:46:ILE:CG2	1:A:47:GLU:H	1.98	0.76
1:B:148:GLN:O	1:B:152:ARG:HD2	1.85	0.76
1:A:115:TRP:CZ2	1:D:77:PRO:CD	2.67	0.76
1:B:131:SER:HB3	1:B:201:ARG:HD2	1.67	0.76
1:C:89:HIS:O	1:C:91:LEU:O	2.04	0.76
1:D:228:ILE:HD13	1:D:267:ILE:HG12	1.68	0.76
1:A:42:GLN:CG	1:A:43:PRO:HD2	2.15	0.76
1:A:60:VAL:HG11	1:A:65:ILE:CD1	2.04	0.76
1:D:207:GLN:HG3	1:D:209:TYR:CE1	2.20	0.76
1:C:231:HIS:O	1:C:235:GLU:HG3	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:THR:CG2	1:D:6:GLN:CD	2.59	0.76
1:A:51:ARG:NH1	1:A:80:LEU:HD11	2.00	0.75
1:C:71:ASP:H	1:C:72:GLY:HA2	1.50	0.75
1:B:28:VAL:HG23	1:B:29:PRO:HD2	1.68	0.75
1:A:2:LEU:HD12	1:A:7:LEU:HB2	1.66	0.75
1:B:228:ILE:N	1:B:232:LEU:HD12	2.00	0.75
1:D:214:HIS:ND1	1:D:215:LYS:N	2.35	0.75
1:B:72:GLY:CA	1:B:73:ALA:HB2	2.15	0.75
1:A:13:ILE:CG1	1:A:14:SER:HA	2.17	0.75
1:D:64:ALA:O	1:D:67:ARG:CG	2.34	0.75
1:A:57:ARG:O	1:D:101:LEU:HD21	1.87	0.74
1:A:55:LEU:O	1:A:57:ARG:N	2.19	0.74
1:A:80:LEU:HA	1:A:83:PHE:HB3	1.67	0.74
1:B:18:LEU:CD2	1:B:41:TYR:OH	2.35	0.74
1:C:206:ALA:C	1:C:207:GLN:HG3	2.13	0.74
1:A:13:ILE:H	1:A:13:ILE:CD1	1.97	0.73
1:B:14:SER:OG	1:B:17:THR:OG1	1.98	0.73
1:D:3:THR:HG22	1:D:6:GLN:CD	2.12	0.73
1:D:110:ALA:O	1:D:114:HIS:CD2	2.41	0.73
1:D:172:ILE:CG2	1:D:184:VAL:HB	2.17	0.73
1:C:178:ASN:H	1:C:179:GLY:HA2	1.52	0.73
1:A:7:LEU:CD2	1:A:9:ARG:NE	2.52	0.73
1:A:108:THR:O	1:A:112:LEU:CD2	2.36	0.73
1:B:52:ILE:O	1:B:54:ALA:N	2.22	0.72
1:C:9:ARG:NH1	1:D:225:PHE:CE2	2.56	0.72
1:A:191:GLU:HA	1:A:201:ARG:HH21	1.53	0.72
1:A:7:LEU:HD23	1:A:9:ARG:HE	1.52	0.72
1:A:87:HIS:O	1:A:88:GLN:C	2.31	0.72
1:B:229:TYR:OH	1:B:245:ASP:OD1	2.08	0.72
1:A:214:HIS:CD2	1:A:221:ILE:CG1	2.67	0.72
1:B:18:LEU:HD21	1:B:41:TYR:OH	1.89	0.72
1:C:64:ALA:O	1:C:66:ASP:N	2.22	0.72
1:A:2:LEU:HD12	1:A:7:LEU:CB	2.20	0.72
1:A:207:GLN:HE22	1:A:244:VAL:H	1.36	0.72
1:A:248:TYR:HB3	1:A:264:ASP:HB2	1.70	0.72
1:D:7:LEU:O	1:D:10:ILE:HG13	1.89	0.72
1:B:107:ARG:HH21	1:C:57:ARG:HH11	1.35	0.72
1:B:65:ILE:CG1	1:B:66:ASP:H	2.03	0.71
1:B:69:LYS:HG3	1:B:74:LEU:HD23	1.71	0.71
1:A:9:ARG:NH1	1:A:9:ARG:HG2	2.06	0.71
1:D:215:LYS:HA	1:D:262:GLN:HA	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:TRP:O	1:B:118:ARG:CG	2.37	0.71
1:D:145:THR:OG1	1:D:146:ILE:N	2.24	0.71
1:A:26:LEU:C	1:A:26:LEU:HD12	2.16	0.71
1:A:80:LEU:HD23	1:A:80:LEU:N	2.04	0.71
1:B:65:ILE:HD12	1:B:66:ASP:N	2.04	0.71
1:D:200:VAL:HG22	1:D:201:ARG:N	2.05	0.71
1:B:42:GLN:CG	1:B:44:GLU:OE2	2.39	0.71
1:D:27:PHE:CE2	1:D:49:LEU:HD22	2.08	0.71
1:D:135:MET:HE3	1:D:153:PHE:HD1	1.55	0.71
1:B:108:THR:C	1:B:112:LEU:HD21	2.14	0.70
1:D:153:PHE:O	1:D:154:ILE:C	2.33	0.70
1:B:11:PHE:HE2	1:B:49:LEU:CD1	2.02	0.70
1:B:116:ARG:HA	1:B:119:ASN:HB2	1.71	0.70
1:C:227:ALA:CA	1:C:230:SER:OG	2.39	0.70
1:B:11:PHE:CD2	1:B:49:LEU:HD13	2.26	0.70
1:D:106:ASP:HA	1:D:109:LEU:HD21	1.72	0.70
1:B:29:PRO:CA	1:B:41:TYR:CE1	2.75	0.70
1:D:105:LEU:O	1:D:107:ARG:N	2.24	0.70
1:A:7:LEU:CD2	1:A:9:ARG:HE	2.04	0.70
1:D:65:ILE:HG22	1:D:66:ASP:N	2.06	0.70
1:D:78:GLN:HA	1:D:81:ARG:HG2	1.72	0.70
1:D:29:PRO:CB	1:D:41:TYR:CE1	2.75	0.70
1:A:52:ILE:HA	1:A:55:LEU:HG	1.74	0.69
1:B:98:ARG:HA	1:B:101:LEU:HB2	1.74	0.69
1:C:132:VAL:HG23	1:C:187:PHE:O	1.92	0.69
1:C:227:ALA:HA	1:C:230:SER:OG	1.92	0.69
1:C:7:LEU:CD1	1:C:41:TYR:CE1	2.75	0.69
1:C:245:ASP:N	1:C:245:ASP:OD1	2.25	0.69
1:D:4:ILE:H	1:D:4:ILE:CD1	1.96	0.69
1:D:86:ARG:O	1:D:88:GLN:N	2.25	0.69
1:B:214:HIS:CD2	1:B:215:LYS:N	2.59	0.69
1:B:65:ILE:O	1:B:68:LEU:N	2.18	0.69
1:C:130:PHE:CZ	1:C:204:VAL:HG21	2.28	0.69
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.58	0.68
1:C:133:VAL:CG2	1:C:201:ARG:HA	2.19	0.68
1:A:7:LEU:HD23	1:A:9:ARG:NE	2.09	0.68
1:C:65:ILE:HA	1:C:68:LEU:HB3	1.75	0.68
1:D:69:LYS:HE3	1:D:70:ARG:HD2	1.74	0.68
1:D:172:ILE:HD13	1:D:202:PHE:HD1	1.57	0.68
1:D:81:ARG:O	1:D:85:GLN:HB3	1.93	0.68
1:C:53:LEU:HD13	1:C:57:ARG:NH2	2.05	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASN:H	1:A:179:GLY:HA2	1.58	0.68
1:B:14:SER:OG	1:B:17:THR:CB	2.42	0.68
1:B:132:VAL:HG11	1:B:172:ILE:HD11	1.75	0.68
1:C:110:ALA:O	1:C:113:ALA:HB3	1.94	0.68
1:A:252:ARG:NE	1:A:262:GLN:HE21	1.92	0.67
1:C:5:GLY:O	1:C:8:ALA:N	2.26	0.67
1:C:236:ARG:O	1:C:236:ARG:HG3	1.94	0.67
1:C:53:LEU:CD1	1:C:57:ARG:NH2	2.57	0.67
1:C:182:HIS:CD2	1:C:183:TYR:H	2.12	0.67
1:D:69:LYS:HG2	1:D:70:ARG:N	2.09	0.67
1:A:180:GLU:HG3	1:A:181:PHE:H	1.59	0.67
1:D:65:ILE:O	1:D:67:ARG:HD2	1.94	0.67
1:A:7:LEU:HD22	1:A:7:LEU:O	1.95	0.67
1:D:122:ALA:CB	1:D:212:PHE:CE1	2.76	0.67
1:A:76:ASP:C	1:A:78:GLN:N	2.50	0.67
1:B:144:ASP:HA	1:B:148:GLN:HG2	1.75	0.67
1:B:160:ILE:HG23	1:B:163:LYS:CD	2.24	0.67
1:D:149:LEU:HD12	1:D:152:ARG:HH21	1.60	0.67
1:A:43:PRO:O	1:A:46:ILE:HG22	1.94	0.67
1:A:85:GLN:HA	1:A:88:GLN:HB3	1.77	0.67
1:C:79:ARG:HG3	1:C:80:LEU:HD12	1.76	0.67
1:C:247:GLU:OE1	1:D:9:ARG:NH2	2.27	0.67
1:D:112:LEU:N	1:D:112:LEU:HD22	2.09	0.67
1:B:28:VAL:HG23	1:B:29:PRO:CD	2.24	0.67
1:D:3:THR:CG2	1:D:6:GLN:HG3	2.23	0.67
1:D:153:PHE:C	1:D:155:PRO:CD	2.61	0.67
1:A:2:LEU:HD12	1:A:7:LEU:CA	2.25	0.67
1:A:87:HIS:O	1:A:89:HIS:N	2.28	0.67
1:A:191:GLU:CD	1:A:203:GLN:HE22	2.02	0.67
1:B:116:ARG:C	1:B:118:ARG:N	2.52	0.66
1:B:220:GLN:HE22	1:C:81:ARG:NH1	1.92	0.66
1:A:13:ILE:HD13	1:A:13:ILE:N	2.05	0.66
1:C:42:GLN:HG3	1:C:43:PRO:HD2	1.77	0.66
1:D:29:PRO:HB2	1:D:41:TYR:HD1	1.59	0.66
1:A:52:ILE:C	1:A:54:ALA:N	2.44	0.66
1:B:29:PRO:HA	1:B:41:TYR:CE1	2.30	0.66
1:D:88:GLN:NE2	1:D:92:ARG:HH11	1.59	0.66
1:C:134:GLY:C	1:C:199:MET:HB3	2.20	0.66
1:C:181:PHE:CE2	1:D:15:THR:HG23	2.31	0.65
1:A:60:VAL:HG12	1:A:65:ILE:HD13	1.72	0.65
1:A:115:TRP:CZ2	1:D:77:PRO:HG3	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:THR:O	1:C:7:LEU:HB2	1.96	0.65
1:C:96:SER:O	1:C:100:ARG:HG3	1.97	0.65
1:B:226:GLN:O	1:B:230:SER:HB3	1.96	0.65
1:D:214:HIS:N	1:D:263:VAL:O	2.29	0.65
1:D:104:GLU:OE2	1:D:105:LEU:CD1	2.38	0.65
1:B:116:ARG:HH11	1:B:116:ARG:C	2.05	0.65
1:B:153:PHE:O	1:B:156:ARG:N	2.21	0.65
1:C:161:ALA:O	1:C:189:VAL:HG11	1.96	0.65
1:A:75:ASP:HB2	1:D:115:TRP:CZ3	2.32	0.65
1:B:248:TYR:HB3	1:B:264:ASP:HB2	1.79	0.65
1:D:83:PHE:HD1	1:D:84:LEU:N	1.93	0.64
1:D:106:ASP:CA	1:D:109:LEU:HD23	2.27	0.64
1:D:152:ARG:O	1:D:155:PRO:CG	2.44	0.64
1:D:223:GLU:HA	1:D:226:GLN:HB3	1.78	0.64
1:B:195:VAL:HG22	1:B:199:MET:HB2	1.78	0.64
1:B:49:LEU:CD2	1:B:53:LEU:CD2	2.73	0.64
1:B:214:HIS:HE1	1:B:221:ILE:CG2	2.01	0.64
1:C:134:GLY:O	1:C:199:MET:CA	2.45	0.64
1:B:150:TRP:O	1:B:154:ILE:HG13	1.98	0.64
1:A:13:ILE:HB	1:A:14:SER:CA	2.26	0.64
1:A:46:ILE:HD12	1:B:230:SER:HA	1.80	0.64
1:A:9:ARG:CD	1:A:9:ARG:H	2.11	0.64
1:B:11:PHE:CE2	1:B:49:LEU:CD1	2.75	0.64
1:D:160:ILE:O	1:D:163:LYS:CE	2.46	0.64
1:A:207:GLN:HB2	1:A:209:TYR:CZ	2.33	0.64
1:D:245:ASP:HB3	1:D:268:PRO:HD3	1.79	0.63
1:A:3:THR:O	1:A:7:LEU:HB2	1.99	0.63
1:B:14:SER:HG	1:B:17:THR:HG1	1.27	0.63
1:B:172:ILE:HD13	1:B:202:PHE:CD2	2.34	0.63
1:D:88:GLN:O	1:D:92:ARG:CD	2.46	0.63
1:B:109:LEU:HA	1:B:112:LEU:HD21	1.79	0.63
1:D:71:ASP:OD1	1:D:72:GLY:N	2.31	0.63
1:B:220:GLN:NE2	1:C:81:ARG:NH1	2.46	0.63
1:A:17:THR:O	1:A:21:TYR:HE1	1.79	0.63
1:D:132:VAL:HB	1:D:188:GLU:HA	1.79	0.63
1:A:115:TRP:CZ2	1:D:77:PRO:CG	2.82	0.63
1:D:4:ILE:HD12	1:D:4:ILE:N	2.05	0.62
1:D:181:PHE:O	1:D:182:HIS:HB2	1.98	0.62
1:A:6:GLN:C	1:A:8:ALA:H	2.07	0.62
1:A:78:GLN:OE1	1:D:260:ASN:HA	1.98	0.62
1:B:69:LYS:HG2	1:B:74:LEU:HD23	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLU:C	1:B:153:PHE:H	2.08	0.62
1:A:109:LEU:CA	1:A:112:LEU:HD23	2.28	0.62
1:C:87:HIS:ND1	1:C:91:LEU:HD12	2.15	0.62
1:D:69:LYS:HZ1	1:D:70:ARG:NH1	1.97	0.62
1:D:73:ALA:HB1	1:D:79:ARG:HD2	1.81	0.62
1:C:79:ARG:C	1:C:81:ARG:H	2.07	0.62
1:D:172:ILE:HG21	1:D:184:VAL:HB	1.81	0.62
1:A:105:LEU:HD22	1:D:84:LEU:CD2	2.29	0.62
1:B:52:ILE:C	1:B:54:ALA:H	2.08	0.62
1:A:250:ASP:OD2	1:A:252:ARG:NH1	2.32	0.62
1:D:149:LEU:HA	1:D:152:ARG:HD2	1.78	0.62
1:D:149:LEU:HD12	1:D:152:ARG:NH2	2.15	0.62
1:A:119:ASN:O	1:A:119:ASN:ND2	2.22	0.61
1:A:85:GLN:HG3	1:A:85:GLN:O	1.99	0.61
1:A:214:HIS:NE2	1:A:221:ILE:HA	2.14	0.61
1:C:133:VAL:CG2	1:C:201:ARG:CA	2.74	0.61
1:C:195:VAL:HG23	1:C:195:VAL:O	1.99	0.61
1:C:89:HIS:O	1:C:90:THR:C	2.41	0.61
1:B:230:SER:OG	1:B:231:HIS:N	2.33	0.61
1:C:26:LEU:HD12	1:C:69:LYS:HE3	1.83	0.61
1:C:213:THR:OG1	1:C:264:ASP:OD1	2.13	0.61
1:C:71:ASP:OD1	1:C:72:GLY:O	2.18	0.61
1:D:69:LYS:CE	1:D:70:ARG:HD2	2.30	0.61
1:D:106:ASP:C	1:D:109:LEU:HD23	2.25	0.61
1:B:116:ARG:NH1	1:B:116:ARG:HG3	2.13	0.61
1:D:130:PHE:CE1	1:D:204:VAL:HG13	2.36	0.61
1:A:228:ILE:HG21	1:A:267:ILE:HD13	1.83	0.61
1:B:123:ARG:HH21	1:B:125:VAL:CG2	2.11	0.61
1:C:65:ILE:O	1:C:65:ILE:HG22	2.01	0.61
1:A:23:ALA:O	1:A:25:GLY:N	2.29	0.60
1:A:53:LEU:HD23	1:A:53:LEU:O	2.01	0.60
1:D:124:ILE:CG2	1:D:208:LYS:NZ	2.64	0.60
1:D:214:HIS:O	1:D:263:VAL:N	2.32	0.60
1:B:69:LYS:HG3	1:B:74:LEU:CD2	2.29	0.60
1:C:9:ARG:CG	1:C:10:ILE:N	2.45	0.60
1:A:115:TRP:CE3	1:D:77:PRO:HG3	2.36	0.60
1:B:65:ILE:C	1:B:67:ARG:H	2.09	0.60
1:A:180:GLU:HG3	1:A:181:PHE:N	2.15	0.60
1:D:130:PHE:CE1	1:D:204:VAL:CG1	2.84	0.60
1:D:28:VAL:O	1:D:28:VAL:HG13	2.02	0.60
1:A:70:ARG:HD3	1:A:74:LEU:HD12	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:N	1:A:72:GLY:HA2	2.15	0.60
1:A:149:LEU:HD12	1:A:149:LEU:H	1.66	0.59
1:D:83:PHE:CD1	1:D:84:LEU:N	2.70	0.59
1:D:170:TYR:HE2	1:D:188:GLU:HB2	1.66	0.59
1:A:46:ILE:O	1:A:49:LEU:N	2.36	0.59
1:C:55:LEU:HB3	1:C:60:VAL:HG11	1.84	0.59
1:D:214:HIS:ND1	1:D:216:GLY:N	2.50	0.59
1:A:65:ILE:N	1:A:65:ILE:HD12	2.17	0.59
1:A:105:LEU:CD2	1:D:84:LEU:CD2	2.81	0.59
1:C:47:GLU:HA	1:C:50:SER:HB3	1.84	0.59
1:C:71:ASP:OD1	1:C:72:GLY:C	2.45	0.59
1:C:87:HIS:CE1	1:C:91:LEU:HD12	2.36	0.59
1:B:149:LEU:HA	1:B:152:ARG:HH21	1.65	0.59
1:D:213:THR:HG23	1:D:213:THR:O	2.01	0.59
1:B:92:ARG:O	1:B:96:SER:N	2.31	0.59
1:D:200:VAL:HG22	1:D:201:ARG:H	1.67	0.59
1:A:252:ARG:HE	1:A:262:GLN:NE2	1.97	0.59
1:B:88:GLN:NE2	1:B:92:ARG:HD3	2.18	0.59
1:A:57:ARG:HE	1:D:104:GLU:HG3	1.66	0.59
1:B:56:ARG:HD2	1:B:62:LEU:HD21	1.83	0.59
1:C:65:ILE:HG12	1:C:68:LEU:HD23	1.85	0.59
1:C:196:PRO:HG2	1:C:199:MET:HE3	1.83	0.59
1:B:52:ILE:C	1:B:54:ALA:N	2.60	0.59
1:D:228:ILE:HA	1:D:232:LEU:HB2	1.83	0.59
1:C:62:LEU:HD12	1:C:62:LEU:N	2.15	0.58
1:C:136:GLU:HG2	1:C:137:TYR:N	2.16	0.58
1:B:29:PRO:CA	1:B:41:TYR:HE1	2.17	0.58
1:C:6:GLN:C	1:C:8:ALA:H	2.11	0.58
1:A:42:GLN:CD	1:A:43:PRO:HD2	2.28	0.58
1:B:16:LYS:HE2	1:B:20:HIS:HB2	1.86	0.58
1:D:84:LEU:O	1:D:88:GLN:HB3	2.03	0.58
1:A:42:GLN:HG3	1:A:43:PRO:N	2.17	0.58
1:A:108:THR:O	1:A:112:LEU:HD21	2.04	0.58
1:A:164:HIS:HD2	1:A:165:ASP:CG	2.12	0.58
1:D:26:LEU:HG	1:D:27:PHE:N	2.18	0.58
1:A:11:PHE:HD1	1:B:181:PHE:HE2	1.51	0.58
1:B:228:ILE:C	1:B:230:SER:H	2.12	0.58
1:C:182:HIS:O	1:C:183:TYR:HB2	2.03	0.58
1:D:105:LEU:C	1:D:107:ARG:H	2.12	0.58
1:A:18:LEU:O	1:A:21:TYR:HB2	2.04	0.57
1:A:53:LEU:O	1:A:54:ALA:HB2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:O	1:B:70:ARG:HG3	2.03	0.57
1:A:62:LEU:O	1:A:65:ILE:N	2.36	0.57
1:B:44:GLU:OE2	1:B:44:GLU:N	2.30	0.57
1:B:228:ILE:HA	1:B:232:LEU:HD12	1.86	0.57
1:D:207:GLN:OE1	1:D:209:TYR:HE1	1.87	0.57
1:A:55:LEU:HD13	1:A:55:LEU:C	2.29	0.57
1:A:80:LEU:H	1:A:80:LEU:CD2	2.08	0.57
1:B:18:LEU:HD22	1:B:41:TYR:OH	2.03	0.57
1:C:79:ARG:CG	1:C:80:LEU:HD12	2.35	0.57
1:C:253:PHE:HA	1:C:261:SER:HB2	1.86	0.57
1:D:124:ILE:CG2	1:D:208:LYS:HZ3	2.18	0.57
1:A:77:PRO:HD3	1:D:115:TRP:HZ3	1.69	0.57
1:A:111:THR:HG22	1:A:111:THR:O	2.03	0.57
1:A:149:LEU:HD12	1:A:149:LEU:N	2.19	0.57
1:B:150:TRP:HE1	1:B:183:TYR:HE2	1.52	0.57
1:A:23:ALA:C	1:A:24:ILE:CG1	2.76	0.57
1:A:105:LEU:HD13	1:D:88:GLN:HB2	1.85	0.57
1:A:122:ALA:HB2	1:A:212:PHE:CE1	2.39	0.57
1:D:90:THR:HA	1:D:93:GLU:HB2	1.87	0.57
1:D:231:HIS:ND1	1:D:235:GLU:OE1	2.33	0.57
1:D:130:PHE:N	1:D:130:PHE:HD1	2.02	0.57
1:D:27:PHE:CZ	1:D:49:LEU:CD1	2.80	0.57
1:B:110:ALA:HB2	1:D:107:ARG:O	2.04	0.57
1:C:6:GLN:CD	1:C:6:GLN:H	2.13	0.57
1:D:130:PHE:N	1:D:130:PHE:CD1	2.71	0.57
1:A:26:LEU:C	1:A:69:LYS:HE2	2.30	0.56
1:B:49:LEU:O	1:B:51:ARG:N	2.37	0.56
1:B:241:LYS:HA	1:B:270:TYR:CE1	2.40	0.56
1:D:69:LYS:HE3	1:D:70:ARG:NH1	2.16	0.56
1:D:109:LEU:N	1:D:109:LEU:HD22	2.19	0.56
1:B:29:PRO:HA	1:B:41:TYR:CD1	2.39	0.56
1:D:172:ILE:HG22	1:D:184:VAL:HB	1.85	0.56
1:D:27:PHE:CD2	1:D:49:LEU:CG	2.78	0.56
1:C:178:ASN:N	1:C:179:GLY:HA2	2.18	0.56
1:D:72:GLY:CA	1:D:73:ALA:CB	2.63	0.56
1:A:148:GLN:HE21	1:A:148:GLN:C	2.13	0.56
1:B:97:ALA:O	1:B:101:LEU:HD23	2.05	0.56
1:B:228:ILE:CA	1:B:232:LEU:HD12	2.35	0.56
1:C:69:LYS:HB2	1:C:74:LEU:HA	1.86	0.56
1:D:51:ARG:NH2	1:D:75:ASP:OD2	0.47	0.56
1:A:126:GLU:HG2	1:A:208:LYS:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:C	1:B:51:ARG:N	2.64	0.56
1:B:64:ALA:O	1:B:65:ILE:O	2.24	0.56
1:B:172:ILE:O	1:B:183:TYR:HA	2.05	0.56
1:C:227:ALA:C	1:C:230:SER:OG	2.48	0.55
1:C:228:ILE:HG21	1:C:267:ILE:HD13	1.87	0.55
1:A:115:TRP:CH2	1:D:77:PRO:CD	2.81	0.55
1:A:214:HIS:HB3	1:A:263:VAL:HG22	1.87	0.55
1:B:253:PHE:C	1:B:254:ARG:HG3	2.30	0.55
1:B:253:PHE:C	1:B:253:PHE:CD1	2.85	0.55
1:A:58:LEU:CD1	1:A:60:VAL:CG2	2.79	0.55
1:B:104:GLU:OE2	1:B:107:ARG:NH2	2.34	0.55
1:B:127:ARG:NH2	1:B:170:TYR:OH	2.40	0.55
1:A:85:GLN:OE1	1:A:88:GLN:HB3	2.05	0.55
1:C:182:HIS:CD2	1:C:183:TYR:N	2.75	0.55
1:C:250:ASP:OD1	1:C:250:ASP:N	2.40	0.55
1:D:195:VAL:HG13	1:D:195:VAL:O	2.06	0.55
1:A:9:ARG:HG2	1:A:9:ARG:HH11	1.69	0.55
1:B:252:ARG:NH2	1:B:264:ASP:OD1	2.39	0.55
1:C:64:ALA:C	1:C:66:ASP:H	2.11	0.55
1:C:196:PRO:CG	1:C:199:MET:CE	2.68	0.55
1:B:26:LEU:O	1:B:69:LYS:NZ	2.22	0.55
1:C:228:ILE:HA	1:C:232:LEU:HB2	1.88	0.55
1:D:27:PHE:CD1	1:D:27:PHE:C	2.85	0.55
1:D:159:GLU:HB3	1:D:196:PRO:HG2	1.89	0.55
1:B:148:GLN:O	1:B:152:ARG:CD	2.55	0.54
1:D:73:ALA:HB2	1:D:79:ARG:NH1	2.22	0.54
1:D:112:LEU:O	1:D:113:ALA:O	2.26	0.54
1:A:88:GLN:HA	1:D:102:LEU:HD21	1.90	0.54
1:C:190:GLN:O	1:C:193:TRP:HD1	1.90	0.54
1:D:105:LEU:HG	1:D:108:THR:HG21	1.88	0.54
1:A:105:LEU:CD1	1:D:88:GLN:HB2	2.37	0.54
1:D:65:ILE:HG22	1:D:66:ASP:H	1.71	0.54
1:D:83:PHE:CD1	1:D:83:PHE:C	2.84	0.54
1:B:156:ARG:HA	1:B:159:GLU:OE1	2.08	0.54
1:C:250:ASP:OD2	1:C:252:ARG:CZ	2.55	0.54
1:D:149:LEU:HD12	1:D:152:ARG:HD2	1.88	0.54
1:D:214:HIS:O	1:D:262:GLN:HA	2.08	0.54
1:B:160:ILE:HG21	1:B:163:LYS:HD2	1.88	0.54
1:C:154:ILE:N	1:C:155:PRO:HD2	2.23	0.54
1:A:23:ALA:O	1:A:24:ILE:HG12	2.08	0.54
1:C:160:ILE:HD13	1:C:199:MET:HE3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LYS:NZ	1:D:70:ARG:HH11	2.05	0.54
1:B:214:HIS:CD2	1:B:214:HIS:C	2.85	0.54
1:A:133:VAL:HG23	1:A:189:VAL:HG21	1.89	0.53
1:A:135:MET:SD	1:A:152:ARG:HD2	2.48	0.53
1:C:73:ALA:CB	1:C:79:ARG:HE	2.14	0.53
1:D:172:ILE:CG2	1:D:184:VAL:CB	2.84	0.53
1:D:172:ILE:CG2	1:D:184:VAL:HG23	2.39	0.53
1:A:65:ILE:HG22	1:A:65:ILE:O	2.07	0.53
1:B:137:TYR:HD2	1:B:183:TYR:HB3	1.73	0.53
1:C:10:ILE:HD13	1:D:226:GLN:HA	1.90	0.53
1:C:86:ARG:O	1:C:90:THR:HG23	2.08	0.53
1:D:69:LYS:HG2	1:D:70:ARG:H	1.73	0.53
1:A:55:LEU:HD13	1:A:56:ARG:N	2.22	0.53
1:B:107:ARG:NH2	1:C:57:ARG:NH1	2.51	0.53
1:D:130:PHE:CD1	1:D:204:VAL:HG13	2.44	0.53
1:C:173:CYS:HB3	1:D:9:ARG:NH1	2.23	0.53
1:A:250:ASP:OD2	1:A:252:ARG:HG3	2.09	0.53
1:B:145:THR:H	1:B:148:GLN:HB2	1.74	0.53
1:B:151:GLU:O	1:B:155:PRO:HD2	2.08	0.53
1:A:56:ARG:CG	1:A:56:ARG:HH11	2.19	0.53
1:A:66:ASP:O	1:A:69:LYS:N	2.38	0.53
1:B:22:ASP:OD2	1:B:39:ARG:NH2	2.42	0.53
1:C:79:ARG:C	1:C:81:ARG:N	2.65	0.53
1:A:65:ILE:CD1	1:A:65:ILE:N	2.71	0.53
1:A:105:LEU:CD2	1:D:84:LEU:HD22	2.37	0.53
1:C:131:SER:CB	1:C:203:GLN:HE22	2.22	0.53
1:D:182:HIS:HD1	1:D:182:HIS:C	2.15	0.53
1:D:149:LEU:CD1	1:D:152:ARG:NH2	2.72	0.53
1:D:207:GLN:CG	1:D:209:TYR:CE1	2.91	0.53
1:B:18:LEU:HD23	1:B:18:LEU:O	2.10	0.52
1:B:132:VAL:CG1	1:B:172:ILE:HD11	2.38	0.52
1:B:104:GLU:O	1:B:108:THR:HG23	2.09	0.52
1:B:174:ALA:HB3	1:B:182:HIS:HB3	1.90	0.52
1:C:73:ALA:CB	1:C:76:ASP:HB2	2.39	0.52
1:D:146:ILE:HG23	1:D:150:TRP:CB	2.39	0.52
1:D:172:ILE:O	1:D:183:TYR:HA	2.08	0.52
1:C:173:CYS:HB3	1:D:9:ARG:HH12	1.74	0.52
1:D:146:ILE:HG23	1:D:150:TRP:HB2	1.91	0.52
1:A:112:LEU:CD2	1:A:112:LEU:N	2.72	0.52
1:C:132:VAL:CG2	1:C:187:PHE:O	2.57	0.52
1:C:152:ARG:O	1:C:156:ARG:HG3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:H	1:A:149:LEU:CD1	2.22	0.52
1:B:148:GLN:C	1:B:152:ARG:HH21	2.15	0.52
1:C:136:GLU:OE2	1:C:200:VAL:HG11	2.10	0.52
1:C:191:GLU:HG3	1:C:201:ARG:NH1	2.25	0.52
1:D:112:LEU:CD2	1:D:112:LEU:N	2.72	0.52
1:A:55:LEU:CD1	1:A:56:ARG:N	2.73	0.52
1:B:28:VAL:HG23	1:B:29:PRO:N	2.25	0.52
1:B:241:LYS:HA	1:B:270:TYR:HE1	1.74	0.52
1:C:7:LEU:HD12	1:C:41:TYR:CE1	2.44	0.52
1:B:94:GLU:OE1	1:C:98:ARG:NH1	2.43	0.52
1:B:108:THR:C	1:B:112:LEU:CD2	2.81	0.52
1:C:4:ILE:CD1	1:C:4:ILE:N	2.73	0.52
1:C:7:LEU:CD2	1:C:18:LEU:HD21	2.40	0.52
1:A:9:ARG:HH11	1:A:9:ARG:CG	2.22	0.52
1:A:10:ILE:HD12	1:B:222:ALA:O	2.10	0.52
1:B:116:ARG:NH1	1:B:117:ILE:H	2.05	0.52
1:D:116:ARG:O	1:D:119:ASN:N	2.43	0.52
1:D:173:CYS:O	1:D:174:ALA:HB2	2.09	0.52
1:D:214:HIS:ND1	1:D:215:LYS:C	2.68	0.52
1:A:47:GLU:HG2	1:D:115:TRP:CE2	2.45	0.52
1:B:116:ARG:HH11	1:B:116:ARG:HG3	1.75	0.52
1:B:149:LEU:HA	1:B:152:ARG:CD	2.32	0.52
1:C:7:LEU:HD12	1:C:41:TYR:CD1	2.44	0.52
1:A:156:ARG:HA	1:A:159:GLU:HG3	1.92	0.51
1:B:26:LEU:HD12	1:B:69:LYS:HD2	1.92	0.51
1:D:27:PHE:CZ	1:D:49:LEU:HD13	2.46	0.51
1:D:69:LYS:NZ	1:D:70:ARG:NH1	2.58	0.51
1:D:109:LEU:CD2	1:D:109:LEU:N	2.73	0.51
1:D:152:ARG:O	1:D:155:PRO:HD2	2.10	0.51
1:A:23:ALA:O	1:A:24:ILE:CG1	2.58	0.51
1:A:109:LEU:HA	1:A:112:LEU:HD21	1.90	0.51
1:B:149:LEU:CA	1:B:152:ARG:HH21	2.23	0.51
1:C:150:TRP:O	1:C:154:ILE:HG12	2.10	0.51
1:D:15:THR:OG1	1:D:19:ARG:NH2	2.43	0.51
1:D:78:GLN:O	1:D:81:ARG:HG3	2.11	0.51
1:D:133:VAL:HG21	1:D:201:ARG:CA	2.34	0.51
1:A:172:ILE:O	1:A:183:TYR:HA	2.09	0.51
1:B:65:ILE:CG1	1:B:66:ASP:N	2.69	0.51
1:C:46:ILE:HG12	1:D:230:SER:HA	1.92	0.51
1:C:91:LEU:HA	1:C:94:GLU:HG3	1.91	0.51
1:D:214:HIS:CE1	1:D:215:LYS:C	2.88	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PRO:HG2	1:B:44:GLU:CD	2.36	0.51
1:B:49:LEU:C	1:B:51:ARG:H	2.18	0.51
1:D:29:PRO:CG	1:D:41:TYR:HE1	1.85	0.51
1:D:218:ALA:O	1:D:221:ILE:HG12	2.10	0.51
1:A:85:GLN:CD	1:A:88:GLN:HG2	2.35	0.51
1:B:67:ARG:HG2	1:B:67:ARG:NH1	2.23	0.51
1:C:3:THR:C	1:C:5:GLY:N	2.64	0.51
1:D:153:PHE:O	1:D:155:PRO:CG	2.59	0.51
1:A:87:HIS:C	1:A:89:HIS:N	2.68	0.51
1:A:112:LEU:N	1:A:112:LEU:HD22	2.26	0.51
1:B:208:LYS:HZ2	1:B:270:TYR:C	2.17	0.51
1:C:3:THR:C	1:C:5:GLY:H	2.17	0.51
1:D:27:PHE:C	1:D:27:PHE:HD1	2.18	0.51
1:D:135:MET:CE	1:D:153:PHE:CD1	2.84	0.51
1:B:42:GLN:O	1:B:45:GLN:HG2	2.11	0.51
1:B:105:LEU:O	1:B:109:LEU:HD12	2.10	0.51
1:C:76:ASP:HB3	1:C:78:GLN:OE1	2.11	0.51
1:D:88:GLN:O	1:D:92:ARG:HD2	2.09	0.51
1:D:214:HIS:ND1	1:D:214:HIS:C	2.68	0.51
1:C:206:ALA:C	1:C:207:GLN:CG	2.84	0.51
1:A:231:HIS:O	1:A:235:GLU:HG3	2.11	0.50
1:D:149:LEU:HD12	1:D:152:ARG:CD	2.41	0.50
1:D:200:VAL:CG2	1:D:201:ARG:N	2.74	0.50
1:A:13:ILE:HG12	1:A:14:SER:HA	1.94	0.50
1:A:251:GLN:OE1	1:A:251:GLN:N	2.33	0.50
1:B:228:ILE:HG13	1:B:229:TYR:N	2.20	0.50
1:A:148:GLN:O	1:A:151:GLU:N	2.45	0.50
1:C:16:LYS:O	1:C:20:HIS:HB2	2.11	0.50
1:C:65:ILE:CG1	1:C:68:LEU:HD23	2.40	0.50
1:C:192:GLY:N	1:C:201:ARG:HH12	2.03	0.50
1:A:15:THR:O	1:A:16:LYS:C	2.53	0.50
1:C:6:GLN:C	1:C:8:ALA:N	2.69	0.50
1:A:52:ILE:CA	1:A:55:LEU:HG	2.37	0.50
1:A:56:ARG:CG	1:A:56:ARG:NH1	2.73	0.50
1:A:75:ASP:HB2	1:D:115:TRP:CH2	2.47	0.50
1:D:135:MET:HE1	1:D:153:PHE:HD1	1.76	0.50
1:D:227:ALA:O	1:D:232:LEU:HD12	2.11	0.50
1:C:225:PHE:HB3	1:D:10:ILE:HG22	1.93	0.50
1:A:147:GLY:O	1:A:150:TRP:HB2	2.11	0.50
1:B:251:GLN:C	1:B:253:PHE:H	2.19	0.50
1:D:172:ILE:HG21	1:D:184:VAL:CG2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ILE:HG13	1:D:173:CYS:N	2.26	0.50
1:A:109:LEU:C	1:A:112:LEU:HD23	2.37	0.50
1:A:149:LEU:O	1:A:153:PHE:HB2	2.12	0.50
1:B:115:TRP:NE1	1:C:47:GLU:OE1	2.45	0.50
1:C:55:LEU:C	1:C:57:ARG:H	2.19	0.50
1:C:132:VAL:HA	1:C:187:PHE:O	2.11	0.50
1:C:131:SER:OG	1:C:203:GLN:NE2	2.41	0.50
1:B:68:LEU:O	1:B:70:ARG:N	2.45	0.49
1:B:212:PHE:CD2	1:B:228:ILE:HG21	2.47	0.49
1:D:13:ILE:HD13	1:D:53:LEU:HD21	1.94	0.49
1:D:124:ILE:HG23	1:D:208:LYS:NZ	2.26	0.49
1:A:164:HIS:CD2	1:A:165:ASP:CG	2.89	0.49
1:B:137:TYR:CD2	1:B:183:TYR:HB3	2.46	0.49
1:D:183:TYR:C	1:D:184:VAL:CG2	2.86	0.49
1:C:7:LEU:HD22	1:C:18:LEU:CD2	2.43	0.49
1:C:225:PHE:CD1	1:D:10:ILE:HG22	2.47	0.49
1:C:5:GLY:C	1:C:7:LEU:N	2.69	0.49
1:C:108:THR:O	1:C:108:THR:HG22	2.12	0.49
1:B:42:GLN:H	1:B:45:GLN:HE21	1.60	0.49
1:C:251:GLN:H	1:C:251:GLN:CD	2.08	0.49
1:D:172:ILE:CG2	1:D:184:VAL:CG2	2.91	0.49
1:B:160:ILE:HG23	1:B:160:ILE:O	2.11	0.49
1:D:254:ARG:NH2	1:D:260:ASN:OD1	2.45	0.49
1:C:52:ILE:O	1:C:56:ARG:HB2	2.12	0.49
1:C:73:ALA:HB2	1:C:79:ARG:NE	2.17	0.49
1:D:64:ALA:C	1:D:67:ARG:HE	2.19	0.49
1:A:222:ALA:O	1:A:226:GLN:HG3	2.12	0.49
1:A:85:GLN:OE1	1:A:88:GLN:OE1	2.29	0.49
1:A:86:ARG:O	1:A:89:HIS:CB	2.52	0.49
1:A:110:ALA:C	1:A:112:LEU:H	2.19	0.49
1:B:48:GLN:NE2	1:B:75:ASP:OD2	2.24	0.49
1:D:133:VAL:HG11	1:D:195:VAL:HG23	1.94	0.49
1:D:86:ARG:HA	1:D:86:ARG:HE	1.77	0.49
1:D:130:PHE:CE1	1:D:204:VAL:HG11	2.48	0.49
1:A:55:LEU:C	1:A:57:ARG:N	2.69	0.48
1:A:75:ASP:OD1	1:A:75:ASP:N	2.46	0.48
1:A:78:GLN:HG2	1:D:215:LYS:O	2.13	0.48
1:B:207:GLN:HG3	1:B:209:TYR:CZ	2.47	0.48
1:C:167:GLU:HG2	1:C:251:GLN:CD	2.37	0.48
1:C:172:ILE:O	1:C:183:TYR:HA	2.13	0.48
1:D:132:VAL:HG22	1:D:133:VAL:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:C	1:D:151:GLU:H	2.20	0.48
1:C:91:LEU:C	1:C:93:GLU:N	2.71	0.48
1:B:228:ILE:O	1:B:230:SER:N	2.47	0.48
1:C:78:GLN:OE1	1:C:78:GLN:N	2.44	0.48
1:D:69:LYS:CG	1:D:70:ARG:N	2.71	0.48
1:A:250:ASP:HB2	1:A:251:GLN:OE1	2.12	0.48
1:C:241:LYS:HB2	1:C:270:TYR:CE2	2.49	0.48
1:A:57:ARG:HE	1:D:104:GLU:CG	2.26	0.48
1:B:212:PHE:CE2	1:B:228:ILE:HG21	2.49	0.48
1:C:53:LEU:HD12	1:C:57:ARG:NH2	2.29	0.48
1:A:86:ARG:HD3	1:A:86:ARG:HA	1.73	0.48
1:C:62:LEU:C	1:C:64:ALA:N	2.70	0.48
1:B:49:LEU:O	1:B:52:ILE:N	2.47	0.48
1:D:239:GLU:HG2	1:D:270:TYR:HD2	1.79	0.48
1:A:71:ASP:H	1:A:72:GLY:HA2	1.78	0.48
1:B:187:PHE:O	1:B:189:VAL:HG13	2.13	0.48
1:B:208:LYS:NZ	1:B:270:TYR:C	2.72	0.48
1:D:65:ILE:C	1:D:67:ARG:N	2.69	0.48
1:A:57:ARG:NE	1:D:104:GLU:CG	2.76	0.48
1:B:96:SER:HA	1:B:99:GLN:HG2	1.95	0.48
1:B:133:VAL:HG21	1:B:160:ILE:HD11	1.91	0.48
1:D:88:GLN:O	1:D:88:GLN:HG3	2.12	0.48
1:A:181:PHE:CG	1:A:182:HIS:N	2.81	0.47
1:B:101:LEU:O	1:B:105:LEU:HB2	2.14	0.47
1:B:149:LEU:HA	1:B:152:ARG:NH2	2.30	0.47
1:C:228:ILE:C	1:C:230:SER:H	2.21	0.47
1:D:86:ARG:C	1:D:88:GLN:N	2.72	0.47
1:D:102:LEU:O	1:D:106:ASP:HB2	2.13	0.47
1:D:170:TYR:CE2	1:D:188:GLU:HB2	2.48	0.47
1:B:228:ILE:C	1:B:230:SER:N	2.72	0.47
1:B:228:ILE:HA	1:B:232:LEU:CD1	2.45	0.47
1:C:4:ILE:HG13	1:C:41:TYR:OH	2.10	0.47
1:C:62:LEU:O	1:C:64:ALA:N	2.47	0.47
1:D:132:VAL:CB	1:D:188:GLU:HA	2.44	0.47
1:A:23:ALA:C	1:A:25:GLY:H	2.18	0.47
1:A:77:PRO:HG3	1:D:115:TRP:HE3	1.79	0.47
1:B:56:ARG:C	1:B:58:LEU:H	2.21	0.47
1:C:55:LEU:C	1:C:57:ARG:N	2.72	0.47
1:C:90:THR:OG1	1:C:91:LEU:N	2.47	0.47
1:D:144:ASP:CG	1:D:148:GLN:HB3	2.39	0.47
1:D:172:ILE:HG23	1:D:184:VAL:HG23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLU:HG2	1:C:51:ARG:NH1	2.29	0.47
1:A:56:ARG:O	1:A:57:ARG:HG3	2.14	0.47
1:A:66:ASP:O	1:A:69:LYS:HB2	2.14	0.47
1:B:205:PRO:O	1:B:207:GLN:HG2	2.15	0.47
1:B:212:PHE:CE2	1:B:228:ILE:CG2	2.97	0.47
1:B:230:SER:OG	1:B:231:HIS:ND1	2.48	0.47
1:C:48:GLN:HG2	1:C:49:LEU:HD23	1.96	0.47
1:D:3:THR:HG21	1:D:6:GLN:CD	2.38	0.47
1:A:10:ILE:HD11	1:B:226:GLN:HG3	1.97	0.47
1:A:54:ALA:N	1:A:55:LEU:CB	2.73	0.47
1:A:54:ALA:HA	1:A:56:ARG:N	2.30	0.47
1:A:57:ARG:NE	1:D:104:GLU:HG3	2.30	0.47
1:A:78:GLN:CD	1:D:260:ASN:HA	2.39	0.47
1:A:172:ILE:HA	1:A:246:PHE:HB3	1.96	0.47
1:B:109:LEU:CA	1:B:112:LEU:HD21	2.45	0.47
1:C:73:ALA:HB1	1:C:76:ASP:HB2	1.97	0.47
1:C:168:VAL:HG13	1:C:249:TYR:O	2.15	0.47
1:D:105:LEU:C	1:D:107:ARG:N	2.70	0.47
1:D:254:ARG:HH21	1:D:258:ASP:CG	2.23	0.47
1:A:22:ASP:CG	1:A:23:ALA:N	2.72	0.47
1:A:57:ARG:HG2	1:D:104:GLU:HG3	1.96	0.47
1:B:65:ILE:HG13	1:B:66:ASP:H	1.80	0.47
1:C:12:GLU:OE2	1:C:12:GLU:HA	2.15	0.47
1:C:249:TYR:CE1	1:C:263:VAL:HG11	2.50	0.47
1:A:3:THR:HG23	1:A:6:GLN:H	1.80	0.47
1:B:29:PRO:CB	1:B:41:TYR:CD1	2.98	0.47
1:C:64:ALA:C	1:C:66:ASP:N	2.72	0.47
1:D:15:THR:O	1:D:19:ARG:HG3	2.15	0.47
1:D:153:PHE:CE2	1:D:157:GLU:HA	2.49	0.47
1:B:14:SER:HG	1:B:17:THR:CB	2.20	0.47
1:C:9:ARG:HD3	1:D:225:PHE:CE2	2.50	0.47
1:C:233:LEU:HD21	1:C:267:ILE:HD11	1.96	0.47
1:C:245:ASP:HB3	1:C:268:PRO:HD3	1.97	0.47
1:D:51:ARG:HH21	1:D:75:ASP:CG	1.77	0.46
1:A:115:TRP:HH2	1:D:75:ASP:HA	1.79	0.46
1:D:132:VAL:HG22	1:D:187:PHE:H	1.20	0.46
1:C:153:PHE:CD1	1:C:153:PHE:C	2.89	0.46
1:B:62:LEU:HA	1:B:65:ILE:HG12	1.97	0.46
1:C:4:ILE:HD12	1:C:4:ILE:N	2.31	0.46
1:D:231:HIS:HD1	1:D:235:GLU:CD	2.23	0.46
1:C:175:GLN:HB2	1:C:243:GLY:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ARG:HA	1:D:86:ARG:NE	2.31	0.46
1:A:112:LEU:O	1:A:116:ARG:HB2	2.15	0.46
1:D:67:ARG:O	1:D:71:ASP:CB	2.58	0.46
1:D:217:THR:HG22	1:D:259:PRO:HA	1.98	0.46
1:A:127:ARG:NH2	1:A:188:GLU:OE2	2.49	0.46
1:C:7:LEU:CD2	1:C:18:LEU:CD2	2.94	0.46
1:C:98:ARG:HA	1:C:101:LEU:HD12	1.98	0.46
1:C:181:PHE:HE2	1:D:15:THR:HG23	1.76	0.46
1:D:65:ILE:C	1:D:67:ARG:H	2.23	0.46
1:D:183:TYR:C	1:D:184:VAL:HG23	2.41	0.46
1:B:104:GLU:CD	1:B:107:ARG:HG2	2.41	0.46
1:C:167:GLU:CG	1:C:251:GLN:OE1	2.64	0.46
1:C:249:TYR:HE1	1:C:263:VAL:HG11	1.80	0.46
1:D:183:TYR:O	1:D:184:VAL:HG22	2.16	0.46
1:A:236:ARG:HE	1:A:236:ARG:HB3	1.62	0.46
1:B:121:HIS:ND1	1:B:122:ALA:N	2.63	0.46
1:C:84:LEU:HD12	1:C:84:LEU:HA	1.72	0.46
1:C:95:ILE:CG2	1:C:99:GLN:NE2	2.67	0.46
1:A:55:LEU:HD22	1:A:55:LEU:HA	1.76	0.45
1:B:49:LEU:O	1:B:50:SER:C	2.57	0.45
1:B:56:ARG:C	1:B:58:LEU:N	2.73	0.45
1:C:6:GLN:OE1	1:C:6:GLN:HA	2.16	0.45
1:C:153:PHE:CD1	1:C:153:PHE:O	2.70	0.45
1:A:110:ALA:C	1:A:112:LEU:N	2.72	0.45
1:A:119:ASN:HD22	1:A:119:ASN:C	2.09	0.45
1:B:68:LEU:C	1:B:70:ARG:N	2.74	0.45
1:C:231:HIS:O	1:C:235:GLU:CG	2.62	0.45
1:D:27:PHE:CD1	1:D:27:PHE:O	2.69	0.45
1:D:74:LEU:HD12	1:D:74:LEU:O	2.16	0.45
1:D:193:TRP:HA	1:D:194:PRO:HD3	1.77	0.45
1:B:58:LEU:C	1:B:60:VAL:N	2.74	0.45
1:C:110:ALA:O	1:C:113:ALA:CB	2.64	0.45
1:C:132:VAL:HG23	1:C:187:PHE:C	2.41	0.45
1:D:153:PHE:O	1:D:155:PRO:CA	2.60	0.45
1:A:10:ILE:HA	1:A:11:PHE:HA	1.72	0.45
1:A:214:HIS:NE2	1:A:221:ILE:HG12	2.23	0.45
1:C:9:ARG:CG	1:C:10:ILE:H	2.06	0.45
1:D:254:ARG:NH2	1:D:258:ASP:OD2	2.49	0.45
1:D:6:GLN:O	1:D:10:ILE:HG12	2.16	0.45
1:A:60:VAL:HB	1:A:65:ILE:HD11	1.95	0.45
1:B:95:ILE:O	1:B:99:GLN:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ASP:OD2	1:C:252:ARG:NH2	2.50	0.45
1:B:133:VAL:HG12	1:B:201:ARG:HG3	1.99	0.45
1:C:14:SER:HB3	1:C:17:THR:HG23	1.99	0.45
1:C:136:GLU:HB2	1:C:184:VAL:HG22	1.98	0.45
1:C:163:LYS:HD2	1:C:166:PRO:HA	1.98	0.45
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.78	0.45
1:C:90:THR:O	1:C:91:LEU:C	2.40	0.45
1:C:160:ILE:HG22	1:C:161:ALA:N	2.31	0.45
1:D:130:PHE:HD1	1:D:130:PHE:H	1.64	0.45
1:D:148:GLN:O	1:D:152:ARG:HD2	2.17	0.45
1:A:42:GLN:CG	1:A:43:PRO:CD	2.85	0.45
1:A:170:TYR:N	1:A:170:TYR:CD2	2.85	0.45
1:D:3:THR:HG22	1:D:6:GLN:HG3	1.89	0.45
1:D:248:TYR:CE2	1:D:250:ASP:HB2	2.52	0.45
1:A:18:LEU:O	1:A:21:TYR:N	2.50	0.44
1:A:122:ALA:O	1:A:236:ARG:NH2	2.49	0.44
1:C:150:TRP:CH2	1:C:185:ALA:HB1	2.53	0.44
1:C:225:PHE:HB3	1:D:10:ILE:CB	2.47	0.44
1:D:121:HIS:O	1:D:212:PHE:HD1	2.00	0.44
1:D:231:HIS:O	1:D:235:GLU:HG3	2.17	0.44
1:B:67:ARG:NH1	1:B:67:ARG:CG	2.80	0.44
1:D:95:ILE:C	1:D:99:GLN:HB2	2.43	0.44
1:A:98:ARG:HB2	1:D:95:ILE:HD11	2.00	0.44
1:B:112:LEU:HD23	1:B:112:LEU:N	2.17	0.44
1:C:51:ARG:O	1:C:54:ALA:HB3	2.17	0.44
1:D:152:ARG:O	1:D:155:PRO:CD	2.65	0.44
1:D:154:ILE:HD12	1:D:154:ILE:H	1.82	0.44
1:A:2:LEU:CD1	1:A:7:LEU:N	2.81	0.44
1:A:71:ASP:N	1:A:72:GLY:CA	2.81	0.44
1:A:214:HIS:O	1:A:262:GLN:HA	2.16	0.44
1:A:11:PHE:HD1	1:B:181:PHE:CE2	2.33	0.44
1:A:178:ASN:N	1:A:179:GLY:HA2	2.24	0.44
1:B:68:LEU:C	1:B:70:ARG:H	2.25	0.44
1:B:220:GLN:NE2	1:C:81:ARG:HH12	2.14	0.44
1:D:105:LEU:C	1:D:108:THR:HG22	2.43	0.44
1:D:212:PHE:CE2	1:D:267:ILE:HD11	2.53	0.44
1:A:105:LEU:HD21	1:D:84:LEU:CD2	2.48	0.44
1:B:4:ILE:HG12	1:B:15:THR:HG23	1.98	0.44
1:B:214:HIS:HD2	1:B:215:LYS:H	1.63	0.44
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.74	0.44
1:B:151:GLU:C	1:B:153:PHE:N	2.72	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:PHE:CD1	1:B:246:PHE:C	2.96	0.44
1:D:54:ALA:HA	1:D:57:ARG:HD2	2.00	0.44
1:B:207:GLN:HB3	1:B:241:LYS:HZ1	1.83	0.43
1:C:61:PRO:O	1:C:62:LEU:HD12	2.13	0.43
1:A:7:LEU:HD23	1:A:9:ARG:CD	2.48	0.43
1:A:22:ASP:CG	1:A:23:ALA:H	2.26	0.43
1:B:42:GLN:HB3	1:B:45:GLN:HG2	2.00	0.43
1:C:165:ASP:OD2	1:C:167:GLU:HB3	2.19	0.43
1:D:69:LYS:CE	1:D:70:ARG:NH1	2.69	0.43
1:D:153:PHE:HB3	1:D:154:ILE:H	1.51	0.43
1:D:228:ILE:HA	1:D:232:LEU:HD13	2.00	0.43
1:A:41:TYR:HD1	1:A:41:TYR:O	2.00	0.43
1:A:228:ILE:HA	1:A:232:LEU:HB2	1.99	0.43
1:B:18:LEU:HD11	1:B:41:TYR:CE2	2.53	0.43
1:D:3:THR:HG23	1:D:6:GLN:H	1.83	0.43
1:A:42:GLN:NE2	1:A:43:PRO:CD	2.73	0.43
1:A:75:ASP:CB	1:D:115:TRP:CH2	3.01	0.43
1:A:77:PRO:HG3	1:D:115:TRP:CE3	2.53	0.43
1:A:62:LEU:O	1:A:63:GLU:C	2.61	0.43
1:B:1:MET:SD	1:B:40:TYR:HB3	2.58	0.43
1:B:268:PRO:O	1:B:269:ILE:HD13	2.19	0.43
1:C:42:GLN:HB3	1:C:44:GLU:HG2	2.00	0.43
1:C:179:GLY:O	1:D:15:THR:HG21	2.18	0.43
1:D:3:THR:HG23	1:D:3:THR:O	2.18	0.43
1:A:79:ARG:O	1:A:81:ARG:N	2.51	0.43
1:A:247:GLU:OE1	1:A:249:TYR:OH	2.37	0.43
1:C:67:ARG:C	1:C:69:LYS:H	2.26	0.43
1:A:11:PHE:O	1:A:11:PHE:CD1	2.72	0.43
1:A:147:GLY:O	1:A:150:TRP:N	2.47	0.43
1:A:217:THR:HB	1:A:257:LEU:HA	2.00	0.43
1:B:89:HIS:HA	1:B:92:ARG:HG3	1.99	0.43
1:D:96:SER:O	1:D:100:ARG:HG2	2.19	0.43
1:A:4:ILE:HG13	1:A:5:GLY:N	2.33	0.43
1:C:56:ARG:HD3	1:C:56:ARG:HA	1.91	0.43
1:D:39:ARG:H	1:D:39:ARG:HG3	1.58	0.43
1:A:52:ILE:HG23	1:A:55:LEU:HG	2.00	0.43
1:B:116:ARG:HH11	1:B:116:ARG:CG	2.28	0.43
1:B:207:GLN:HE21	1:B:241:LYS:NZ	2.17	0.43
1:D:229:TYR:HD1	1:D:233:LEU:HD11	1.84	0.43
1:D:241:LYS:HG2	1:D:270:TYR:CD2	2.54	0.42
1:C:130:PHE:CZ	1:C:204:VAL:CG2	2.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LEU:CA	1:B:152:ARG:HD3	2.37	0.42
1:B:172:ILE:HD13	1:B:202:PHE:HD2	1.82	0.42
1:B:245:ASP:O	1:B:246:PHE:HB3	2.19	0.42
1:D:86:ARG:C	1:D:88:GLN:H	2.27	0.42
1:C:12:GLU:OE2	1:C:12:GLU:CA	2.67	0.42
1:A:6:GLN:O	1:A:8:ALA:N	2.51	0.42
1:A:52:ILE:O	1:A:53:LEU:C	2.47	0.42
1:A:154:ILE:N	1:A:155:PRO:HD2	2.34	0.42
1:B:58:LEU:C	1:B:60:VAL:H	2.26	0.42
1:D:122:ALA:HB2	1:D:212:PHE:CD1	2.50	0.42
1:A:181:PHE:O	1:A:182:HIS:HB2	2.20	0.42
1:D:147:GLY:H	1:D:150:TRP:H	1.67	0.42
1:B:101:LEU:HD13	1:C:58:LEU:HA	2.01	0.42
1:D:3:THR:HG21	1:D:6:GLN:CG	2.20	0.42
1:A:71:ASP:H	1:A:72:GLY:CA	2.32	0.42
1:C:134:GLY:O	1:C:199:MET:HA	2.19	0.42
1:C:167:GLU:HG2	1:C:251:GLN:OE1	2.19	0.42
1:A:46:ILE:CG2	1:A:47:GLU:N	2.49	0.42
1:A:61:PRO:HG2	1:A:64:ALA:CB	2.50	0.42
1:B:29:PRO:HD3	1:B:39:ARG:HH22	1.84	0.42
1:B:42:GLN:H	1:B:45:GLN:NE2	2.18	0.42
1:C:157:GLU:O	1:C:163:LYS:NZ	2.53	0.42
1:C:225:PHE:HB3	1:D:10:ILE:CG2	2.49	0.42
1:C:262:GLN:HE21	1:C:262:GLN:HB2	1.58	0.42
1:D:112:LEU:O	1:D:113:ALA:C	2.63	0.42
1:D:207:GLN:OE1	1:D:209:TYR:CE1	2.70	0.42
1:B:14:SER:OG	1:B:17:THR:HB	2.19	0.42
1:B:48:GLN:O	1:B:48:GLN:CG	2.68	0.42
1:B:90:THR:O	1:B:94:GLU:HG3	2.20	0.42
1:C:6:GLN:CD	1:C:6:GLN:N	2.76	0.42
1:C:206:ALA:O	1:C:207:GLN:HG3	2.20	0.42
1:D:112:LEU:HD13	1:D:112:LEU:HA	1.74	0.42
1:A:78:GLN:NE2	1:D:215:LYS:HB3	2.35	0.41
1:B:27:PHE:CE2	1:B:49:LEU:HG	2.55	0.41
1:B:110:ALA:HB3	1:D:110:ALA:HB3	2.01	0.41
1:B:154:ILE:HG13	1:B:154:ILE:H	1.57	0.41
1:B:207:GLN:HG3	1:B:209:TYR:CE1	2.55	0.41
1:B:217:THR:OG1	1:B:219:PRO:HD2	2.21	0.41
1:A:41:TYR:OH	1:B:239:GLU:CD	2.58	0.41
1:A:117:ILE:HG23	1:A:232:LEU:HD11	2.02	0.41
1:C:160:ILE:H	1:C:160:ILE:HG12	1.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:HG2	1:B:67:ARG:O	2.20	0.41
1:D:215:LYS:HE2	1:D:262:GLN:OE1	2.20	0.41
1:D:228:ILE:O	1:D:233:LEU:HG	2.20	0.41
1:C:66:ASP:O	1:C:69:LYS:HG2	2.20	0.41
1:A:111:THR:O	1:A:111:THR:CG2	2.69	0.41
1:A:224:SER:O	1:A:228:ILE:HG12	2.20	0.41
1:D:152:ARG:H	1:D:152:ARG:HG3	1.57	0.41
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.71	0.41
1:D:135:MET:HE3	1:D:153:PHE:CD1	2.44	0.41
1:B:221:ILE:HA	1:B:224:SER:HB2	2.01	0.41
1:B:228:ILE:CG1	1:B:229:TYR:H	2.21	0.41
1:A:75:ASP:HB2	1:D:115:TRP:HZ3	1.81	0.41
1:A:135:MET:HB2	1:A:153:PHE:CD1	2.56	0.41
1:B:84:LEU:O	1:B:88:GLN:N	2.50	0.41
1:C:20:HIS:HD2	1:C:21:TYR:CE1	2.39	0.41
1:D:3:THR:HG21	1:D:6:GLN:NE2	2.27	0.41
1:A:22:ASP:OD1	1:A:23:ALA:N	2.54	0.41
1:A:54:ALA:CB	1:A:57:ARG:CD	2.85	0.41
1:B:29:PRO:CD	1:B:29:PRO:O	2.69	0.41
1:C:67:ARG:C	1:C:69:LYS:N	2.77	0.41
1:C:71:ASP:N	1:C:72:GLY:HA2	2.22	0.41
1:C:135:MET:HE2	1:C:135:MET:HB2	1.78	0.41
1:C:154:ILE:O	1:C:157:GLU:HB2	2.20	0.41
1:C:159:GLU:HG2	1:C:196:PRO:HG3	2.02	0.41
1:D:200:VAL:CG2	1:D:201:ARG:H	2.32	0.41
1:B:18:LEU:CD1	1:B:41:TYR:CE2	3.04	0.41
1:B:145:THR:HG22	1:B:148:GLN:OE1	2.21	0.41
1:B:145:THR:O	1:B:148:GLN:HB2	2.21	0.41
1:B:214:HIS:CE1	1:B:221:ILE:HA	2.56	0.41
1:C:218:ALA:HB3	1:C:219:PRO:HD3	2.02	0.41
1:D:174:ALA:C	1:D:182:HIS:HB3	2.45	0.41
1:A:64:ALA:C	1:A:65:ILE:HD12	2.46	0.40
1:B:116:ARG:C	1:B:118:ARG:H	2.28	0.40
1:D:172:ILE:O	1:D:172:ILE:HG23	2.21	0.40
1:A:2:LEU:HD12	1:A:7:LEU:N	2.36	0.40
1:A:120:MET:HE3	1:A:228:ILE:HD11	2.03	0.40
1:B:93:GLU:HA	1:B:96:SER:HB2	2.03	0.40
1:D:208:LYS:HB3	1:D:269:ILE:O	2.21	0.40
1:A:9:ARG:H	1:A:9:ARG:HD3	1.84	0.40
1:A:65:ILE:O	1:A:65:ILE:CG2	2.68	0.40
1:B:110:ALA:O	1:B:113:ALA:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:HA	1:B:198:GLY:HA2	1.48	0.40
1:B:210:ALA:HB2	1:B:269:ILE:HD11	2.03	0.40
1:C:6:GLN:OE1	1:C:6:GLN:CA	2.68	0.40
1:C:154:ILE:N	1:C:155:PRO:CD	2.85	0.40
1:C:213:THR:CG2	1:C:262:GLN:HE21	2.35	0.40
1:D:156:ARG:HE	1:D:156:ARG:HB3	1.78	0.40
1:C:71:ASP:OD1	1:C:72:GLY:CA	2.69	0.40
1:D:183:TYR:O	1:D:184:VAL:CG2	2.70	0.40

All (7) 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:B:203:GLN:OE1	1:D:38:TYR:O[5_555]	1.36	0.84
1:A:119:ASN:ND2	1:C:164:HIS:CD2[5_445]	1.83	0.37
1:A:158:HIS:ND1	1:B:70:ARG:NH1[5_445]	1.89	0.31
1:B:203:GLN:OE1	1:D:38:TYR:C[5_555]	1.98	0.22
1:A:158:HIS:CB	1:B:70:ARG:NH1[5_445]	2.04	0.16
1:A:119:ASN:ND2	1:C:164:HIS:NE2[5_445]	2.17	0.03
1:A:158:HIS:CG	1:B:70:ARG:NH1[5_445]	2.19	0.01

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	243/291 (84%)	195 (80%)	31 (13%)	17 (7%)	1	2
1	B	246/291 (84%)	203 (82%)	33 (13%)	10 (4%)	2	9
1	C	243/291 (84%)	185 (76%)	44 (18%)	14 (6%)	1	4
1	D	246/291 (84%)	196 (80%)	29 (12%)	21 (8%)	0	1
All	All	978/1164 (84%)	779 (80%)	137 (14%)	62 (6%)	1	3

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	13	ILE
1	A	16	LYS
1	A	23	ALA
1	A	24	ILE
1	A	53	LEU
1	A	57	ARG
1	A	80	LEU
1	A	181	PHE
1	A	182	HIS
1	B	53	LEU
1	B	59	ASP
1	B	66	ASP
1	B	73	ALA
1	B	117	ILE
1	C	6	GLN
1	C	65	ILE
1	C	91	LEU
1	C	92	ARG
1	C	196	PRO
1	C	252	ARG
1	D	65	ILE
1	D	66	ASP
1	D	73	ALA
1	D	87	HIS
1	D	106	ASP
1	D	113	ALA
1	D	153	PHE
1	D	154	ILE
1	D	182	HIS
1	D	262	GLN
1	A	54	ALA
1	B	65	ILE
1	B	229	TYR
1	B	252	ARG
1	C	10	ILE
1	D	114	HIS
1	D	115	TRP
1	D	120	MET
1	D	180	GLU
1	D	196	PRO
1	A	79	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	88	GLN
1	B	52	ILE
1	C	57	ARG
1	C	63	GLU
1	C	64	ALA
1	C	177	PRO
1	C	183	TYR
1	D	26	LEU
1	D	86	ARG
1	D	183	TYR
1	D	213	THR
1	A	15	THR
1	A	46	ILE
1	A	52	ILE
1	A	56	ARG
1	C	12	GLU
1	B	50	SER
1	C	181	PHE
1	D	97	ALA
1	D	184	VAL

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	213/245 (87%)	191 (90%)	22 (10%)	7	23
1	B	217/245 (89%)	196 (90%)	21 (10%)	8	25
1	C	213/245 (87%)	186 (87%)	27 (13%)	4	14
1	D	217/245 (89%)	181 (83%)	36 (17%)	2	7
All	All	860/980 (88%)	754 (88%)	106 (12%)	4	15

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	9	ARG
1	A	13	ILE
1	A	16	LYS
1	A	18	LEU
1	A	24	ILE
1	A	26	LEU
1	A	44	GLU
1	A	46	ILE
1	A	51	ARG
1	A	56	ARG
1	A	57	ARG
1	A	78	GLN
1	A	80	LEU
1	A	86	ARG
1	A	87	HIS
1	A	112	LEU
1	A	124	ILE
1	A	145	THR
1	A	148	GLN
1	A	180	GLU
1	A	240	PRO
1	B	28	VAL
1	B	29	PRO
1	B	42	GLN
1	B	47	GLU
1	B	49	LEU
1	B	65	ILE
1	B	105	LEU
1	B	106	ASP
1	B	108	THR
1	B	109	LEU
1	B	116	ARG
1	B	152	ARG
1	B	160	ILE
1	B	199	MET
1	B	211	VAL
1	B	224	SER
1	B	228	ILE
1	B	241	LYS
1	B	245	ASP
1	B	247	GLU
1	B	253	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4	ILE
1	C	7	LEU
1	C	9	ARG
1	C	56	ARG
1	C	61	PRO
1	C	63	GLU
1	C	91	LEU
1	C	99	GLN
1	C	107	ARG
1	C	119	ASN
1	C	120	MET
1	C	133	VAL
1	C	135	MET
1	C	136	GLU
1	C	157	GLU
1	C	159	GLU
1	C	163	LYS
1	C	169	SER
1	C	188	GLU
1	C	189	VAL
1	C	199	MET
1	C	230	SER
1	C	235	GLU
1	C	241	LYS
1	C	245	ASP
1	C	251	GLN
1	C	262	GLN
1	D	7	LEU
1	D	9	ARG
1	D	27	PHE
1	D	50	SER
1	D	61	PRO
1	D	62	LEU
1	D	63	GLU
1	D	67	ARG
1	D	70	ARG
1	D	71	ASP
1	D	79	ARG
1	D	81	ARG
1	D	85	GLN
1	D	88	GLN
1	D	95	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	96	SER
1	D	99	GLN
1	D	107	ARG
1	D	114	HIS
1	D	116	ARG
1	D	120	MET
1	D	130	PHE
1	D	133	VAL
1	D	150	TRP
1	D	163	LYS
1	D	172	ILE
1	D	180	GLU
1	D	197	GLU
1	D	203	GLN
1	D	204	VAL
1	D	205	PRO
1	D	208	LYS
1	D	211	VAL
1	D	214	HIS
1	D	238	LEU
1	D	267	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	87	HIS
1	A	148	GLN
1	A	164	HIS
1	A	207	GLN
1	A	220	GLN
1	A	226	GLN
1	A	231	HIS
1	B	45	GLN
1	B	48	GLN
1	B	87	HIS
1	B	88	GLN
1	B	89	HIS
1	B	207	GLN
1	B	214	HIS
1	B	220	GLN
1	C	20	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	87	HIS
1	C	114	HIS
1	C	158	HIS
1	C	182	HIS
1	C	203	GLN
1	C	262	GLN
1	D	6	GLN
1	D	88	GLN
1	D	89	HIS
1	D	114	HIS
1	D	121	HIS
1	D	207	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	249/291 (85%)	-0.45	1 (0%) 88 85	25, 55, 113, 169	0
1	B	254/291 (87%)	-0.37	0 100 100	33, 59, 93, 134	0
1	C	249/291 (85%)	-0.40	3 (1%) 76 69	16, 58, 111, 160	0
1	D	254/291 (87%)	0.09	10 (3%) 43 35	39, 70, 104, 135	0
All	All	1006/1164 (86%)	-0.28	14 (1%) 73 65	16, 62, 110, 169	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	ALA	3.5
1	C	78	GLN	3.1
1	D	99	GLN	2.5
1	D	114	HIS	2.5
1	D	182	HIS	2.5
1	A	8	ALA	2.4
1	D	77	PRO	2.4
1	C	178	ASN	2.2
1	D	100	ARG	2.2
1	D	198	GLY	2.1
1	D	102	LEU	2.1
1	D	225	PHE	2.1
1	D	178	ASN	2.1
1	C	52	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.