



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:37 am BST

PDB ID : 2YPI
Title : CRYSTALLOGRAPHIC ANALYSIS OF THE COMPLEX BETWEEN
TRIOSEPHOSPHATE ISOMERASE AND 2-PHOSPHOGLYCOLATE AT
2.5-ANGSTROMS RESOLUTION. IMPLICATIONS FOR CATALYSIS
Authors : Lolis, E.; Petsko, G.A.
Deposited on : 1990-01-12
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

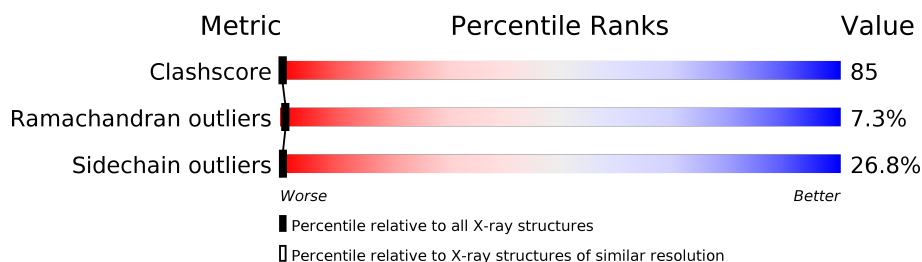
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGA	B	249	-	X	-	-

2 Entry composition [i](#)

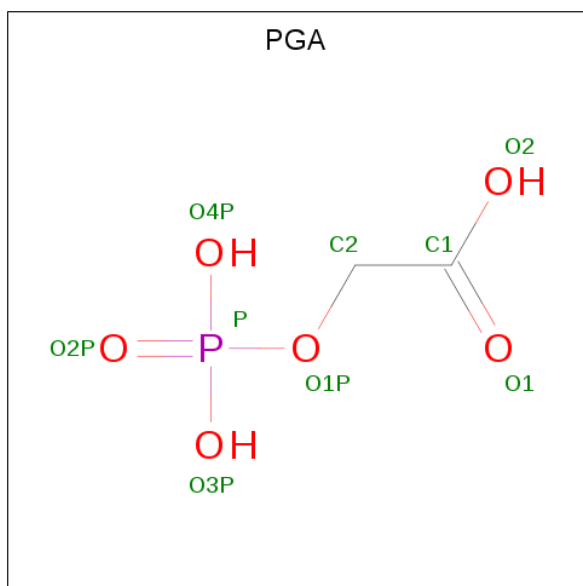
There are 3 unique types of molecules in this entry. The entry contains 3809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			
1	B	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is water.

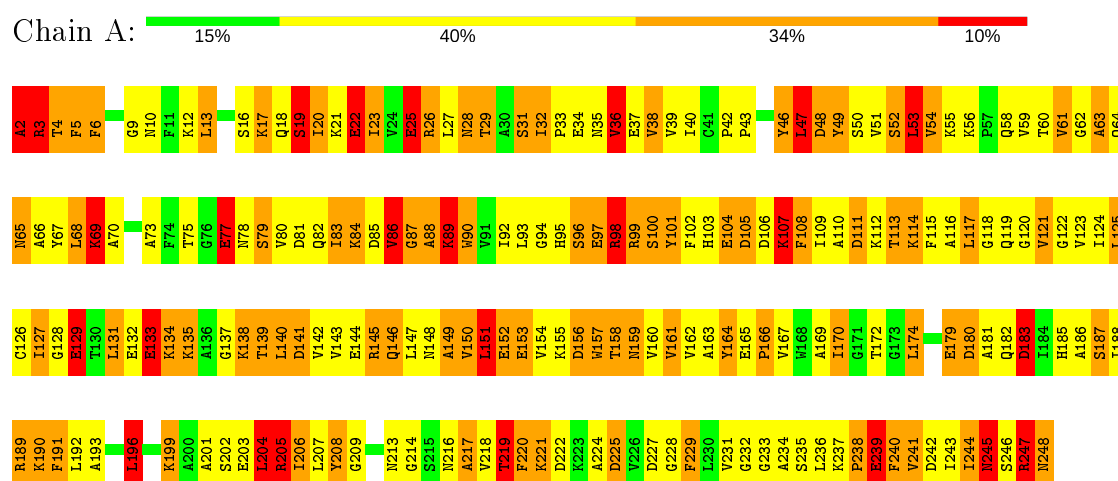
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	13	Total 13	O 13	0	0

3 Residue-property plots

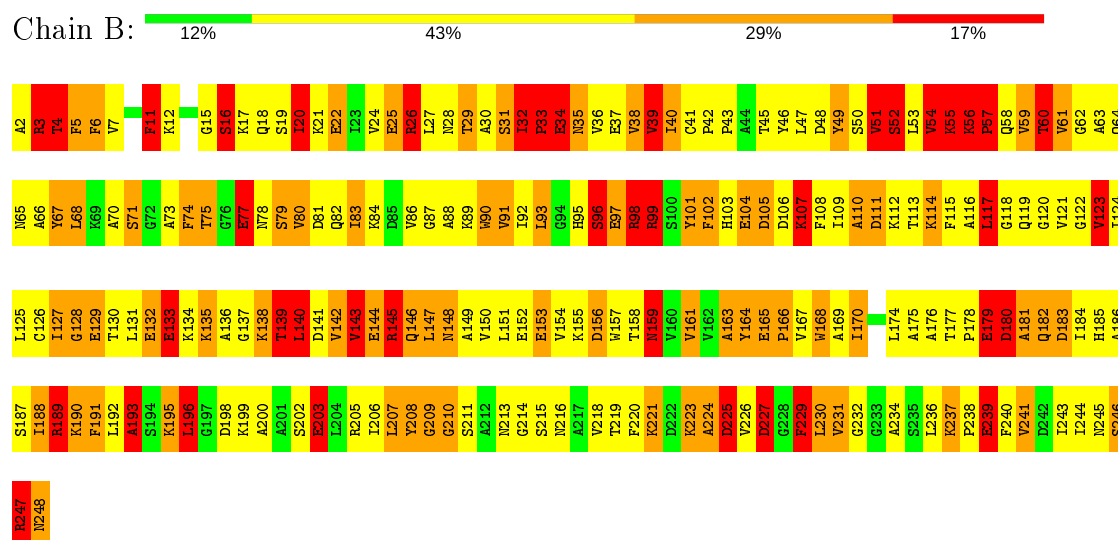
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: TRIOSEPHOSPHATE ISOMERASE



- Molecule 1: TRIOSEPHOSPHATE ISOMERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.35Å 83.97Å 38.67Å 90.00° 99.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3809	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2.08	44/1915 (2.3%)	2.70	165/2590 (6.4%)
1	B	2.12	45/1915 (2.3%)	2.66	136/2590 (5.3%)
All	All	2.10	89/3830 (2.3%)	2.68	301/5180 (5.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	GLU	CD-OE2	12.20	1.39	1.25
1	A	132	GLU	CD-OE2	11.91	1.38	1.25
1	A	25	GLU	CD-OE2	11.33	1.38	1.25
1	B	25	GLU	CD-OE2	11.02	1.37	1.25
1	A	133	GLU	CD-OE2	10.73	1.37	1.25
1	B	179	GLU	CD-OE2	10.21	1.36	1.25
1	A	203	GLU	CD-OE2	10.13	1.36	1.25
1	B	152	GLU	CD-OE1	-9.18	1.15	1.25
1	B	34	GLU	CD-OE2	9.11	1.35	1.25
1	A	239	GLU	CD-OE2	9.06	1.35	1.25
1	B	153	GLU	CD-OE2	8.66	1.35	1.25
1	B	133	GLU	CD-OE2	8.54	1.35	1.25
1	A	132	GLU	CG-CD	-8.50	1.39	1.51
1	A	22	GLU	CD-OE2	8.15	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	GLU	CB-CG	8.08	1.67	1.52
1	A	77	GLU	CD-OE2	7.99	1.34	1.25
1	B	203	GLU	CD-OE2	7.92	1.34	1.25
1	A	34	GLU	CB-CG	7.84	1.67	1.52
1	A	104	GLU	CD-OE2	7.51	1.33	1.25
1	A	239	GLU	CD-OE1	-7.45	1.17	1.25
1	B	129	GLU	CD-OE2	7.39	1.33	1.25
1	B	165	GLU	CB-CG	7.26	1.66	1.52
1	A	87	GLY	N-CA	7.20	1.56	1.46
1	B	96	SER	CB-OG	7.08	1.51	1.42
1	B	97	GLU	CG-CD	-7.01	1.41	1.51
1	B	247	ARG	NE-CZ	6.95	1.42	1.33
1	B	129	GLU	CG-CD	-6.92	1.41	1.51
1	B	139	THR	C-O	6.89	1.36	1.23
1	A	104	GLU	CD-OE1	-6.85	1.18	1.25
1	B	98	ARG	NE-CZ	6.85	1.42	1.33
1	B	97	GLU	CD-OE2	6.75	1.33	1.25
1	A	108	PHE	N-CA	6.67	1.59	1.46
1	A	162	VAL	CA-CB	-6.64	1.40	1.54
1	A	129	GLU	CG-CD	-6.55	1.42	1.51
1	A	120	GLY	N-CA	6.53	1.55	1.46
1	A	48	ASP	N-CA	6.51	1.59	1.46
1	A	3	ARG	N-CA	-6.46	1.33	1.46
1	A	34	GLU	CD-OE2	6.41	1.32	1.25
1	B	239	GLU	CD-OE2	6.33	1.32	1.25
1	A	129	GLU	CD-OE2	6.29	1.32	1.25
1	B	205	ARG	CD-NE	-6.27	1.35	1.46
1	A	100	SER	N-CA	6.25	1.58	1.46
1	A	46	TYR	CG-CD1	6.20	1.47	1.39
1	B	229	PHE	CG-CD2	6.20	1.48	1.38
1	A	179	GLU	CD-OE2	6.17	1.32	1.25
1	A	203	GLU	CB-CG	6.15	1.63	1.52
1	B	209	GLY	C-O	6.15	1.33	1.23
1	A	187	SER	CB-OG	6.07	1.50	1.42
1	B	33	PRO	CA-CB	6.00	1.65	1.53
1	A	62	GLY	N-CA	6.00	1.55	1.46
1	A	166	PRO	N-CD	5.97	1.56	1.47
1	A	141	ASP	CA-CB	-5.95	1.40	1.53
1	A	219	THR	CB-OG1	-5.92	1.31	1.43
1	B	74	PHE	N-CA	5.91	1.58	1.46
1	B	99	ARG	CD-NE	-5.89	1.36	1.46
1	A	245	ASN	C-O	5.86	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	GLU	CB-CG	-5.79	1.41	1.52
1	A	19	SER	CB-OG	5.75	1.49	1.42
1	B	87	GLY	C-O	5.68	1.32	1.23
1	A	31	SER	CA-C	5.67	1.67	1.52
1	B	229	PHE	CE2-CZ	5.67	1.48	1.37
1	A	26	ARG	CD-NE	-5.66	1.36	1.46
1	A	145	ARG	NE-CZ	5.66	1.40	1.33
1	B	214	GLY	C-O	5.62	1.32	1.23
1	B	31	SER	CB-OG	-5.58	1.35	1.42
1	B	25	GLU	CB-CG	5.57	1.62	1.52
1	A	133	GLU	CA-CB	-5.55	1.41	1.53
1	A	79	SER	CB-OG	5.51	1.49	1.42
1	B	104	GLU	CD-OE2	5.49	1.31	1.25
1	B	179	GLU	CB-CG	5.46	1.62	1.52
1	B	5	PHE	CE1-CZ	5.41	1.47	1.37
1	A	153	GLU	CG-CD	-5.36	1.44	1.51
1	A	170	ILE	CA-CB	-5.35	1.42	1.54
1	A	153	GLU	CD-OE1	5.34	1.31	1.25
1	B	208	TYR	CE1-CZ	5.33	1.45	1.38
1	B	22	GLU	CD-OE1	-5.32	1.19	1.25
1	B	33	PRO	N-CA	-5.29	1.38	1.47
1	B	49	TYR	CE1-CZ	5.26	1.45	1.38
1	A	157	TRP	CD2-CE2	5.22	1.47	1.41
1	B	67	TYR	CE1-CZ	5.20	1.45	1.38
1	B	246	SER	CB-OG	5.20	1.49	1.42
1	B	74	PHE	CA-CB	-5.18	1.42	1.53
1	B	63	ALA	CA-CB	5.18	1.63	1.52
1	A	247	ARG	C-N	-5.15	1.22	1.34
1	B	248	ASN	C-OXT	5.09	1.33	1.23
1	B	248	ASN	CB-CG	5.08	1.62	1.51
1	A	3	ARG	C-O	5.05	1.32	1.23
1	B	41	CYS	CB-SG	-5.05	1.73	1.81
1	B	90	TRP	CG-CD1	5.03	1.43	1.36

All (301) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ARG	CD-NE-CZ	26.91	161.27	123.60
1	A	2	ALA	C-N-CA	21.34	175.06	121.70
1	A	17	LYS	CA-CB-CG	15.39	147.25	113.40
1	B	247	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	B	145	ARG	NE-CZ-NH2	13.28	126.94	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH2	12.94	126.77	120.30
1	A	99	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	A	189	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	B	227	ASP	CB-CG-OD1	12.21	129.29	118.30
1	A	242	ASP	CB-CG-OD2	-12.07	107.44	118.30
1	A	164	TYR	CB-CG-CD2	12.01	128.21	121.00
1	B	101	TYR	CA-CB-CG	11.96	136.12	113.40
1	A	117	LEU	CA-CB-CG	11.51	141.76	115.30
1	A	132	GLU	OE1-CD-OE2	-11.38	109.64	123.30
1	A	26	ARG	NE-CZ-NH2	11.29	125.94	120.30
1	B	99	ARG	CG-CD-NE	11.15	135.22	111.80
1	A	152	GLU	CA-CB-CG	11.02	137.63	113.40
1	B	99	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	B	37	GLU	OE1-CD-OE2	10.79	136.25	123.30
1	A	141	ASP	CB-CG-OD1	10.79	128.01	118.30
1	B	33	PRO	N-CA-C	10.70	139.91	112.10
1	A	101	TYR	CB-CG-CD1	10.31	127.18	121.00
1	A	31	SER	N-CA-CB	10.22	125.83	110.50
1	A	132	GLU	CA-CB-CG	10.20	135.83	113.40
1	B	145	ARG	NE-CZ-NH1	-10.01	115.30	120.30
1	A	145	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	B	33	PRO	CA-C-O	9.72	143.53	120.20
1	A	132	GLU	CB-CG-CD	9.69	140.36	114.20
1	B	156	ASP	CB-CG-OD2	9.64	126.97	118.30
1	A	225	ASP	CB-CG-OD1	9.56	126.90	118.30
1	B	54	VAL	C-N-CA	9.54	145.56	121.70
1	A	164	TYR	CB-CG-CD1	-9.48	115.31	121.00
1	B	223	LYS	CB-CG-CD	9.33	135.85	111.60
1	B	152	GLU	OE1-CD-OE2	9.19	134.33	123.30
1	A	132	GLU	CG-CD-OE1	9.17	136.65	118.30
1	B	147	LEU	CA-CB-CG	9.06	136.15	115.30
1	B	26	ARG	CG-CD-NE	9.01	130.71	111.80
1	B	60	THR	CA-CB-CG2	8.96	124.95	112.40
1	B	111	ASP	CA-CB-CG	8.82	132.80	113.40
1	A	133	GLU	CA-CB-CG	8.74	132.62	113.40
1	A	138	LYS	C-N-CA	8.67	143.38	121.70
1	A	225	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	A	46	TYR	CA-CB-CG	8.57	129.69	113.40
1	A	26	ARG	NH1-CZ-NH2	-8.53	110.02	119.40
1	B	3	ARG	C-N-CA	8.52	143.01	121.70
1	B	3	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	B	26	ARG	NE-CZ-NH2	8.49	124.55	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ARG	CD-NE-CZ	8.38	135.33	123.60
1	A	96	SER	N-CA-CB	8.33	122.99	110.50
1	B	99	ARG	NH1-CZ-NH2	-8.16	110.42	119.40
1	A	81	ASP	CB-CG-OD2	8.12	125.61	118.30
1	B	33	PRO	CA-C-N	-8.12	99.35	117.20
1	A	48	ASP	CB-CA-C	8.00	126.40	110.40
1	A	105	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	A	25	GLU	CG-CD-OE1	7.96	134.22	118.30
1	A	101	TYR	CG-CD1-CE1	7.96	127.67	121.30
1	B	99	ARG	CD-NE-CZ	7.96	134.74	123.60
1	A	146	GLN	CA-CB-CG	7.95	130.89	113.40
1	A	181	ALA	N-CA-CB	7.87	121.12	110.10
1	A	121	VAL	CB-CA-C	7.81	126.24	111.40
1	A	131	LEU	CA-CB-CG	7.81	133.26	115.30
1	B	148	ASN	CB-CA-C	7.74	125.87	110.40
1	A	196	LEU	CB-CG-CD2	7.69	124.07	111.00
1	A	61	VAL	CG1-CB-CG2	-7.61	98.72	110.90
1	A	101	TYR	CG-CD2-CE2	7.59	127.37	121.30
1	A	189	ARG	NH1-CZ-NH2	-7.55	111.09	119.40
1	A	69	LYS	CB-CG-CD	7.54	131.19	111.60
1	A	2	ALA	O-C-N	-7.49	110.71	122.70
1	B	226	VAL	O-C-N	7.48	134.67	122.70
1	A	22	GLU	CA-CB-CG	7.44	129.77	113.40
1	B	55	LYS	N-CA-CB	7.41	123.94	110.60
1	B	22	GLU	CA-CB-CG	7.38	129.65	113.40
1	B	205	ARG	CD-NE-CZ	7.34	133.88	123.60
1	A	31	SER	O-C-N	7.34	134.44	122.70
1	B	230	LEU	N-CA-CB	7.33	125.06	110.40
1	A	107	LYS	CA-CB-CG	7.32	129.50	113.40
1	B	102	PHE	C-N-CA	7.28	139.89	121.70
1	A	101	TYR	CZ-CE2-CD2	-7.27	113.26	119.80
1	A	141	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	A	247	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	101	TYR	CA-CB-CG	7.19	127.07	113.40
1	A	84	LYS	CA-CB-CG	7.19	129.22	113.40
1	B	133	GLU	CB-CA-C	7.18	124.77	110.40
1	A	69	LYS	CA-CB-CG	7.15	129.13	113.40
1	B	180	ASP	CB-CG-OD1	7.14	124.72	118.30
1	B	52	SER	N-CA-CB	-7.11	99.84	110.50
1	A	29	THR	CA-CB-CG2	7.08	122.32	112.40
1	B	110	ALA	N-CA-CB	-7.08	100.18	110.10
1	B	63	ALA	N-CA-CB	-7.08	100.18	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	GLU	CG-CD-OE2	-7.04	104.22	118.30
1	B	22	GLU	CG-CD-OE2	-7.04	104.23	118.30
1	A	26	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	203	GLU	OE1-CD-OE2	-7.02	114.87	123.30
1	B	3	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	11	PHE	CB-CG-CD1	-7.00	115.90	120.80
1	B	207	LEU	O-C-N	6.98	133.87	122.70
1	B	203	GLU	CA-CB-CG	6.96	128.71	113.40
1	A	205	ARG	NH1-CZ-NH2	-6.94	111.77	119.40
1	B	193	ALA	CB-CA-C	-6.93	99.70	110.10
1	B	99	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	B	37	GLU	CG-CD-OE2	-6.90	104.51	118.30
1	B	15	GLY	C-N-CA	6.86	138.85	121.70
1	A	141	ASP	CA-CB-CG	6.86	128.49	113.40
1	A	153	GLU	CA-CB-CG	6.85	128.48	113.40
1	B	129	GLU	CG-CD-OE1	6.81	131.92	118.30
1	B	247	ARG	O-C-N	-6.80	111.82	122.70
1	B	214	GLY	C-N-CA	6.75	138.58	121.70
1	B	180	ASP	CB-CA-C	6.74	123.88	110.40
1	B	181	ALA	N-CA-CB	6.73	119.53	110.10
1	B	101	TYR	CZ-CE2-CD2	-6.68	113.78	119.80
1	B	117	LEU	CB-CA-C	6.68	122.89	110.20
1	B	144	GLU	CA-CB-CG	6.66	128.05	113.40
1	A	108	PHE	CA-CB-CG	6.64	129.84	113.90
1	B	129	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	A	217	ALA	CB-CA-C	6.64	120.06	110.10
1	A	98	ARG	CD-NE-CZ	6.61	132.85	123.60
1	B	39	VAL	N-CA-CB	6.60	126.03	111.50
1	A	36	VAL	CA-C-O	6.57	133.90	120.10
1	A	111	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	168	TRP	CB-CG-CD1	6.55	135.52	127.00
1	A	5	PHE	CB-CA-C	6.53	123.46	110.40
1	A	111	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	151	LEU	O-C-N	6.51	133.12	122.70
1	A	129	GLU	CG-CD-OE1	6.48	131.26	118.30
1	A	129	GLU	CA-CB-CG	6.46	127.62	113.40
1	A	156	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	81	ASP	OD1-CG-OD2	-6.45	111.04	123.30
1	B	59	VAL	CA-CB-CG2	-6.44	101.24	110.90
1	B	49	TYR	CD1-CE1-CZ	-6.43	114.01	119.80
1	A	36	VAL	CA-C-N	-6.42	103.08	117.20
1	B	164	TYR	N-CA-CB	6.42	122.16	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ALA	O-C-N	6.42	132.97	122.70
1	B	128	GLY	CA-C-O	-6.41	109.06	120.60
1	A	163	ALA	CB-CA-C	6.39	119.69	110.10
1	B	34	GLU	CG-CD-OE2	-6.38	105.54	118.30
1	B	195	LYS	N-CA-C	-6.36	93.83	111.00
1	B	3	ARG	CB-CA-C	6.31	123.02	110.40
1	B	225	ASP	O-C-N	6.31	132.80	122.70
1	A	25	GLU	CG-CD-OE2	-6.29	105.71	118.30
1	B	73	ALA	O-C-N	6.26	132.71	122.70
1	B	68	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	111	ASP	OD1-CG-OD2	-6.25	111.43	123.30
1	A	240	PHE	CB-CG-CD2	-6.24	116.43	120.80
1	A	238	PRO	C-N-CA	6.23	137.27	121.70
1	A	220	PHE	C-N-CA	6.22	137.25	121.70
1	A	164	TYR	O-C-N	6.22	132.65	122.70
1	B	47	LEU	O-C-N	-6.21	112.77	122.70
1	B	51	VAL	CB-CA-C	6.19	123.16	111.40
1	A	87	GLY	C-N-CA	6.18	137.14	121.70
1	B	183	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	99	ARG	CD-NE-CZ	-6.16	114.98	123.60
1	B	105	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	247	ARG	N-CA-CB	-6.14	99.55	110.60
1	B	54	VAL	CA-CB-CG2	6.14	120.11	110.90
1	A	29	THR	C-N-CA	6.14	137.04	121.70
1	A	180	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	200	ALA	O-C-N	6.12	132.50	122.70
1	A	201	ALA	N-CA-CB	-6.12	101.53	110.10
1	B	198	ASP	CA-C-O	-6.08	107.34	120.10
1	B	163	ALA	N-CA-CB	6.07	118.60	110.10
1	A	68	LEU	C-N-CA	6.07	136.87	121.70
1	A	69	LYS	N-CA-CB	6.07	121.52	110.60
1	B	99	ARG	CA-CB-CG	6.05	126.70	113.40
1	A	111	ASP	CB-CA-C	6.03	122.46	110.40
1	A	170	ILE	C-N-CA	6.01	134.93	122.30
1	B	111	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	5	PHE	CB-CG-CD1	6.01	125.01	120.80
1	B	152	GLU	CG-CD-OE2	-6.01	106.29	118.30
1	A	54	VAL	CG1-CB-CG2	6.00	120.51	110.90
1	B	179	GLU	CG-CD-OE1	6.00	130.29	118.30
1	A	196	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	5	PHE	CG-CD2-CE2	5.97	127.36	120.80
1	A	86	VAL	N-CA-CB	5.93	124.55	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	HIS	CA-CB-CG	-5.93	103.51	113.60
1	B	241	VAL	CB-CA-C	5.91	122.62	111.40
1	B	157	TRP	CG-CD1-NE1	5.90	116.00	110.10
1	B	49	TYR	CG-CD1-CE1	5.90	126.02	121.30
1	B	229	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	A	28	ASN	O-C-N	5.90	132.14	122.70
1	A	100	SER	N-CA-CB	-5.90	101.66	110.50
1	B	22	GLU	CG-CD-OE1	5.89	130.09	118.30
1	B	189	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	86	VAL	CB-CA-C	-5.88	100.22	111.40
1	B	101	TYR	N-CA-CB	5.88	121.19	110.60
1	A	83	ILE	CA-CB-CG2	5.88	122.65	110.90
1	B	140	LEU	CB-CA-C	5.88	121.36	110.20
1	A	89	LYS	C-N-CA	5.87	136.38	121.70
1	B	232	GLY	N-CA-C	-5.85	98.48	113.10
1	A	47	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	47	LEU	CA-CB-CG	5.83	128.72	115.30
1	B	57	PRO	N-CA-C	-5.80	97.01	112.10
1	A	49	TYR	CA-CB-CG	5.79	124.40	113.40
1	A	224	ALA	O-C-N	-5.79	113.44	122.70
1	A	162	VAL	CB-CA-C	5.78	122.38	111.40
1	A	204	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	A	232	GLY	C-N-CA	5.77	134.41	122.30
1	A	4	THR	CA-CB-CG2	-5.76	104.33	112.40
1	B	71	SER	CB-CA-C	5.76	121.05	110.10
1	A	48	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	5	PHE	CG-CD2-CE2	5.73	127.10	120.80
1	B	75	THR	N-CA-CB	-5.73	99.42	110.30
1	A	5	PHE	CZ-CE2-CD2	-5.72	113.24	120.10
1	A	247	ARG	N-CA-C	5.67	126.30	111.00
1	A	180	ASP	CB-CA-C	5.66	121.72	110.40
1	A	90	TRP	CH2-CZ2-CE2	-5.61	111.79	117.40
1	A	6	PHE	CB-CG-CD1	-5.61	116.88	120.80
1	B	4	THR	CA-CB-OG1	-5.60	97.24	109.00
1	B	182	GLN	CB-CA-C	-5.60	99.20	110.40
1	B	183	ASP	CB-CA-C	5.60	121.60	110.40
1	A	121	VAL	N-CA-CB	-5.60	99.19	111.50
1	A	229	PHE	CB-CG-CD1	-5.58	116.90	120.80
1	A	3	ARG	N-CA-C	5.57	126.05	111.00
1	B	166	PRO	N-CA-C	-5.57	97.62	112.10
1	B	26	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
1	B	16	SER	CB-CA-C	5.55	120.65	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	PRO	O-C-N	-5.54	113.83	122.70
1	B	5	PHE	CA-CB-CG	5.54	127.19	113.90
1	A	31	SER	CA-C-N	-5.53	105.03	117.20
1	A	181	ALA	O-C-N	5.53	131.55	122.70
1	B	146	GLN	C-N-CA	5.53	135.52	121.70
1	B	123	VAL	CB-CA-C	5.53	121.90	111.40
1	A	183	ASP	O-C-N	5.52	131.53	122.70
1	A	124	ILE	C-N-CA	5.51	135.48	121.70
1	A	2	ALA	CA-C-N	5.49	129.29	117.20
1	A	199	LYS	N-CA-CB	5.45	120.41	110.60
1	A	88	ALA	O-C-N	5.45	131.42	122.70
1	A	133	GLU	CG-CD-OE1	5.45	129.19	118.30
1	A	26	ARG	CA-CB-CG	5.44	125.37	113.40
1	A	133	GLU	N-CA-CB	5.43	120.37	110.60
1	B	148	ASN	CA-CB-CG	-5.41	101.49	113.40
1	B	59	VAL	CB-CA-C	5.41	121.67	111.40
1	A	222	ASP	CB-CA-C	5.40	121.20	110.40
1	B	91	VAL	O-C-N	5.40	131.33	122.70
1	B	163	ALA	CA-C-N	-5.38	105.36	117.20
1	A	202	SER	O-C-N	5.37	131.29	122.70
1	A	222	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	246	SER	N-CA-CB	-5.35	102.48	110.50
1	B	231	VAL	CA-CB-CG2	5.34	118.91	110.90
1	A	167	VAL	CA-CB-CG1	5.34	118.91	110.90
1	B	205	ARG	CA-C-O	5.34	131.31	120.10
1	B	175	ALA	CB-CA-C	5.34	118.10	110.10
1	A	229	PHE	N-CA-CB	-5.33	101.00	110.60
1	B	196	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	B	140	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	53	LEU	CB-CA-C	5.31	120.29	110.20
1	A	204	LEU	O-C-N	5.30	131.19	122.70
1	A	62	GLY	N-CA-C	-5.29	99.86	113.10
1	B	92	ILE	N-CA-C	-5.29	96.72	111.00
1	A	53	LEU	CA-CB-CG	-5.28	103.15	115.30
1	A	183	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	132	GLU	OE1-CD-OE2	5.28	129.64	123.30
1	A	63	ALA	CB-CA-C	5.25	117.97	110.10
1	A	129	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	A	150	VAL	CA-CB-CG1	5.23	118.75	110.90
1	A	13	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	74	PHE	CB-CA-C	5.22	120.84	110.40
1	B	226	VAL	CB-CA-C	5.22	121.32	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLU	CB-CG-CD	5.22	128.29	114.20
1	A	141	ASP	N-CA-C	-5.20	96.97	111.00
1	A	81	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	189	ARG	CB-CG-CD	5.19	125.09	111.60
1	B	189	ARG	CB-CA-C	5.19	120.77	110.40
1	B	128	GLY	O-C-N	5.18	130.99	122.70
1	B	247	ARG	CD-NE-CZ	-5.18	116.35	123.60
1	B	107	LYS	O-C-N	5.17	130.97	122.70
1	B	3	ARG	N-CA-C	-5.16	97.06	111.00
1	A	34	GLU	N-CA-CB	5.16	119.89	110.60
1	A	97	GLU	OE1-CD-OE2	5.15	129.49	123.30
1	A	35	ASN	O-C-N	5.15	130.94	122.70
1	A	139	THR	CA-CB-OG1	-5.15	98.19	109.00
1	B	176	ALA	N-CA-C	-5.14	97.12	111.00
1	A	22	GLU	CA-C-O	5.13	130.87	120.10
1	A	126	CYS	CA-C-O	5.13	130.87	120.10
1	A	247	ARG	CA-CB-CG	-5.12	102.13	113.40
1	B	77	GLU	O-C-N	5.11	130.88	122.70
1	A	156	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	61	VAL	CB-CA-C	5.11	121.10	111.40
1	B	166	PRO	CB-CA-C	5.11	124.77	112.00
1	A	28	ASN	N-CA-CB	5.10	119.78	110.60
1	A	101	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
1	A	32	ILE	CB-CA-C	5.09	121.79	111.60
1	A	65	ASN	CB-CA-C	5.09	120.57	110.40
1	A	190	LYS	CA-C-N	-5.08	106.02	117.20
1	A	208	TYR	CB-CG-CD1	5.08	124.05	121.00
1	B	168	TRP	CG-CD1-NE1	5.07	115.17	110.10
1	B	5	PHE	CB-CG-CD2	5.07	124.35	120.80
1	A	19	SER	CB-CA-C	-5.05	100.50	110.10
1	B	39	VAL	CA-CB-CG1	5.05	118.48	110.90
1	A	152	GLU	CG-CD-OE2	-5.05	108.19	118.30
1	B	224	ALA	CA-C-O	-5.04	109.51	120.10
1	A	101	TYR	CD1-CG-CD2	-5.04	112.36	117.90
1	B	56	LYS	N-CA-C	5.04	124.60	111.00
1	A	179	GLU	CA-CB-CG	5.03	124.46	113.40
1	A	225	ASP	CB-CA-C	5.02	120.44	110.40
1	B	156	ASP	CA-CB-CG	5.02	124.44	113.40
1	B	246	SER	O-C-N	-5.02	114.67	122.70
1	A	146	GLN	O-C-N	5.01	130.72	122.70
1	B	223	LYS	CB-CA-C	5.01	120.42	110.40
1	B	159	ASN	O-C-N	5.00	130.71	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	VAL	N-CA-C	-5.00	97.49	111.00
1	B	147	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ALA	Peptide
1	A	205	ARG	Sidechain
1	B	189	ARG	Sidechain
1	B	247	ARG	Sidechain

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	1883	0	1881	274	0
1	B	1883	0	1886	393	0
2	A	9	0	2	0	0
2	B	9	0	3	2	0
3	A	12	0	0	5	0
3	B	13	0	0	6	0
All	All	3809	0	3772	641	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 85.

All (641) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:HA	1:B:225:ASP:OD1	1.28	1.27
1:A:111:ASP:HA	1:A:114:LYS:CE	1.65	1.25
1:A:28:ASN:ND2	1:A:55:LYS:H	1.35	1.23
1:B:3:ARG:NH2	1:B:203:GLU:HA	1.51	1.21
1:A:28:ASN:HD21	1:A:55:LYS:N	1.38	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:O	1:B:225:ASP:HB2	1.37	1.18
1:B:178:PRO:O	1:B:181:ALA:HB3	1.46	1.14
1:B:32:ILE:N	1:B:33:PRO:HD3	1.65	1.12
1:B:3:ARG:HH22	1:B:203:GLU:CA	1.62	1.11
1:A:2:ALA:N	3:A:612:HOH:O	1.83	1.11
1:A:192:LEU:HD22	1:A:196:LEU:HD21	1.31	1.10
1:B:142:VAL:HG12	1:B:143:VAL:H	1.16	1.06
1:B:56:LYS:NZ	1:B:56:LYS:HB3	1.70	1.04
1:B:91:VAL:CG1	1:B:93:LEU:HD22	1.88	1.04
1:B:91:VAL:HG13	1:B:93:LEU:HD22	1.35	1.03
1:B:186:ALA:CA	1:B:225:ASP:OD1	2.07	1.02
1:A:111:ASP:HA	1:A:114:LYS:HE2	1.06	1.02
1:B:179:GLU:HG3	1:B:180:ASP:H	1.25	1.01
1:A:111:ASP:CA	1:A:114:LYS:HE2	1.90	1.01
1:B:127:ILE:HG13	1:B:143:VAL:HG22	1.38	1.01
1:A:105:ASP:O	1:A:109:ILE:HD12	1.61	1.01
1:B:32:ILE:HG22	1:B:245:ASN:ND2	1.76	1.01
1:B:56:LYS:HA	1:B:59:VAL:O	1.61	1.01
1:B:24:VAL:HG11	1:B:53:LEU:HB3	1.41	1.01
1:B:70:ALA:HB2	1:B:115:PHE:HZ	1.25	0.99
1:B:32:ILE:HG21	1:B:241:VAL:CG1	1.92	0.99
1:A:2:ALA:CA	3:A:612:HOH:O	2.10	0.98
1:A:17:LYS:HB3	1:A:49:TYR:CE1	1.99	0.98
1:B:127:ILE:CG1	1:B:143:VAL:HG22	1.95	0.96
1:B:142:VAL:O	1:B:145:ARG:HG2	1.66	0.96
1:B:190:LYS:O	1:B:193:ALA:N	1.98	0.95
1:B:56:LYS:HB3	1:B:56:LYS:HZ3	1.25	0.95
1:B:104:GLU:HB3	1:B:108:PHE:HD2	1.31	0.95
1:B:32:ILE:HG12	1:B:244:ILE:HD11	1.49	0.95
1:B:246:SER:C	1:B:247:ARG:HG3	1.85	0.94
1:B:16:SER:OG	1:B:18:GLN:HG2	1.66	0.93
1:A:221:LYS:O	1:A:221:LYS:HG2	1.66	0.93
1:B:54:VAL:HB	1:B:59:VAL:HG12	1.50	0.93
1:B:51:VAL:HG12	1:B:61:VAL:HG11	1.51	0.92
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.00	0.92
1:B:32:ILE:HG22	1:B:245:ASN:HD21	1.35	0.92
1:B:218:VAL:O	1:B:221:LYS:HB2	1.69	0.92
1:A:70:ALA:HB2	1:A:115:PHE:HZ	1.34	0.92
1:B:148:ASN:HD21	1:B:191:PHE:HE1	1.03	0.92
1:A:56:LYS:O	1:A:59:VAL:HG12	1.70	0.91
1:B:51:VAL:O	1:B:53:LEU:N	2.04	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:O	1:B:225:ASP:CB	2.20	0.90
1:B:182:GLN:HG2	1:B:223:LYS:HG2	1.55	0.89
1:B:32:ILE:H	1:B:33:PRO:HD3	1.37	0.89
1:B:164:TYR:CZ	1:B:166:PRO:HG3	2.08	0.89
1:A:142:VAL:O	1:A:146:GLN:HG3	1.71	0.89
1:B:182:GLN:CG	1:B:223:LYS:HG2	2.02	0.88
1:B:189:ARG:NH1	1:B:227:ASP:OD2	2.07	0.87
1:B:247:ARG:HG2	1:B:247:ARG:HH11	1.34	0.87
1:B:56:LYS:CB	1:B:56:LYS:NZ	2.32	0.86
1:A:86:VAL:O	1:A:86:VAL:HG23	1.75	0.86
1:A:110:ALA:O	1:A:114:LYS:HG2	1.75	0.86
1:A:131:LEU:O	1:A:135:LYS:HG2	1.77	0.85
1:B:114:LYS:HG3	1:B:153:GLU:OE2	1.76	0.85
1:B:24:VAL:HG11	1:B:53:LEU:CB	2.06	0.85
1:B:60:THR:HG21	1:B:89:LYS:NZ	1.92	0.85
1:A:85:ASP:OD1	1:B:46:TYR:OH	1.94	0.84
1:A:87:GLY:O	1:A:89:LYS:NZ	2.10	0.84
1:A:28:ASN:ND2	1:A:55:LYS:N	2.08	0.84
1:B:32:ILE:N	1:B:33:PRO:CD	2.40	0.84
1:B:213:ASN:OD1	1:B:213:ASN:C	2.13	0.84
1:B:60:THR:HG21	1:B:89:LYS:HZ2	1.42	0.84
1:A:88:ALA:O	1:A:89:LYS:NZ	2.08	0.84
1:B:148:ASN:ND2	1:B:191:PHE:CE1	2.46	0.84
1:B:244:ILE:HG21	3:B:620:HOH:O	1.76	0.83
1:B:32:ILE:HG21	1:B:241:VAL:HG12	1.59	0.83
1:A:188:ILE:O	1:A:191:PHE:HB3	1.78	0.83
1:B:136:ALA:HB3	1:B:138:LYS:NZ	1.94	0.83
1:B:142:VAL:HG12	1:B:143:VAL:N	1.87	0.83
1:B:56:LYS:HE2	1:B:89:LYS:HD2	1.61	0.83
1:A:47:LEU:HD23	1:A:61:VAL:HG12	1.61	0.83
1:A:73:ALA:HA	1:B:12:LYS:HD3	1.59	0.82
1:B:20:ILE:O	1:B:24:VAL:HG23	1.77	0.82
1:B:231:VAL:HG11	1:B:234:ALA:HB3	1.61	0.82
1:B:40:ILE:HD11	1:B:54:VAL:HG11	1.60	0.82
1:B:142:VAL:CG1	1:B:143:VAL:H	1.92	0.82
1:B:177:THR:OG1	1:B:179:GLU:HG2	1.80	0.82
1:A:127:ILE:HG13	1:A:146:GLN:OE1	1.78	0.81
1:B:6:PHE:CZ	1:B:39:VAL:HG13	2.16	0.81
1:B:104:GLU:HB3	1:B:108:PHE:CD2	2.16	0.81
1:B:244:ILE:HD13	3:B:620:HOH:O	1.80	0.81
1:A:111:ASP:HA	1:A:114:LYS:NZ	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ALA:CB	1:B:138:LYS:HZ2	1.93	0.81
1:A:67:TYR:HB2	1:A:77:GLU:HG2	1.61	0.81
1:B:196:LEU:HD13	1:B:196:LEU:N	1.95	0.81
1:A:143:VAL:O	1:A:147:LEU:HB2	1.80	0.81
1:B:54:VAL:CG2	1:B:55:LYS:N	2.41	0.80
1:B:216:ASN:O	1:B:219:THR:OG1	1.99	0.80
1:A:86:VAL:HG11	1:B:45:THR:CG2	2.11	0.80
1:B:145:ARG:HG3	1:B:146:GLN:N	1.94	0.80
1:B:185:HIS:ND1	1:B:206:ILE:HG22	1.96	0.80
1:A:66:ALA:O	1:A:112:LYS:HE2	1.81	0.80
1:B:51:VAL:O	1:B:54:VAL:N	2.15	0.80
1:A:238:PRO:O	1:A:241:VAL:HG12	1.82	0.80
1:B:129:GLU:HB3	1:B:139:THR:HG23	1.63	0.79
1:B:79:SER:O	1:B:80:VAL:C	2.20	0.79
1:B:32:ILE:CG1	1:B:244:ILE:HD11	2.12	0.79
1:B:56:LYS:CB	1:B:56:LYS:HZ2	1.93	0.78
1:A:127:ILE:HG23	1:A:143:VAL:HG22	1.64	0.78
1:B:83:ILE:O	1:B:88:ALA:HB3	1.83	0.78
1:B:55:LYS:O	1:B:56:LYS:HG2	1.82	0.78
1:A:186:ALA:O	1:A:190:LYS:N	2.15	0.78
1:A:52:SER:C	1:A:53:LEU:HD23	2.04	0.77
1:B:54:VAL:HG23	1:B:55:LYS:N	2.00	0.77
1:A:138:LYS:HD3	1:A:141:ASP:OD1	1.85	0.77
1:A:188:ILE:HD13	1:A:206:ILE:HD13	1.65	0.76
1:A:78:ASN:ND2	3:A:632:HOH:O	2.07	0.76
1:B:17:LYS:O	1:B:49:TYR:HE1	1.68	0.76
1:B:56:LYS:HD2	1:B:89:LYS:HD3	1.68	0.76
1:A:92:ILE:O	1:A:93:LEU:HD23	1.86	0.75
1:A:40:ILE:O	1:A:42:PRO:HD3	1.86	0.75
1:B:136:ALA:HB3	1:B:138:LYS:HZ2	1.49	0.75
1:A:47:LEU:O	1:A:51:VAL:HG23	1.86	0.75
1:A:65:ASN:HD21	1:A:112:LYS:NZ	1.85	0.75
1:B:188:ILE:HD12	1:B:192:LEU:CD1	2.17	0.75
1:B:33:PRO:HB3	1:B:34:GLU:OE1	1.86	0.75
1:A:3:ARG:HB3	1:A:3:ARG:CZ	2.16	0.74
1:A:115:PHE:HZ	1:A:119:GLN:HE21	1.32	0.74
1:B:129:GLU:CG	1:B:139:THR:HG23	2.18	0.74
1:B:5:PHE:CE1	1:B:248:ASN:HA	2.23	0.74
1:B:33:PRO:O	1:B:36:VAL:HG12	1.86	0.74
1:B:32:ILE:HG21	1:B:241:VAL:HG13	1.69	0.73
1:B:142:VAL:CG1	1:B:143:VAL:N	2.49	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ALA:HB2	1:B:115:PHE:CZ	2.16	0.73
1:A:238:PRO:O	1:A:241:VAL:CG1	2.37	0.73
1:A:86:VAL:CG1	1:B:45:THR:CG2	2.66	0.73
1:A:6:PHE:CD2	1:A:207:LEU:HD11	2.24	0.73
1:A:32:ILE:HA	1:A:245:ASN:HD21	1.53	0.73
1:A:151:LEU:HD13	1:A:157:TRP:HZ2	1.54	0.72
1:A:216:ASN:O	1:A:219:THR:HG22	1.90	0.72
1:B:136:ALA:CB	1:B:138:LYS:NZ	2.51	0.72
1:B:17:LYS:O	1:B:49:TYR:CE1	2.43	0.71
1:B:247:ARG:O	1:B:248:ASN:HB2	1.90	0.71
1:B:170:ILE:HA	2:B:249:PGA:O3P	1.90	0.71
1:B:96:SER:HA	1:B:99:ARG:HG3	1.71	0.71
1:A:190:LYS:O	1:A:193:ALA:HB3	1.90	0.71
1:B:106:ASP:O	1:B:110:ALA:HB2	1.90	0.71
1:A:32:ILE:HG21	1:A:244:ILE:HD11	1.71	0.71
1:A:70:ALA:HB2	1:A:115:PHE:CZ	2.22	0.71
1:B:21:LYS:HG3	1:B:53:LEU:CD1	2.21	0.71
1:B:165:GLU:HG2	1:B:209:GLY:C	2.12	0.70
1:B:24:VAL:CG1	1:B:53:LEU:HB3	2.19	0.70
1:A:128:GLY:HA3	1:A:165:GLU:O	1.91	0.70
1:A:47:LEU:HD23	1:A:61:VAL:CG1	2.21	0.70
1:B:113:THR:O	1:B:117:LEU:HG	1.91	0.70
1:B:51:VAL:HG22	1:B:52:SER:H	1.55	0.70
1:A:82:GLN:HB3	1:B:46:TYR:CE1	2.26	0.70
1:B:190:LYS:O	1:B:191:PHE:C	2.29	0.70
1:A:21:LYS:O	1:A:25:GLU:HB2	1.91	0.70
1:A:39:VAL:HA	1:A:60:THR:O	1.91	0.70
1:A:28:ASN:O	1:A:56:LYS:HE3	1.91	0.70
1:B:148:ASN:ND2	1:B:191:PHE:HE1	1.83	0.70
1:B:5:PHE:CD1	1:B:248:ASN:HA	2.27	0.70
1:A:105:ASP:OD2	1:A:107:LYS:HB3	1.92	0.70
1:A:111:ASP:CB	1:A:114:LYS:HE2	2.22	0.70
1:B:21:LYS:HG3	1:B:53:LEU:HD13	1.72	0.70
1:A:217:ALA:O	1:A:248:ASN:ND2	2.24	0.69
1:B:131:LEU:O	1:B:135:LYS:HD3	1.92	0.69
1:B:117:LEU:O	1:B:120:GLY:N	2.22	0.69
1:B:213:ASN:OD1	1:B:213:ASN:O	2.10	0.69
1:A:188:ILE:HD13	1:A:206:ILE:CD1	2.23	0.69
1:A:28:ASN:HD22	1:A:55:LYS:C	1.96	0.69
1:B:20:ILE:O	1:B:24:VAL:CG2	2.40	0.69
1:B:147:LEU:HD13	1:B:191:PHE:CE2	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLU:CB	1:B:139:THR:HG23	2.24	0.68
1:B:182:GLN:HG3	1:B:223:LYS:HG2	1.74	0.68
1:B:3:ARG:HB3	1:B:3:ARG:NH2	2.08	0.68
1:A:38:VAL:O	1:A:59:VAL:HA	1.92	0.68
1:A:42:PRO:C	1:A:64:GLN:NE2	2.46	0.68
1:A:96:SER:O	1:A:100:SER:OG	2.10	0.68
1:A:66:ALA:O	1:A:112:LYS:CE	2.41	0.68
1:A:2:ALA:CB	3:A:612:HOH:O	2.40	0.68
1:A:134:LYS:O	1:A:137:GLY:N	2.26	0.68
1:B:31:SER:C	1:B:32:ILE:HG23	2.14	0.68
1:A:2:ALA:HB2	3:A:612:HOH:O	1.93	0.68
1:A:28:ASN:HA	1:A:56:LYS:HG3	1.75	0.68
1:B:238:PRO:O	1:B:240:PHE:N	2.27	0.68
1:B:49:TYR:O	1:B:52:SER:HB3	1.94	0.68
1:A:65:ASN:HD21	1:A:112:LYS:HZ3	1.41	0.68
1:B:164:TYR:CE2	1:B:166:PRO:HG3	2.28	0.68
1:A:157:TRP:O	1:A:159:ASN:N	2.28	0.67
1:B:2:ALA:C	1:B:3:ARG:HG2	2.14	0.67
1:A:52:SER:O	1:A:53:LEU:HD23	1.94	0.67
1:B:48:ASP:HB2	1:B:86:VAL:CG1	2.24	0.67
1:B:67:TYR:O	3:B:622:HOH:O	2.12	0.67
1:A:28:ASN:ND2	1:A:55:LYS:CA	2.57	0.67
1:B:188:ILE:HD11	1:B:206:ILE:HD11	1.77	0.67
1:B:7:VAL:HG21	1:B:244:ILE:HG22	1.76	0.67
1:B:33:PRO:HB2	1:B:34:GLU:HG2	1.77	0.67
1:B:179:GLU:CG	1:B:180:ASP:H	1.99	0.66
1:A:129:GLU:HB2	1:A:133:GLU:HG3	1.76	0.66
1:A:22:GLU:O	1:A:23:ILE:C	2.33	0.66
1:B:129:GLU:HG3	1:B:139:THR:HG23	1.75	0.66
1:B:56:LYS:HB2	1:B:56:LYS:HZ2	1.59	0.66
1:A:90:TRP:CZ3	1:A:161:VAL:HG13	2.29	0.66
1:A:2:ALA:N	1:A:227:ASP:OD1	2.29	0.66
1:A:36:VAL:HG12	1:A:58:GLN:HG2	1.77	0.66
1:A:207:LEU:HD22	1:A:228:GLY:HA3	1.78	0.65
1:B:113:THR:HG23	1:B:123:VAL:HG11	1.78	0.65
1:B:56:LYS:HE2	1:B:89:LYS:CD	2.25	0.65
1:A:83:ILE:HG23	1:A:88:ALA:HB3	1.76	0.65
1:A:129:GLU:HB2	1:A:133:GLU:CG	2.26	0.65
1:B:140:LEU:O	1:B:144:GLU:HB3	1.96	0.65
1:A:151:LEU:HD13	1:A:157:TRP:CZ2	2.32	0.65
1:A:56:LYS:O	1:A:59:VAL:CG1	2.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD13	1:B:191:PHE:HE2	1.59	0.65
1:A:182:GLN:O	1:A:182:GLN:HG3	1.94	0.65
1:B:108:PHE:CZ	1:B:112:LYS:HE2	2.32	0.65
1:B:188:ILE:HD12	1:B:192:LEU:HD11	1.77	0.65
1:B:142:VAL:O	1:B:145:ARG:CG	2.45	0.64
1:A:16:SER:O	1:A:20:ILE:HG23	1.96	0.64
1:A:113:THR:HG23	1:A:123:VAL:HG11	1.79	0.64
1:B:61:VAL:CG2	1:B:62:GLY:N	2.61	0.64
1:A:79:SER:O	1:A:83:ILE:HD12	1.98	0.64
1:B:142:VAL:O	1:B:145:ARG:N	2.31	0.64
1:B:98:ARG:HA	1:B:102:PHE:HB2	1.80	0.64
1:A:5:PHE:CD1	1:A:248:ASN:O	2.51	0.64
1:B:178:PRO:O	1:B:181:ALA:CB	2.35	0.64
1:B:51:VAL:O	1:B:52:SER:C	2.34	0.64
1:A:147:LEU:O	1:A:151:LEU:HD22	1.98	0.64
1:B:48:ASP:HB2	1:B:86:VAL:HG11	1.79	0.63
1:A:141:ASP:HB3	1:A:145:ARG:CZ	2.28	0.63
1:A:75:THR:HG23	1:B:64:GLN:HB3	1.79	0.63
1:A:75:THR:OG1	1:B:97:GLU:OE1	2.16	0.63
1:B:177:THR:OG1	1:B:179:GLU:CG	2.46	0.63
1:A:156:ASP:OD1	1:A:158:THR:HG22	1.98	0.63
1:B:190:LYS:O	1:B:193:ALA:CB	2.46	0.63
1:B:90:TRP:CZ3	1:B:122:GLY:HA3	2.33	0.63
1:B:148:ASN:OD1	1:B:151:LEU:HD12	1.98	0.63
1:B:185:HIS:ND1	1:B:206:ILE:CG2	2.62	0.63
1:A:32:ILE:CG2	1:A:244:ILE:HD11	2.29	0.62
1:A:53:LEU:N	1:A:53:LEU:HD23	2.14	0.62
1:B:129:GLU:HG3	1:B:139:THR:CG2	2.28	0.62
1:B:133:GLU:HG2	1:B:142:VAL:HG21	1.81	0.62
1:A:47:LEU:CD2	1:A:61:VAL:HG12	2.27	0.62
1:B:107:LYS:O	1:B:110:ALA:HB3	1.98	0.62
1:B:179:GLU:HG3	1:B:180:ASP:CG	2.19	0.62
1:B:5:PHE:CE1	1:B:248:ASN:CA	2.81	0.62
1:A:185:HIS:HB3	1:A:225:ASP:HB3	1.80	0.62
1:B:165:GLU:HG2	1:B:209:GLY:O	1.99	0.62
1:B:18:GLN:CG	1:B:19:SER:N	2.62	0.62
1:A:32:ILE:HA	1:A:245:ASN:ND2	2.14	0.62
1:A:47:LEU:HD11	1:A:63:ALA:HB2	1.81	0.62
1:B:132:GLU:O	1:B:133:GLU:C	2.39	0.61
1:B:32:ILE:HA	1:B:245:ASN:OD1	2.00	0.61
1:B:80:VAL:HG23	1:B:81:ASP:N	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:O	1:A:51:VAL:CG2	2.49	0.61
1:A:42:PRO:C	1:A:64:GLN:HE21	2.03	0.61
1:A:129:GLU:OE1	1:A:164:TYR:OH	2.17	0.61
1:B:114:LYS:HZ2	1:B:153:GLU:HB3	1.64	0.61
1:B:127:ILE:CD1	1:B:143:VAL:HG22	2.29	0.61
1:A:127:ILE:HG21	1:A:143:VAL:HG13	1.82	0.61
1:B:140:LEU:HD22	1:B:141:ASP:N	2.15	0.61
1:B:179:GLU:HG3	1:B:180:ASP:OD1	2.00	0.61
1:B:80:VAL:HG21	1:B:119:GLN:HG3	1.81	0.61
1:B:244:ILE:CG2	3:B:620:HOH:O	2.43	0.60
1:B:18:GLN:HG3	1:B:19:SER:N	2.15	0.60
1:B:246:SER:C	1:B:247:ARG:CG	2.66	0.60
1:A:148:ASN:O	1:A:150:VAL:N	2.34	0.60
1:B:179:GLU:C	1:B:181:ALA:N	2.54	0.60
1:B:56:LYS:CD	1:B:89:LYS:HD3	2.31	0.60
1:B:112:LYS:O	1:B:116:ALA:HB2	2.01	0.60
1:B:188:ILE:O	1:B:192:LEU:HB2	2.02	0.60
1:B:31:SER:O	1:B:32:ILE:CG2	2.49	0.60
1:B:140:LEU:O	1:B:144:GLU:CB	2.50	0.60
1:A:127:ILE:CG1	1:A:146:GLN:OE1	2.48	0.60
1:B:91:VAL:HG11	1:B:93:LEU:HD22	1.78	0.60
1:B:99:ARG:NH1	1:B:109:ILE:HD12	2.16	0.60
1:A:221:LYS:O	1:A:221:LYS:CG	2.47	0.60
1:A:156:ASP:CG	1:A:158:THR:HG22	2.22	0.59
1:B:239:GLU:O	1:B:243:ILE:HG13	2.02	0.59
1:B:91:VAL:HG13	1:B:91:VAL:O	2.01	0.59
1:A:28:ASN:ND2	1:A:55:LYS:C	2.55	0.59
1:A:95:HIS:CG	1:B:75:THR:HG21	2.37	0.59
1:A:139:THR:HG22	1:A:140:LEU:HD23	1.85	0.59
1:A:247:ARG:HH21	1:A:247:ARG:HG3	1.66	0.59
1:B:56:LYS:HD2	1:B:60:THR:OG1	2.03	0.59
1:B:185:HIS:CE1	1:B:206:ILE:HG22	2.38	0.58
1:A:10:ASN:ND2	1:A:12:LYS:HE2	2.18	0.58
1:B:107:LYS:HZ2	1:B:110:ALA:HB3	1.67	0.58
1:B:247:ARG:HG2	1:B:247:ARG:NH1	2.13	0.58
1:A:77:GLU:HG3	1:A:78:ASN:H	1.68	0.58
1:A:220:PHE:HB3	1:A:248:ASN:HD22	1.68	0.58
1:B:99:ARG:NH1	1:B:109:ILE:CD1	2.67	0.58
1:A:2:ALA:HB2	1:A:189:ARG:CZ	2.34	0.58
1:B:117:LEU:HD23	1:B:123:VAL:CG1	2.34	0.58
1:A:86:VAL:HG11	1:B:45:THR:HG23	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASN:ND2	3:B:630:HOH:O	2.31	0.58
1:A:40:ILE:HG13	1:A:61:VAL:HG22	1.85	0.57
1:A:115:PHE:CZ	1:A:119:GLN:NE2	2.66	0.57
1:A:115:PHE:O	1:A:118:GLY:N	2.37	0.57
1:B:126:CYS:HA	1:B:163:ALA:O	2.04	0.57
1:B:134:LYS:HE2	1:B:168:TRP:CZ2	2.39	0.57
1:A:105:ASP:OD2	1:A:107:LYS:CB	2.52	0.57
1:B:138:LYS:O	1:B:141:ASP:HB2	2.04	0.57
1:B:25:GLU:HA	1:B:28:ASN:HB2	1.86	0.57
1:A:83:ILE:HG23	1:A:88:ALA:CB	2.34	0.57
1:B:184:ILE:O	1:B:185:HIS:C	2.40	0.57
1:B:99:ARG:CZ	1:B:109:ILE:CD1	2.83	0.57
1:A:53:LEU:O	1:A:55:LYS:HG3	2.04	0.57
1:B:33:PRO:C	1:B:36:VAL:HG12	2.24	0.57
1:B:179:GLU:O	1:B:181:ALA:N	2.38	0.56
1:B:247:ARG:CG	1:B:247:ARG:HH11	2.09	0.56
1:A:95:HIS:CB	1:B:75:THR:HG21	2.35	0.56
1:B:48:ASP:CB	1:B:86:VAL:HG13	2.35	0.56
1:B:164:TYR:OH	1:B:166:PRO:HG3	2.04	0.56
1:B:169:ALA:HB1	1:B:210:GLY:O	2.05	0.56
1:B:77:GLU:HA	1:B:77:GLU:OE2	2.01	0.56
1:B:182:GLN:HG2	1:B:223:LYS:CG	2.32	0.56
1:B:48:ASP:CB	1:B:86:VAL:CG1	2.84	0.56
1:A:148:ASN:C	1:A:150:VAL:N	2.59	0.56
1:A:9:GLY:HA2	1:A:231:VAL:O	2.06	0.56
1:B:165:GLU:OE2	1:B:209:GLY:HA3	2.05	0.56
1:B:64:GLN:O	1:B:65:ASN:HB2	2.05	0.56
1:A:90:TRP:HZ3	1:A:161:VAL:HG13	1.72	0.55
1:A:140:LEU:HD11	1:A:187:SER:HB3	1.87	0.55
1:A:6:PHE:HD2	1:A:207:LEU:HD11	1.68	0.55
1:A:180:ASP:O	1:A:183:ASP:HB2	2.06	0.55
1:B:179:GLU:O	1:B:180:ASP:C	2.45	0.55
1:B:50:SER:O	1:B:51:VAL:O	2.24	0.55
1:A:114:LYS:HB3	1:A:154:VAL:HG22	1.89	0.55
1:B:114:LYS:HG3	1:B:153:GLU:HB3	1.87	0.55
1:B:3:ARG:HH22	1:B:203:GLU:HA	0.66	0.55
1:A:46:TYR:CE1	1:B:82:GLN:HG2	2.41	0.55
1:B:112:LYS:O	1:B:116:ALA:CB	2.55	0.55
1:A:111:ASP:HB3	1:A:114:LYS:HE2	1.88	0.55
1:B:188:ILE:O	1:B:192:LEU:HD12	2.06	0.55
1:A:141:ASP:OD2	1:A:145:ARG:NH2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:O	1:A:199:LYS:HG2	2.06	0.55
1:A:247:ARG:NH2	1:A:247:ARG:HG3	2.22	0.55
1:A:83:ILE:CG2	1:A:88:ALA:HB3	2.37	0.55
1:A:82:GLN:HA	1:B:46:TYR:OH	2.07	0.55
1:A:31:SER:O	1:A:245:ASN:OD1	2.25	0.55
1:B:107:LYS:NZ	1:B:111:ASP:OD2	2.40	0.55
1:A:169:ALA:HB2	1:A:174:LEU:O	2.07	0.54
1:A:86:VAL:HG11	1:B:45:THR:HG22	1.88	0.54
1:A:31:SER:C	1:A:32:ILE:HG23	2.27	0.54
1:A:46:TYR:OH	1:B:82:GLN:HG2	2.08	0.54
1:A:31:SER:O	1:A:32:ILE:HG23	2.08	0.54
1:B:11:PHE:N	1:B:11:PHE:CD2	2.74	0.54
1:B:179:GLU:HG3	1:B:180:ASP:N	2.09	0.54
1:B:31:SER:C	1:B:32:ILE:CG2	2.75	0.54
1:A:79:SER:HB3	1:A:82:GLN:HG3	1.90	0.54
1:B:104:GLU:CB	1:B:108:PHE:HD2	2.12	0.54
1:A:111:ASP:CA	1:A:114:LYS:NZ	2.69	0.54
1:B:199:LYS:HG2	1:B:203:GLU:OE1	2.07	0.54
1:B:20:ILE:HD13	1:B:42:PRO:HB3	1.90	0.54
1:A:190:LYS:O	1:A:191:PHE:C	2.46	0.54
1:A:40:ILE:O	1:A:42:PRO:CD	2.54	0.54
1:B:117:LEU:O	1:B:118:GLY:C	2.45	0.54
1:B:148:ASN:ND2	1:B:191:PHE:CZ	2.76	0.54
1:A:75:THR:CG2	1:B:64:GLN:HB3	2.37	0.54
1:A:80:VAL:HG22	1:A:121:VAL:HG11	1.89	0.54
1:A:151:LEU:CD1	1:A:157:TRP:CZ2	2.91	0.54
1:A:157:TRP:O	1:A:158:THR:C	2.46	0.53
1:B:31:SER:O	1:B:32:ILE:HG22	2.08	0.53
1:B:48:ASP:CG	1:B:86:VAL:HG13	2.28	0.53
1:A:5:PHE:HE2	1:A:244:ILE:O	1.91	0.53
1:A:86:VAL:CG1	1:B:45:THR:HG22	2.38	0.53
1:A:104:GLU:OE1	1:A:112:LYS:NZ	2.42	0.53
1:A:16:SER:OG	1:A:19:SER:HB3	2.08	0.53
1:B:143:VAL:HG11	1:B:188:ILE:HG21	1.90	0.53
1:A:73:ALA:HA	1:B:12:LYS:CD	2.36	0.53
1:B:114:LYS:NZ	1:B:153:GLU:HB3	2.23	0.53
1:B:188:ILE:CD1	1:B:206:ILE:HD11	2.38	0.53
1:A:98:ARG:HA	1:A:102:PHE:HD1	1.74	0.53
1:B:169:ALA:HB3	1:B:210:GLY:HA3	1.90	0.53
1:B:138:LYS:O	1:B:140:LEU:N	2.42	0.53
1:B:185:HIS:HB3	1:B:225:ASP:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ILE:CG1	1:B:206:ILE:HD11	2.40	0.52
1:A:84:LYS:HG3	1:A:121:VAL:CG2	2.40	0.52
1:B:191:PHE:CD2	1:B:192:LEU:N	2.77	0.52
1:A:125:LEU:HD11	1:A:150:VAL:HG21	1.92	0.52
1:A:17:LYS:CB	1:A:49:TYR:CE1	2.84	0.52
1:B:134:LYS:HE2	1:B:168:TRP:CE2	2.44	0.52
1:A:111:ASP:CA	1:A:114:LYS:CE	2.61	0.52
1:B:11:PHE:N	1:B:11:PHE:HD2	2.07	0.52
1:B:178:PRO:HB3	1:B:223:LYS:HE2	1.92	0.52
1:B:3:ARG:HB3	1:B:3:ARG:CZ	2.40	0.52
1:B:138:LYS:O	1:B:141:ASP:N	2.43	0.52
1:A:155:LYS:O	1:A:157:TRP:HD1	1.93	0.52
1:A:117:LEU:HD21	1:A:160:VAL:HG23	1.92	0.52
1:A:246:SER:O	1:A:247:ARG:HB2	2.10	0.52
1:A:86:VAL:CG2	1:A:86:VAL:O	2.45	0.52
1:B:114:LYS:NZ	1:B:153:GLU:O	2.40	0.52
1:A:95:HIS:O	1:A:99:ARG:HG3	2.10	0.52
1:B:91:VAL:O	1:B:91:VAL:CG1	2.56	0.52
1:A:141:ASP:O	1:A:144:GLU:N	2.35	0.51
1:A:17:LYS:HD3	1:A:49:TYR:CZ	2.45	0.51
1:A:33:PRO:HD3	1:A:245:ASN:ND2	2.25	0.51
1:A:220:PHE:CB	1:A:248:ASN:HD22	2.23	0.51
1:A:114:LYS:NZ	1:A:153:GLU:HG3	2.26	0.51
1:B:135:LYS:C	1:B:137:GLY:H	2.14	0.51
1:B:60:THR:HG21	1:B:89:LYS:HZ3	1.74	0.51
1:A:40:ILE:C	1:A:42:PRO:HD3	2.31	0.51
1:B:91:VAL:CG1	1:B:93:LEU:CD2	2.76	0.51
1:A:151:LEU:HD11	1:A:196:LEU:CD2	2.40	0.51
1:A:147:LEU:HD23	1:A:191:PHE:CD2	2.46	0.51
1:B:133:GLU:HG2	1:B:142:VAL:CG2	2.40	0.51
1:B:83:ILE:O	1:B:88:ALA:CB	2.57	0.51
1:B:95:HIS:O	1:B:99:ARG:HG2	2.11	0.51
1:B:190:LYS:HA	1:B:193:ALA:HB2	1.92	0.51
1:A:234:ALA:C	1:A:236:LEU:N	2.63	0.51
1:B:56:LYS:O	1:B:57:PRO:O	2.28	0.51
1:B:136:ALA:HB1	1:B:138:LYS:HZ2	1.73	0.51
1:B:16:SER:OG	1:B:18:GLN:CG	2.51	0.51
1:A:95:HIS:HB3	1:B:75:THR:HG21	1.93	0.51
1:A:105:ASP:C	1:A:109:ILE:HD12	2.28	0.50
1:A:26:ARG:NE	1:A:238:PRO:HA	2.26	0.50
1:B:195:LYS:C	1:B:196:LEU:HD13	2.31	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ALA:CB	1:B:241:VAL:HG11	2.42	0.50
1:B:51:VAL:CG2	1:B:52:SER:N	2.75	0.50
1:B:5:PHE:CE1	1:B:248:ASN:N	2.79	0.50
1:A:18:GLN:HG3	1:A:18:GLN:O	2.10	0.50
1:A:214:GLY:HA2	1:A:243:ILE:HG13	1.94	0.50
1:B:95:HIS:O	1:B:99:ARG:CG	2.59	0.50
1:B:105:ASP:O	1:B:106:ASP:C	2.50	0.50
1:B:145:ARG:CG	1:B:146:GLN:N	2.69	0.50
1:B:19:SER:O	1:B:20:ILE:C	2.46	0.50
1:B:247:ARG:O	1:B:248:ASN:CB	2.60	0.50
1:B:30:ALA:O	1:B:32:ILE:HG13	2.11	0.50
1:A:50:SER:O	1:A:53:LEU:N	2.31	0.50
1:A:47:LEU:CD2	1:A:88:ALA:HB2	2.42	0.50
1:B:150:VAL:O	1:B:154:VAL:N	2.45	0.50
1:A:148:ASN:O	1:A:149:ALA:C	2.50	0.50
1:A:32:ILE:HD13	1:A:244:ILE:HD11	1.92	0.50
1:B:196:LEU:N	1:B:196:LEU:CD1	2.73	0.50
1:B:32:ILE:HD13	1:B:244:ILE:HD12	1.93	0.50
1:A:94:GLY:O	1:A:99:ARG:NE	2.45	0.49
1:A:2:ALA:CB	1:A:189:ARG:NH2	2.75	0.49
1:B:237:LYS:HB3	1:B:238:PRO:HD2	1.93	0.49
1:B:48:ASP:HB2	1:B:86:VAL:HG13	1.95	0.49
1:A:90:TRP:HA	1:A:122:GLY:O	2.12	0.49
1:A:2:ALA:CB	1:A:204:LEU:O	2.60	0.49
1:A:85:ASP:OD1	1:B:46:TYR:CZ	2.66	0.49
1:B:178:PRO:C	1:B:181:ALA:HB3	2.26	0.49
1:B:61:VAL:HG23	1:B:62:GLY:N	2.27	0.49
1:B:130:THR:HA	1:B:167:VAL:HB	1.94	0.49
1:B:158:THR:HB	1:B:159:ASN:OD1	2.13	0.49
1:B:238:PRO:O	1:B:241:VAL:N	2.35	0.49
1:B:34:GLU:C	1:B:36:VAL:H	2.16	0.49
1:A:191:PHE:CD2	1:A:192:LEU:HG	2.48	0.49
1:B:138:LYS:C	1:B:140:LEU:N	2.64	0.49
1:B:186:ALA:CB	1:B:225:ASP:OD1	2.60	0.49
1:A:33:PRO:HD3	1:A:245:ASN:HD22	1.77	0.49
1:B:20:ILE:HD12	1:B:46:TYR:HB2	1.94	0.49
1:B:143:VAL:O	1:B:147:LEU:HB2	2.12	0.49
1:B:4:THR:HG23	1:B:35:ASN:O	2.13	0.49
1:B:89:LYS:NZ	1:B:90:TRP:HE1	2.11	0.49
1:A:192:LEU:O	1:A:196:LEU:N	2.41	0.48
1:B:39:VAL:HG11	1:B:90:TRP:CD1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ALA:O	1:A:187:SER:C	2.49	0.48
1:B:98:ARG:NH2	1:B:104:GLU:OE1	2.47	0.48
1:A:109:ILE:HG22	1:A:109:ILE:O	2.13	0.48
1:A:235:SER:HA	1:A:240:PHE:CD1	2.49	0.48
1:B:148:ASN:O	1:B:151:LEU:HB2	2.12	0.48
1:A:73:ALA:CA	1:B:12:LYS:HD3	2.40	0.48
1:B:243:ILE:HG22	1:B:243:ILE:O	2.12	0.48
1:B:50:SER:O	1:B:51:VAL:C	2.52	0.48
1:A:111:ASP:O	1:A:114:LYS:HG3	2.14	0.48
1:B:208:TYR:O	1:B:229:PHE:HA	2.14	0.48
1:B:54:VAL:HG23	1:B:55:LYS:C	2.34	0.48
1:A:117:LEU:HD11	1:A:154:VAL:HG11	1.95	0.48
1:B:145:ARG:HG3	1:B:146:GLN:H	1.73	0.47
1:B:68:LEU:HB3	1:B:112:LYS:HG2	1.95	0.47
1:A:235:SER:HA	1:A:240:PHE:CG	2.50	0.47
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.96	0.47
1:B:179:GLU:CG	1:B:180:ASP:N	2.72	0.47
1:A:42:PRO:CB	1:A:43:PRO:HD2	2.45	0.47
1:B:117:LEU:HG	1:B:117:LEU:H	1.46	0.47
1:B:32:ILE:CG2	1:B:241:VAL:HG12	2.38	0.47
1:B:42:PRO:C	1:B:64:GLN:NE2	2.68	0.47
1:A:114:LYS:HZ3	1:A:153:GLU:HG3	1.79	0.47
1:B:51:VAL:HG22	1:B:52:SER:N	2.27	0.47
1:B:140:LEU:HD22	1:B:140:LEU:C	2.35	0.47
1:B:51:VAL:CG2	1:B:52:SER:H	2.24	0.47
1:B:95:HIS:HA	1:B:126:CYS:HB2	1.97	0.47
1:A:169:ALA:CB	1:A:174:LEU:O	2.62	0.47
1:A:189:ARG:O	1:A:193:ALA:HB2	2.14	0.47
1:A:84:LYS:O	1:A:85:ASP:C	2.53	0.47
1:B:190:LYS:O	1:B:193:ALA:CA	2.62	0.47
1:B:188:ILE:HD11	1:B:206:ILE:CD1	2.44	0.47
1:B:96:SER:CA	1:B:99:ARG:HG3	2.42	0.47
1:A:188:ILE:CD1	1:A:206:ILE:CD1	2.92	0.47
1:A:164:TYR:HB2	1:A:206:ILE:HD11	1.95	0.46
1:B:129:GLU:CG	1:B:139:THR:CG2	2.89	0.46
1:A:75:THR:O	1:B:98:ARG:NE	2.42	0.46
1:A:106:ASP:O	1:A:110:ALA:N	2.49	0.46
1:A:247:ARG:NH2	1:A:247:ARG:CG	2.78	0.46
1:B:124:ILE:HG13	1:B:161:VAL:HG23	1.98	0.46
1:B:21:LYS:O	1:B:25:GLU:N	2.39	0.46
1:A:85:ASP:OD1	1:B:46:TYR:CE2	2.68	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:VAL:HG23	1:B:81:ASP:H	1.80	0.46
1:A:129:GLU:HB2	1:A:133:GLU:HG2	1.96	0.46
1:A:170:ILE:O	1:A:172:THR:HG23	2.15	0.46
1:B:107:LYS:HA	1:B:107:LYS:HD2	1.55	0.46
1:B:178:PRO:HA	1:B:181:ALA:CB	2.46	0.46
1:B:80:VAL:CG2	1:B:119:GLN:HG3	2.46	0.46
1:A:140:LEU:HD22	1:A:140:LEU:HA	1.61	0.46
1:B:142:VAL:C	1:B:145:ARG:HG2	2.32	0.46
1:B:67:TYR:CG	1:B:77:GLU:HG3	2.51	0.46
1:B:113:THR:O	1:B:116:ALA:HB3	2.16	0.46
1:B:191:PHE:O	1:B:195:LYS:HG2	2.16	0.46
1:B:165:GLU:HG2	1:B:209:GLY:CA	2.45	0.46
1:A:17:LYS:O	1:A:49:TYR:HE1	1.99	0.46
1:A:75:THR:CB	1:B:97:GLU:OE1	2.64	0.46
1:B:127:ILE:HD12	1:B:127:ILE:HG21	1.79	0.46
1:B:238:PRO:C	1:B:240:PHE:N	2.69	0.46
1:B:32:ILE:O	1:B:36:VAL:HG11	2.15	0.46
1:B:66:ALA:HA	1:B:78:ASN:HB2	1.97	0.46
1:A:114:LYS:HA	1:A:117:LEU:HD12	1.98	0.46
1:B:38:VAL:HG13	1:B:59:VAL:HG22	1.98	0.46
1:B:6:PHE:C	1:B:6:PHE:CD1	2.90	0.45
1:A:157:TRP:CG	1:A:196:LEU:HD13	2.51	0.45
1:A:239:GLU:O	1:A:239:GLU:CG	2.64	0.45
1:B:127:ILE:HD11	1:B:143:VAL:HG22	1.97	0.45
1:B:42:PRO:HG3	1:B:50:SER:OG	2.16	0.45
1:B:51:VAL:C	1:B:53:LEU:N	2.68	0.45
1:A:127:ILE:CG2	1:A:143:VAL:HG13	2.46	0.45
1:A:205:ARG:HB2	1:A:205:ARG:HE	1.60	0.45
1:A:13:LEU:HG	1:B:79:SER:HB2	1.98	0.45
1:A:234:ALA:C	1:A:236:LEU:H	2.17	0.45
1:A:240:PHE:HA	1:A:243:ILE:HD12	1.98	0.45
1:A:82:GLN:O	1:A:86:VAL:N	2.41	0.45
1:B:98:ARG:HG2	1:B:98:ARG:H	1.50	0.45
1:A:165:GLU:OE2	1:A:209:GLY:HA3	2.17	0.45
1:B:136:ALA:HB1	1:B:138:LYS:NZ	2.29	0.45
1:B:230:LEU:HA	1:B:230:LEU:HD12	1.71	0.45
1:A:17:LYS:HD3	1:A:49:TYR:CE2	2.52	0.45
1:B:98:ARG:NH1	1:B:102:PHE:CD2	2.85	0.45
1:B:39:VAL:CG2	1:B:39:VAL:O	2.65	0.45
1:B:93:LEU:HB2	1:B:123:VAL:HG23	1.98	0.45
2:B:249:PGA:H21	3:B:643:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TRP:C	1:A:159:ASN:N	2.68	0.44
1:B:122:GLY:HA2	1:B:159:ASN:O	2.17	0.44
1:B:169:ALA:O	1:B:211:SER:OG	2.20	0.44
1:B:238:PRO:O	1:B:239:GLU:C	2.54	0.44
1:A:190:LYS:O	1:A:193:ALA:CB	2.63	0.44
1:B:247:ARG:CG	1:B:247:ARG:NH1	2.76	0.44
1:A:17:LYS:HB3	1:A:49:TYR:CZ	2.49	0.44
1:B:7:VAL:CG2	1:B:244:ILE:HG22	2.44	0.44
1:A:97:GLU:HG2	1:A:101:TYR:HE2	1.82	0.44
1:A:108:PHE:O	1:A:109:ILE:C	2.54	0.44
1:B:54:VAL:HG23	1:B:55:LYS:O	2.16	0.44
1:B:188:ILE:HG13	1:B:206:ILE:HD11	1.98	0.44
1:B:25:GLU:O	1:B:28:ASN:N	2.50	0.44
1:B:80:VAL:CG2	1:B:81:ASP:N	2.78	0.44
1:A:108:PHE:O	1:A:110:ALA:N	2.50	0.44
1:A:32:ILE:CB	1:A:244:ILE:HD11	2.47	0.44
1:A:127:ILE:HG22	1:A:164:TYR:HD1	1.83	0.44
1:A:2:ALA:HB2	1:A:189:ARG:NH2	2.33	0.44
1:A:97:GLU:HB2	1:B:75:THR:HB	1.98	0.44
1:B:138:LYS:C	1:B:140:LEU:H	2.20	0.44
1:B:3:ARG:HH12	1:B:203:GLU:HB3	1.82	0.44
1:A:213:ASN:O	1:A:214:GLY:C	2.57	0.44
1:A:36:VAL:HG13	1:A:58:GLN:HB3	1.99	0.44
1:A:6:PHE:HA	1:A:37:GLU:O	2.18	0.43
1:B:188:ILE:HD12	1:B:192:LEU:HD12	1.97	0.43
1:A:115:PHE:CZ	1:A:119:GLN:HG3	2.53	0.43
1:B:127:ILE:HG13	1:B:143:VAL:CG2	2.28	0.43
1:B:56:LYS:CD	1:B:89:LYS:CD	2.96	0.43
1:A:84:LYS:HG3	1:A:121:VAL:HG22	2.00	0.43
1:B:215:SER:O	1:B:218:VAL:HG12	2.18	0.43
1:B:90:TRP:CZ3	1:B:161:VAL:HG22	2.54	0.43
1:B:91:VAL:HG11	1:B:93:LEU:CD2	2.46	0.43
1:B:93:LEU:HD13	1:B:93:LEU:HA	1.79	0.43
1:A:247:ARG:HA	1:A:247:ARG:HD3	1.18	0.43
1:B:143:VAL:HG12	1:B:144:GLU:N	2.33	0.43
1:B:34:GLU:CA	1:B:34:GLU:OE1	2.65	0.43
1:A:185:HIS:HB3	1:A:225:ASP:CB	2.48	0.43
1:A:18:GLN:O	1:A:21:LYS:HG2	2.18	0.43
1:A:82:GLN:O	1:A:86:VAL:HG13	2.18	0.43
1:A:22:GLU:O	1:A:23:ILE:O	2.36	0.43
1:B:20:ILE:HD12	1:B:46:TYR:CB	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ALA:CB	1:B:220:PHE:CE2	3.01	0.43
1:B:32:ILE:HD13	1:B:244:ILE:CD1	2.48	0.43
1:A:135:LYS:HG2	1:A:135:LYS:H	1.66	0.42
1:B:185:HIS:N	1:B:185:HIS:CD2	2.87	0.42
1:B:51:VAL:HA	1:B:54:VAL:HG22	2.01	0.42
1:A:243:ILE:O	1:A:246:SER:OG	2.37	0.42
1:A:64:GLN:O	1:A:65:ASN:HB2	2.19	0.42
1:B:6:PHE:HD1	1:B:6:PHE:C	2.22	0.42
1:A:208:TYR:O	1:A:229:PHE:HD2	2.02	0.42
1:A:53:LEU:HD22	1:A:53:LEU:HA	1.51	0.42
1:A:89:LYS:O	1:A:122:GLY:N	2.45	0.42
1:A:25:GLU:O	1:A:26:ARG:C	2.57	0.42
1:A:3:ARG:HB3	1:A:3:ARG:NH1	2.35	0.42
1:A:47:LEU:HD22	1:A:88:ALA:HB2	2.01	0.42
1:B:131:LEU:O	1:B:135:LYS:CD	2.65	0.42
1:B:179:GLU:O	1:B:182:GLN:N	2.52	0.42
1:B:20:ILE:CD1	1:B:42:PRO:HB3	2.48	0.42
1:A:159:ASN:HD22	1:A:159:ASN:HA	1.25	0.42
1:B:129:GLU:OE2	1:B:164:TYR:OH	2.26	0.42
1:B:236:LEU:HA	1:B:236:LEU:HD12	1.75	0.42
1:B:26:ARG:HA	1:B:29:THR:HG22	2.02	0.42
1:A:4:THR:HB	1:A:205:ARG:HH21	1.85	0.42
1:B:183:ASP:O	1:B:186:ALA:HB3	2.20	0.42
1:B:56:LYS:CE	1:B:89:LYS:CD	2.97	0.42
1:B:134:LYS:CE	1:B:168:TRP:CE2	3.03	0.41
1:B:199:LYS:HD3	1:B:203:GLU:OE1	2.20	0.41
1:B:42:PRO:HB2	1:B:43:PRO:CD	2.50	0.41
1:A:165:GLU:HA	1:A:166:PRO:HD3	1.75	0.41
1:B:114:LYS:HZ2	1:B:153:GLU:C	2.24	0.41
1:B:19:SER:O	1:B:21:LYS:N	2.53	0.41
1:A:6:PHE:CD1	1:A:37:GLU:HG2	2.55	0.41
1:B:29:THR:HG23	1:B:29:THR:O	2.20	0.41
1:B:132:GLU:N	1:B:132:GLU:CD	2.74	0.41
1:B:32:ILE:O	1:B:32:ILE:CD1	2.69	0.41
1:A:156:ASP:OD1	1:A:158:THR:CG2	2.67	0.41
1:B:32:ILE:CD1	1:B:32:ILE:C	2.88	0.41
1:A:187:SER:O	1:A:190:LYS:HB3	2.20	0.41
1:A:2:ALA:HB1	1:A:204:LEU:O	2.20	0.41
1:A:2:ALA:CB	1:A:189:ARG:NH1	2.84	0.41
1:A:188:ILE:CD1	1:A:206:ILE:HD11	2.50	0.41
1:B:185:HIS:HD1	1:B:206:ILE:HG22	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:O	1:A:193:ALA:N	2.54	0.41
1:A:229:PHE:HB3	1:A:231:VAL:CG2	2.51	0.41
1:B:128:GLY:HA3	1:B:165:GLU:O	2.21	0.41
1:B:31:SER:O	1:B:32:ILE:HG23	2.19	0.41
1:A:213:ASN:HB2	1:A:239:GLU:OE2	2.21	0.41
1:A:115:PHE:O	1:A:118:GLY:CA	2.69	0.41
1:B:142:VAL:HA	1:B:145:ARG:HG2	2.03	0.41
1:B:165:GLU:O	1:B:166:PRO:C	2.59	0.41
1:B:185:HIS:H	1:B:185:HIS:CD2	2.39	0.40
1:B:219:THR:HG1	1:B:219:THR:H	1.53	0.40
1:B:24:VAL:HG11	1:B:53:LEU:HB2	1.98	0.40
1:B:51:VAL:CG1	1:B:61:VAL:HG11	2.35	0.40
1:B:80:VAL:CG2	1:B:81:ASP:H	2.34	0.40
1:A:187:SER:HA	1:A:190:LYS:HD3	2.02	0.40
1:B:237:LYS:CB	1:B:238:PRO:CD	2.99	0.40
1:A:46:TYR:HE1	1:B:82:GLN:HG2	1.84	0.40
1:A:82:GLN:HB3	1:B:46:TYR:HE1	1.85	0.40
1:B:220:PHE:HA	1:B:223:LYS:HE2	2.04	0.40
1:B:5:PHE:CZ	1:B:248:ASN:N	2.89	0.40
1:B:48:ASP:OD2	1:B:86:VAL:HG13	2.21	0.40
1:B:80:VAL:HG22	1:B:115:PHE:CE2	2.56	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	245/247 (99%)	191 (78%)	43 (18%)	11 (4%)	2	3
1	B	245/247 (99%)	181 (74%)	39 (16%)	25 (10%)	0	0
All	All	490/494 (99%)	372 (76%)	82 (17%)	36 (7%)	1	1

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	23	ILE
1	A	149	ALA
1	B	33	PRO
1	B	51	VAL
1	B	52	SER
1	B	55	LYS
1	B	57	PRO
1	B	77	GLU
1	B	103	HIS
1	B	142	VAL
1	B	179	GLU
1	B	239	GLU
1	A	158	THR
1	A	191	PHE
1	B	4	THR
1	B	54	VAL
1	B	80	VAL
1	B	143	VAL
1	B	225	ASP
1	B	247	ARG
1	A	113	THR
1	A	134	LYS
1	B	34	GLU
1	B	149	ALA
1	B	193	ALA
1	A	135	LYS
1	A	221	LYS
1	B	20	ILE
1	B	139	THR
1	A	22	GLU
1	B	32	ILE
1	B	114	LYS
1	B	133	GLU
1	B	210	GLY
1	A	233	GLY

5.3.2 Protein sidechains [i](#)

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	200/200 (100%)	155 (78%)	45 (22%)	1	1
1	B	200/200 (100%)	138 (69%)	62 (31%)	0	0
All	All	400/400 (100%)	293 (73%)	107 (27%)	0	0

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	20	ILE
1	A	25	GLU
1	A	27	LEU
1	A	29	THR
1	A	36	VAL
1	A	38	VAL
1	A	47	LEU
1	A	48	ASP
1	A	52	SER
1	A	53	LEU
1	A	54	VAL
1	A	68	LEU
1	A	69	LYS
1	A	77	GLU
1	A	86	VAL
1	A	89	LYS
1	A	98	ARG
1	A	107	LYS
1	A	114	LYS
1	A	125	LEU
1	A	127	ILE
1	A	129	GLU
1	A	133	GLU
1	A	140	LEU
1	A	151	LEU
1	A	152	GLU
1	A	159	ASN
1	A	161	VAL
1	A	174	LEU
1	A	179	GLU
1	A	183	ASP
1	A	196	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	204	LEU
1	A	205	ARG
1	A	206	ILE
1	A	218	VAL
1	A	219	THR
1	A	237	LYS
1	A	239	GLU
1	A	241	VAL
1	A	244	ILE
1	A	245	ASN
1	A	247	ARG
1	A	248	ASN
1	B	3	ARG
1	B	6	PHE
1	B	11	PHE
1	B	16	SER
1	B	20	ILE
1	B	22	GLU
1	B	26	ARG
1	B	27	LEU
1	B	29	THR
1	B	32	ILE
1	B	34	GLU
1	B	35	ASN
1	B	38	VAL
1	B	39	VAL
1	B	40	ILE
1	B	56	LYS
1	B	58	GLN
1	B	60	THR
1	B	61	VAL
1	B	71	SER
1	B	74	PHE
1	B	79	SER
1	B	83	ILE
1	B	84	LYS
1	B	93	LEU
1	B	96	SER
1	B	98	ARG
1	B	99	ARG
1	B	101	TYR
1	B	107	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	117	LEU
1	B	121	VAL
1	B	123	VAL
1	B	125	LEU
1	B	127	ILE
1	B	135	LYS
1	B	138	LYS
1	B	139	THR
1	B	140	LEU
1	B	143	VAL
1	B	145	ARG
1	B	155	LYS
1	B	156	ASP
1	B	159	ASN
1	B	161	VAL
1	B	170	ILE
1	B	174	LEU
1	B	180	ASP
1	B	187	SER
1	B	188	ILE
1	B	190	LYS
1	B	191	PHE
1	B	196	LEU
1	B	202	SER
1	B	203	GLU
1	B	207	LEU
1	B	221	LYS
1	B	225	ASP
1	B	227	ASP
1	B	229	PHE
1	B	237	LYS
1	B	247	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	65	ASN
1	A	159	ASN
1	A	245	ASN
1	B	18	GLN
1	B	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	64	GLN
1	B	65	ASN
1	B	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PGA	B	249	-	5,8,8	1.86	3 (60%)	6,11,11	3.22	5 (83%)
2	PGA	A	249	-	5,8,8	1.23	0	6,11,11	2.59	3 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGA	B	249	-	-	3/4/6/6	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGA	A	249	-	-	2/4/6/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	249	PGA	P-O1P	2.74	1.69	1.60
2	B	249	PGA	P-O2P	-2.10	1.43	1.50
2	B	249	PGA	P-O3P	2.05	1.62	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	PGA	O3P-P-O1P	-5.75	91.44	106.73
2	A	249	PGA	O4P-P-O1P	-4.07	95.91	106.73
2	A	249	PGA	O1P-P-O2P	3.76	117.02	106.47
2	B	249	PGA	O3P-P-O2P	3.05	122.63	110.68
2	B	249	PGA	O1P-P-O2P	2.77	114.23	106.47
2	B	249	PGA	O4P-P-O1P	-2.34	100.49	106.73
2	B	249	PGA	O4P-P-O2P	2.28	119.60	110.68
2	A	249	PGA	O3P-P-O1P	-2.19	100.92	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	249	PGA	C2-O1P-P-O3P
2	B	249	PGA	C2-O1P-P-O4P
2	A	249	PGA	C2-O1P-P-O3P
2	A	249	PGA	C2-O1P-P-O4P
2	B	249	PGA	C2-O1P-P-O2P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	249	PGA	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.