



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 AM GMT

PDB ID : 2NVL
Title : Crystal structure of archaeal peroxiredoxin, thioredoxin peroxidase from *Aeropyrum pernix* K1 (sulfonic acid form)
Authors : Nakamura, T.; Yamamoto, T.; Abe, M.; Matsumura, H.; Hagihara, Y.; Goto, T.; Yamaguchi, T.; Inoue, T.
Deposited on : 2006-11-13
Resolution : 2.36 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
<http://wwpdb.org/validation/2016/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:

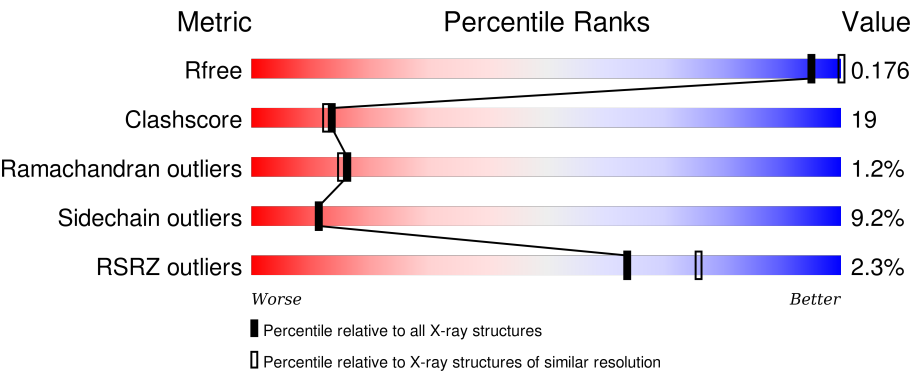
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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	250	<div><div>3%</div><div><div></div><div>63%</div><div>25%</div><div>8%</div><div>••</div></div></div>
1	B	250	<div><div>%</div><div><div></div><div>68%</div><div>22%</div><div>5%</div><div>••</div></div></div>
1	C	250	<div><div>2%</div><div><div></div><div>63%</div><div>26%</div><div>7%</div><div>•</div></div></div>
1	D	250	<div><div>2%</div><div><div></div><div>62%</div><div>28%</div><div>6%</div><div>••</div></div></div>
1	E	250	<div><div>2%</div><div><div></div><div>62%</div><div>29%</div><div>5%</div><div>•</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	250	<div> <div>3%</div> <div>62%</div> <div>29%</div> <div>• • •</div> </div>
1	G	250	<div> <div>%</div> <div>62%</div> <div>30%</div> <div>• • •</div> </div>
1	H	250	<div> <div>2%</div> <div>70%</div> <div>20%</div> <div>6%</div> <div>• •</div> </div>
1	I	250	<div> <div>4%</div> <div>62%</div> <div>28%</div> <div>6%</div> <div>• •</div> </div>
1	J	250	<div> <div>2%</div> <div>69%</div> <div>20%</div> <div>6%</div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20328 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 Probable peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	B	240	Total	C	N	O	S	0	0	0
			1953	1254	343	350	6			
1	C	240	Total	C	N	O	S	0	0	0
			1950	1252	341	351	6			
1	D	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	E	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	F	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	G	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	H	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	I	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			
1	J	242	Total	C	N	O	S	0	0	0
			1965	1261	345	353	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
B	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
C	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
D	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
E	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
F	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
G	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
H	207	SER	CYS	ENGINEERED	UNP Q9Y9L0
I	207	SER	CYS	ENGINEERED	UNP Q9Y9L0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	207	SER	CYS	ENGINEERED	UNP Q9Y9L0

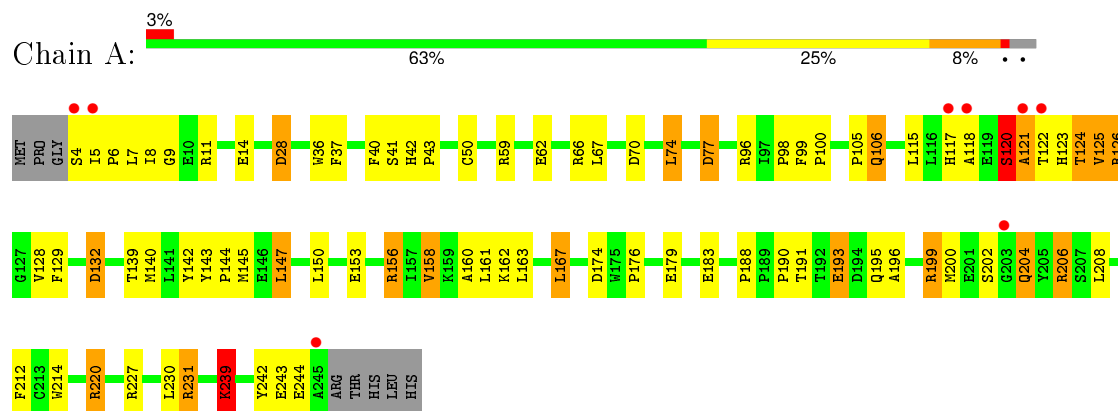
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	83	Total O 83 83	0	0
2	B	64	Total O 64 64	0	0
2	C	58	Total O 58 58	0	0
2	D	44	Total O 44 44	0	0
2	E	66	Total O 66 66	0	0
2	F	75	Total O 75 75	0	0
2	G	82	Total O 82 82	0	0
2	H	82	Total O 82 82	0	0
2	I	75	Total O 75 75	0	0
2	J	76	Total O 76 76	0	0

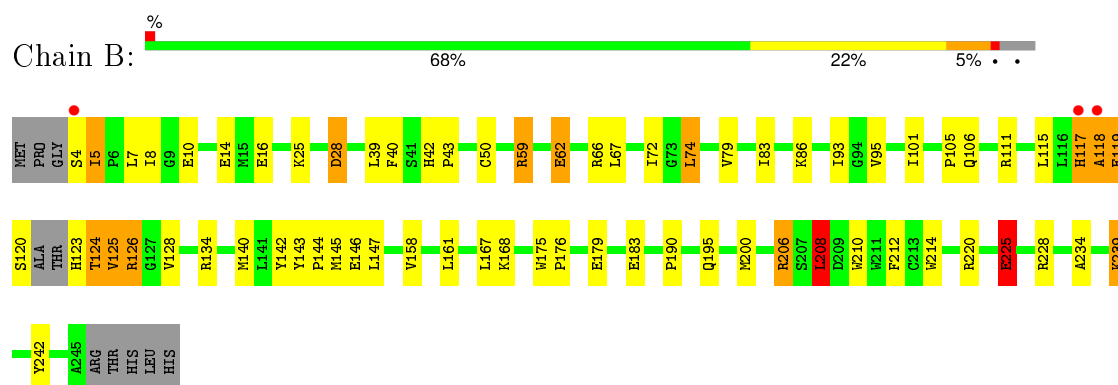
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

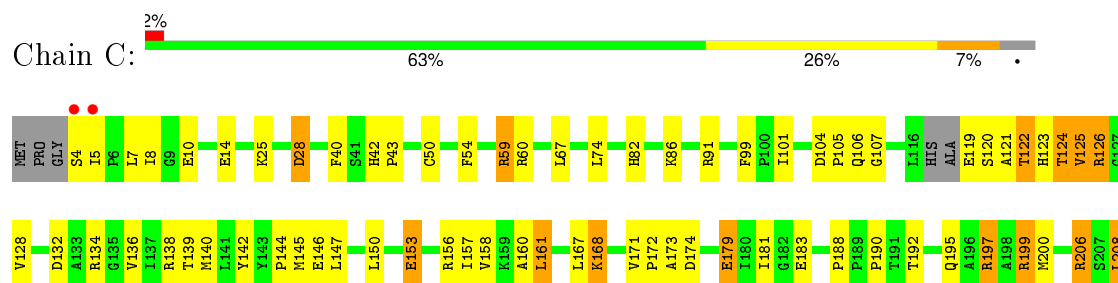
• Molecule 1: Probable peroxiredoxin

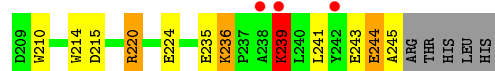


• Molecule 1: Probable peroxiredoxin

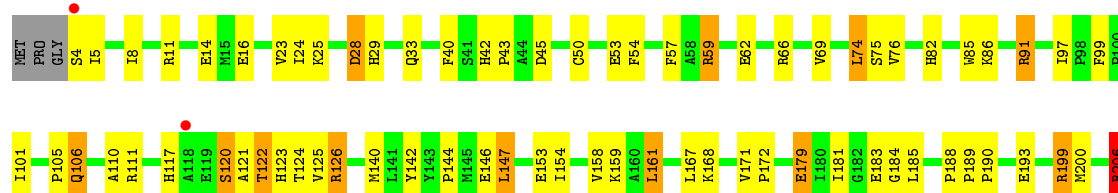


• Molecule 1: Probable peroxiredoxin

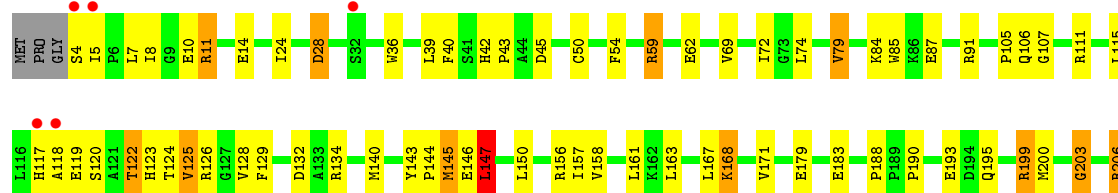




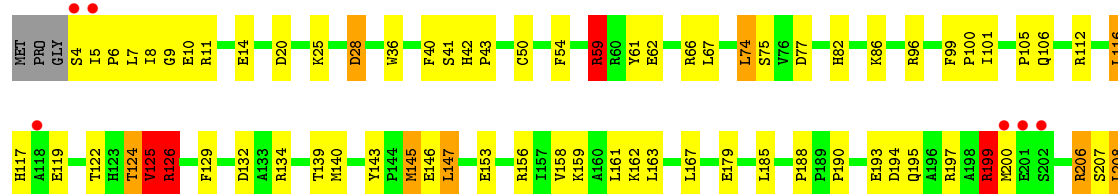
- Molecule 1: Probable peroxiredoxin



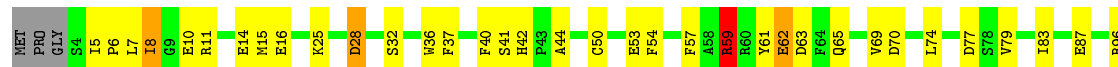
- Molecule 1: Probable peroxiredoxin

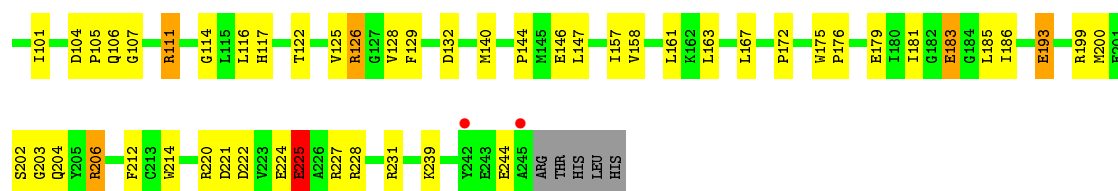


- Molecule 1: Probable peroxiredoxin

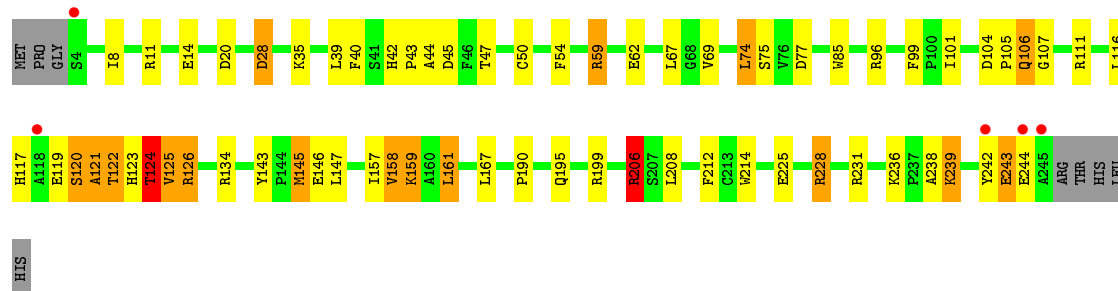


- Molecule 1: Probable peroxiredoxin

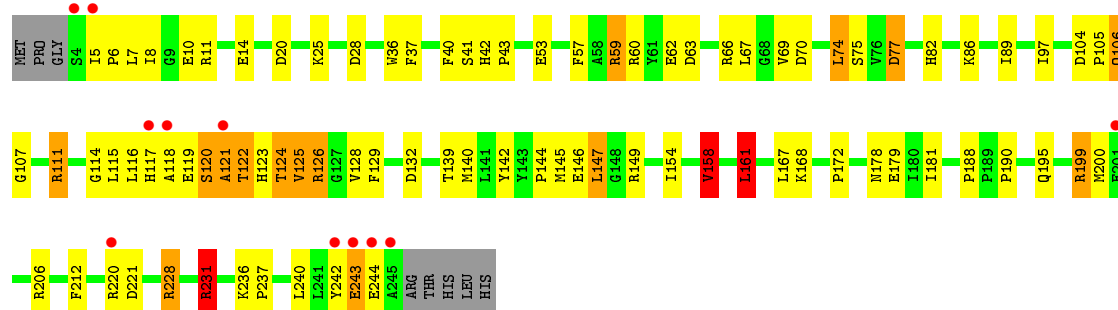




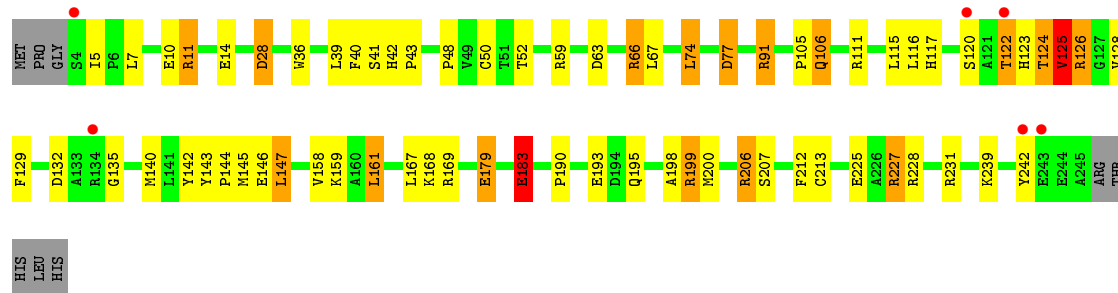
• Molecule 1: Probable peroxiredoxin



• Molecule 1: Probable peroxiredoxin



• Molecule 1: Probable peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.32Å 102.96Å 104.30Å 105.65° 105.26° 92.69°	Depositor
Resolution (Å)	50.00 – 2.36 50.13 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.36) 84.9 (50.13-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.219 0.167 , 0.176	Depositor DCC
R_{free} test set	11666 reflections (11.70%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 116808 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20328	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.19	3/2009 (0.1%)	1.04	8/2730 (0.3%)
1	B	1.20	6/1996 (0.3%)	1.02	5/2710 (0.2%)
1	C	1.17	4/1992 (0.2%)	1.00	7/2705 (0.3%)
1	D	1.13	5/2009 (0.2%)	1.02	8/2730 (0.3%)
1	E	1.18	5/2009 (0.2%)	1.02	7/2730 (0.3%)
1	F	1.22	3/2009 (0.1%)	1.11	17/2730 (0.6%)
1	G	1.28	10/2009 (0.5%)	1.09	11/2730 (0.4%)
1	H	1.17	3/2009 (0.1%)	1.06	7/2730 (0.3%)
1	I	1.16	5/2009 (0.2%)	1.04	12/2730 (0.4%)
1	J	1.17	5/2009 (0.2%)	1.02	6/2730 (0.2%)
All	All	1.19	49/20060 (0.2%)	1.04	88/27255 (0.3%)

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	1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	CD-OE1	9.85	1.36	1.25
1	E	183	GLU	CD-OE2	9.63	1.36	1.25
1	G	225	GLU	CG-CD	7.96	1.63	1.51
1	B	225	GLU	CG-CD	7.62	1.63	1.51
1	G	62	GLU	CG-CD	7.53	1.63	1.51
1	I	158	VAL	CB-CG2	-7.23	1.37	1.52
1	G	179	GLU	CG-CD	7.23	1.62	1.51
1	J	179	GLU	CG-CD	7.11	1.62	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	179	GLU	CD-OE1	6.69	1.33	1.25
1	B	179	GLU	CG-CD	6.36	1.61	1.51
1	B	62	GLU	CG-CD	6.32	1.61	1.51
1	H	243	GLU	CG-CD	6.24	1.61	1.51
1	J	225	GLU	CG-CD	6.14	1.61	1.51
1	C	179	GLU	CD-OE1	6.11	1.32	1.25
1	I	179	GLU	CD-OE1	6.08	1.32	1.25
1	I	57	PHE	CE1-CZ	6.04	1.48	1.37
1	E	225	GLU	CG-CD	6.02	1.60	1.51
1	G	57	PHE	CE1-CZ	6.02	1.48	1.37
1	J	225	GLU	CD-OE1	5.87	1.32	1.25
1	D	57	PHE	CE1-CZ	5.84	1.48	1.37
1	G	225	GLU	CB-CG	5.80	1.63	1.52
1	G	44	ALA	CA-CB	5.75	1.64	1.52
1	B	225	GLU	CD-OE1	5.70	1.31	1.25
1	G	179	GLU	CD-OE2	5.67	1.31	1.25
1	D	179	GLU	CG-CD	5.65	1.60	1.51
1	C	153	GLU	CG-CD	5.61	1.60	1.51
1	D	224	GLU	CG-CD	5.61	1.60	1.51
1	F	214	TRP	CG-CD1	5.56	1.44	1.36
1	J	179	GLU	CB-CG	5.55	1.62	1.52
1	I	243	GLU	CG-CD	5.51	1.60	1.51
1	E	79	VAL	CB-CG2	-5.50	1.41	1.52
1	D	179	GLU	CD-OE1	5.48	1.31	1.25
1	C	183	GLU	CD-OE2	5.45	1.31	1.25
1	G	87	GLU	CB-CG	-5.44	1.41	1.52
1	H	242	TYR	CE1-CZ	5.43	1.45	1.38
1	B	242	TYR	CE1-CZ	5.40	1.45	1.38
1	A	243	GLU	CG-CD	5.39	1.60	1.51
1	E	225	GLU	CD-OE2	5.37	1.31	1.25
1	C	179	GLU	CG-CD	5.36	1.59	1.51
1	J	183	GLU	CG-CD	-5.32	1.44	1.51
1	G	62	GLU	CD-OE1	5.31	1.31	1.25
1	D	171	VAL	CB-CG2	5.28	1.64	1.52
1	F	207	SER	CB-OG	-5.28	1.35	1.42
1	I	53	GLU	CD-OE1	5.18	1.31	1.25
1	E	225	GLU	CB-CG	5.16	1.61	1.52
1	B	62	GLU	CD-OE1	5.12	1.31	1.25
1	G	57	PHE	CD2-CE2	5.06	1.49	1.39
1	A	160	ALA	CA-CB	5.05	1.63	1.52
1	H	214	TRP	CG-CD1	5.05	1.43	1.36

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	59	ARG	NE-CZ-NH1	11.61	126.10	120.30
1	J	231	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	G	126	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	G	231	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	F	227	ARG	NE-CZ-NH1	-9.39	115.60	120.30
1	J	169	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	I	126	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	D	126	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	F	134	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	G	221	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	D	208	LEU	CA-CB-CG	7.82	133.27	115.30
1	G	221	ASP	CB-CG-OD1	7.73	125.26	118.30
1	B	208	LEU	CA-CB-CG	7.66	132.91	115.30
1	F	231	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	D	126	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	E	231	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	E	227	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	F	134	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	J	126	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	I	220	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	E	208	LEU	CA-CB-CG	7.29	132.08	115.30
1	F	116	LEU	CA-CB-CG	-7.25	98.62	115.30
1	G	96	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	28	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	206	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	F	231	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	G	111	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	E	227	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	H	231	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	28	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	220	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	I	126	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	J	126	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	156	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	F	59	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	C	156	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	H	159	LYS	CD-CE-NZ	-6.29	97.22	111.70
1	F	156	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	F	228	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	G	227	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	F	20	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	132	ASP	CB-CG-OD1	6.14	123.83	118.30
1	I	231	ARG	NE-CZ-NH1	6.14	123.37	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	117	HIS	N-CA-C	6.11	127.51	111.00
1	D	221	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	I	228	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	G	231	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	F	228	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	F	74	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	126	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	I	116	LEU	CA-CB-CG	-6.00	101.50	115.30
1	I	77	ASP	CB-CG-OD2	5.96	123.66	118.30
1	H	231	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	74	LEU	CA-CB-CG	5.83	128.72	115.30
1	C	206	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	G	96	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	J	227	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	161	LEU	CA-CB-CG	5.70	128.42	115.30
1	I	221	ASP	CB-CG-OD1	5.66	123.39	118.30
1	F	199	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	I	220	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	I	161	LEU	CA-CB-CG	5.57	128.12	115.30
1	J	74	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	158	VAL	CG1-CB-CG2	-5.57	101.99	110.90
1	H	206	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	220	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	F	96	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	174	ASP	CB-CG-OD1	5.41	123.17	118.30
1	I	20	ASP	CB-CG-OD1	5.40	123.16	118.30
1	G	111	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	I	111	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	241	LEU	CA-CB-CG	5.31	127.51	115.30
1	H	134	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	228	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	F	126	ARG	CB-CA-C	5.24	120.88	110.40
1	H	20	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	74	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	132	ASP	CB-CG-OD1	5.15	122.94	118.30
1	H	126	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	147	LEU	CA-CB-CG	5.13	127.09	115.30
1	C	236	LYS	CD-CE-NZ	5.09	123.42	111.70
1	E	74	LEU	CA-CB-CG	5.04	126.89	115.30
1	F	199	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	74	LEU	CA-CB-CG	5.04	126.88	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	197	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	G	59	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1965	0	1948	93	0
1	B	1953	0	1935	73	0
1	C	1950	0	1935	74	0
1	D	1965	0	1948	99	0
1	E	1965	0	1948	97	0
1	F	1965	0	1948	94	0
1	G	1965	0	1948	70	0
1	H	1965	0	1948	60	0
1	I	1965	0	1948	87	0
1	J	1965	0	1947	84	0
2	A	83	0	0	5	0
2	B	64	0	0	6	0
2	C	58	0	0	6	0
2	D	44	0	0	3	0
2	E	66	0	0	5	0
2	F	75	0	0	5	0
2	G	82	0	0	4	0
2	H	82	0	0	6	0
2	I	75	0	0	3	0
2	J	76	0	0	3	0
All	All	20328	0	19453	727	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 19.

All (727) 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:J:66:ARG:HH11	1:J:66:ARG:HG3	1.05	1.16
1:D:105:PRO:O	1:D:106:GLN:HB3	1.43	1.15
1:G:105:PRO:O	1:G:106:GLN:HB2	1.48	1.13
1:G:14:GLU:HG3	1:G:25:LYS:HZ1	1.00	1.10
1:B:126:ARG:HH11	1:B:145:MET:HA	1.11	1.08
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.18	1.07
1:H:206:ARG:HH11	1:H:206:ARG:HG3	1.08	1.06
1:J:206:ARG:HG3	1:J:206:ARG:HH11	0.91	1.06
1:G:14:GLU:HG3	1:G:25:LYS:NZ	1.71	1.05
1:F:206:ARG:HG3	1:F:206:ARG:HH11	1.18	1.04
1:E:11:ARG:HG2	1:E:11:ARG:HH11	1.25	1.01
1:F:105:PRO:O	1:F:106:GLN:HB2	1.59	0.99
1:J:206:ARG:HG3	1:J:206:ARG:NH1	1.68	0.99
1:J:91:ARG:HH11	1:J:91:ARG:HG2	1.27	0.97
1:J:105:PRO:O	1:J:106:GLN:HB2	1.61	0.97
1:J:11:ARG:HG2	1:J:11:ARG:HH11	1.28	0.96
1:I:5:ILE:HD12	1:I:6:PRO:O	1.64	0.96
1:E:11:ARG:CG	1:E:11:ARG:HH11	1.79	0.94
1:B:228:ARG:HD2	2:B:271:HOH:O	1.67	0.93
1:D:120:SER:CB	1:D:123:HIS:O	2.16	0.92
1:E:59:ARG:HG3	1:E:59:ARG:HH11	1.31	0.92
1:E:168:LYS:O	1:E:168:LYS:HD3	1.69	0.92
1:J:206:ARG:CG	1:J:206:ARG:HH11	1.83	0.91
1:H:106:GLN:O	1:H:111:ARG:NH2	2.04	0.91
1:B:126:ARG:NH1	1:B:145:MET:HA	1.84	0.91
1:E:242:TYR:CD1	1:F:214:TRP:HH2	1.89	0.90
1:C:214:TRP:HH2	1:D:242:TYR:CD1	1.90	0.90
1:H:111:ARG:HE	1:I:106:GLN:NE2	1.68	0.90
1:A:105:PRO:HG2	1:J:122:THR:HG22	1.53	0.89
1:G:206:ARG:HG3	1:G:206:ARG:HH11	1.38	0.88
1:A:7:LEU:HD13	1:B:117:HIS:HB3	1.54	0.88
1:C:14:GLU:OE1	1:C:28:ASP:OD1	1.92	0.88
1:D:188:PRO:O	1:D:199:ARG:NH2	2.07	0.88
1:A:200:MET:HE2	1:A:200:MET:HA	1.52	0.87
1:I:8:ILE:H	1:J:117:HIS:HD2	1.18	0.87
1:F:40:PHE:HD1	1:F:42:HIS:HE2	1.19	0.87
1:I:117:HIS:HB2	1:I:125:VAL:CG1	2.05	0.86
1:A:126:ARG:NH1	1:A:145:MET:O	2.08	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:91:ARG:NH1	1:J:91:ARG:HG2	1.89	0.84
1:C:105:PRO:O	1:C:106:GLN:HB2	1.76	0.84
1:D:105:PRO:O	1:D:106:GLN:CB	2.26	0.84
1:F:66:ARG:NH2	2:F:311:HOH:O	2.11	0.84
1:F:206:ARG:NH1	1:F:206:ARG:HG3	1.89	0.84
1:D:69:VAL:HG21	1:D:158:VAL:HG11	1.60	0.83
1:G:7:LEU:HD12	1:G:10:GLU:OE2	1.78	0.83
1:H:105:PRO:O	1:H:106:GLN:HB2	1.79	0.83
1:G:5:ILE:HD12	1:G:6:PRO:O	1.78	0.83
1:F:238:ALA:O	1:F:239:LYS:HB2	1.77	0.83
1:H:206:ARG:NH1	1:H:206:ARG:HG3	1.85	0.82
1:D:241:LEU:HA	1:D:244:GLU:HG3	1.61	0.82
1:I:8:ILE:N	1:J:117:HIS:HD2	1.77	0.82
1:B:183:GLU:OE2	2:B:301:HOH:O	1.97	0.82
1:E:179:GLU:OE1	1:F:59:ARG:HG2	1.80	0.82
1:J:66:ARG:NH1	1:J:66:ARG:HG3	1.81	0.81
1:A:7:LEU:HB3	1:B:117:HIS:HB2	1.62	0.81
1:J:11:ARG:NH1	1:J:11:ARG:HG2	1.93	0.81
1:D:206:ARG:NH1	1:D:206:ARG:HG3	1.89	0.81
1:F:62:GLU:HG3	1:F:66:ARG:NH2	1.94	0.81
1:E:40:PHE:HD1	1:E:42:HIS:HE2	1.28	0.81
2:C:270:HOH:O	1:D:183:GLU:HG3	1.80	0.81
1:I:59:ARG:HH12	1:J:179:GLU:HG2	1.46	0.81
1:C:5:ILE:HD13	1:D:5:ILE:HD13	1.60	0.80
1:F:14:GLU:OE1	1:F:25:LYS:HE2	1.79	0.80
1:B:126:ARG:HB2	1:B:143:TYR:O	1.80	0.80
1:E:11:ARG:HG2	1:E:11:ARG:NH1	1.96	0.79
1:F:11:ARG:HG2	1:F:11:ARG:HH11	1.45	0.79
1:E:126:ARG:NH1	1:E:145:MET:O	2.17	0.78
1:D:111:ARG:HD2	2:D:273:HOH:O	1.83	0.78
1:B:14:GLU:OE1	1:B:25:LYS:HE2	1.83	0.78
1:I:59:ARG:NH1	1:J:179:GLU:HG2	1.99	0.78
1:J:91:ARG:HH11	1:J:91:ARG:CG	1.97	0.77
1:D:5:ILE:HD12	1:D:140:MET:HE1	1.67	0.77
1:J:115:LEU:O	1:J:125:VAL:HG23	1.85	0.77
1:A:126:ARG:HH12	1:A:145:MET:C	1.88	0.77
1:D:120:SER:HB2	1:D:123:HIS:O	1.85	0.77
1:C:43:PRO:HD2	1:C:50:OCS:OD3	1.85	0.77
1:F:5:ILE:HG13	1:F:6:PRO:O	1.85	0.76
1:A:231:ARG:HH21	1:A:231:ARG:HB2	1.48	0.76
1:G:105:PRO:O	1:G:106:GLN:CB	2.27	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:LEU:O	1:F:10:GLU:HB2	1.86	0.76
1:B:105:PRO:O	1:B:106:GLN:HB2	1.84	0.76
1:D:117:HIS:HB2	1:D:125:VAL:CG1	2.15	0.76
1:I:8:ILE:H	1:J:117:HIS:CD2	2.03	0.75
1:J:145:MET:HE3	2:J:295:HOH:O	1.85	0.75
1:E:200:MET:HA	1:E:200:MET:HE2	1.67	0.75
1:J:7:LEU:HD12	1:J:10:GLU:OE2	1.84	0.75
1:A:200:MET:CE	1:A:200:MET:HA	2.15	0.75
1:J:50:OCS:OD1	1:J:126:ARG:NH2	2.20	0.75
2:A:262:HOH:O	1:B:146:GLU:HG3	1.87	0.75
1:E:43:PRO:HG2	1:E:145:MET:HG2	1.68	0.75
1:I:40:PHE:HD1	1:I:42:HIS:HE2	1.34	0.74
1:H:59:ARG:CG	1:H:59:ARG:HH11	2.00	0.74
1:G:50:OCS:OD1	1:G:126:ARG:NH2	2.19	0.74
1:B:40:PHE:HD1	1:B:42:HIS:HE2	1.35	0.74
1:E:120:SER:HB2	1:E:123:HIS:O	1.88	0.74
1:E:50:OCS:OD1	1:E:126:ARG:NH2	2.20	0.74
1:C:168:LYS:HD3	1:C:168:LYS:O	1.88	0.74
1:C:8:ILE:H	1:D:117:HIS:HD2	1.34	0.73
1:B:206:ARG:HH11	1:B:206:ARG:HG3	1.52	0.73
1:G:5:ILE:HG22	1:G:114:GLY:HA3	1.69	0.73
1:F:206:ARG:HH11	1:F:206:ARG:CG	1.98	0.72
1:A:231:ARG:HH21	1:A:231:ARG:CB	2.02	0.72
1:H:59:ARG:HH11	1:H:59:ARG:HG3	1.53	0.72
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.69	0.72
1:H:11:ARG:NH1	1:H:14:GLU:OE2	2.22	0.72
1:E:117:HIS:CG	1:E:125:VAL:HG21	2.24	0.72
1:D:120:SER:HB3	1:D:123:HIS:O	1.88	0.72
1:C:214:TRP:CH2	1:D:242:TYR:CD1	2.77	0.72
1:I:117:HIS:HB2	1:I:125:VAL:HG11	1.72	0.72
1:G:206:ARG:CG	1:G:206:ARG:HH11	2.02	0.71
1:G:206:ARG:HG3	1:G:206:ARG:NH1	2.06	0.71
1:B:140:MET:CE	1:B:142:TYR:OH	2.39	0.71
2:I:295:HOH:O	1:J:146:GLU:HG3	1.90	0.71
1:I:106:GLN:O	1:I:111:ARG:NH2	2.24	0.71
1:F:124:THR:HG23	1:F:125:VAL:O	1.91	0.70
1:E:59:ARG:HG3	1:E:59:ARG:NH1	1.98	0.70
1:G:8:ILE:H	1:H:117:HIS:HD2	1.38	0.70
1:D:86:LYS:HD3	1:D:97:ILE:HB	1.72	0.70
1:B:126:ARG:NH1	1:B:145:MET:CA	2.55	0.70
1:F:185:LEU:O	1:F:214:TRP:HB2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:GLU:OE1	1:E:28:ASP:OD1	2.10	0.69
1:G:11:ARG:NH1	1:G:14:GLU:OE2	2.22	0.69
1:I:5:ILE:HG22	1:I:114:GLY:HA3	1.72	0.69
1:I:60:ARG:HG3	1:I:60:ARG:HH11	1.58	0.69
1:F:129:PHE:HE2	1:F:140:MET:HE3	1.58	0.69
1:A:7:LEU:HD22	1:B:117:HIS:CG	2.28	0.69
1:E:168:LYS:HD2	2:E:284:HOH:O	1.94	0.68
1:G:117:HIS:HD2	1:H:8:ILE:H	1.40	0.68
1:E:242:TYR:CD1	1:F:214:TRP:CH2	2.77	0.68
1:G:14:GLU:OE1	1:G:28:ASP:OD1	2.12	0.68
1:J:117:HIS:ND1	1:J:125:VAL:HG21	2.09	0.68
1:A:118:ALA:HB2	1:B:10:GLU:HG3	1.75	0.68
1:F:106:GLN:HE22	1:G:107:GLY:HA3	1.56	0.68
1:I:117:HIS:HB2	1:I:125:VAL:HG13	1.74	0.68
1:C:125:VAL:HA	1:C:145:MET:HE2	1.76	0.68
1:D:228:ARG:NH1	2:D:268:HOH:O	2.25	0.68
1:C:214:TRP:HH2	1:D:242:TYR:CE1	2.12	0.68
1:B:106:GLN:O	1:B:111:ARG:NH2	2.26	0.68
1:F:129:PHE:CE2	1:F:140:MET:CE	2.77	0.67
1:G:40:PHE:HD1	1:G:42:HIS:HE2	1.40	0.67
1:A:239:LYS:HD2	1:A:244:GLU:HG2	1.75	0.67
1:A:231:ARG:NH2	1:A:231:ARG:HB2	2.10	0.67
1:H:111:ARG:HE	1:I:106:GLN:HE22	1.40	0.67
1:C:120:SER:O	1:C:122:THR:N	2.27	0.67
1:F:188:PRO:O	1:F:199:ARG:NH2	2.27	0.67
1:E:8:ILE:H	1:F:117:HIS:HD2	1.40	0.67
1:D:50:OCS:OD1	1:D:126:ARG:NH2	2.27	0.67
1:E:115:LEU:HB3	1:E:124:THR:HG23	1.76	0.67
1:B:43:PRO:HB3	1:B:123:HIS:HB3	1.77	0.67
1:B:67:LEU:HD13	1:B:158:VAL:HG23	1.76	0.67
1:D:120:SER:C	1:D:122:THR:H	1.98	0.67
1:E:40:PHE:HD1	1:E:42:HIS:NE2	1.92	0.67
1:J:67:LEU:HD13	1:J:158:VAL:HG23	1.76	0.66
1:E:190:PRO:HB3	1:E:195:GLN:HB3	1.77	0.66
1:G:40:PHE:HD1	1:G:42:HIS:NE2	1.92	0.66
1:A:208:LEU:CD1	1:A:214:TRP:CZ3	2.78	0.66
1:H:69:VAL:HG21	1:H:158:VAL:HG21	1.78	0.66
1:C:125:VAL:HA	1:C:145:MET:CE	2.25	0.66
1:J:105:PRO:O	1:J:106:GLN:CB	2.37	0.66
1:I:14:GLU:OE1	1:I:25:LYS:HE2	1.96	0.66
1:D:167:LEU:HD23	1:D:217:PRO:HG2	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:LEU:HA	1:D:244:GLU:CG	2.27	0.65
1:I:240:LEU:O	1:I:243:GLU:HG2	1.96	0.65
1:H:122:THR:HG22	1:H:123:HIS:CD2	2.32	0.65
1:E:117:HIS:CD2	1:E:125:VAL:HG21	2.31	0.65
1:A:7:LEU:HB3	1:B:117:HIS:CB	2.26	0.65
1:B:59:ARG:HH11	1:B:59:ARG:HG2	1.62	0.65
1:E:129:PHE:CE2	1:E:140:MET:HE2	2.31	0.64
1:A:67:LEU:HD13	1:A:158:VAL:HG23	1.80	0.64
1:B:126:ARG:HH12	1:B:145:MET:CG	2.09	0.64
1:E:129:PHE:HE2	1:E:140:MET:HE3	1.62	0.64
1:F:106:GLN:NE2	1:G:107:GLY:HA3	2.12	0.64
1:H:125:VAL:HA	1:H:145:MET:HE2	1.78	0.64
1:G:40:PHE:CD1	1:G:42:HIS:NE2	2.63	0.64
1:G:63:ASP:CG	1:G:228:ARG:HH12	2.00	0.64
1:I:105:PRO:O	1:I:106:GLN:HB2	1.97	0.64
1:H:67:LEU:HD13	1:H:158:VAL:HG22	1.78	0.64
1:E:129:PHE:CE2	1:E:140:MET:CE	2.80	0.64
1:D:117:HIS:HB2	1:D:125:VAL:HG13	1.80	0.63
1:I:43:PRO:HG3	1:I:145:MET:HG2	1.78	0.63
1:B:126:ARG:HH11	1:B:145:MET:CA	1.99	0.63
1:F:11:ARG:HG2	1:F:11:ARG:NH1	2.11	0.63
1:D:200:MET:HE3	1:D:210:TRP:HA	1.79	0.63
1:B:106:GLN:HE22	1:C:107:GLY:HA3	1.63	0.63
1:F:129:PHE:CE2	1:F:140:MET:HE3	2.33	0.63
1:I:7:LEU:HD12	1:I:10:GLU:OE2	1.98	0.63
1:H:40:PHE:HD1	1:H:42:HIS:HE2	1.47	0.63
1:E:168:LYS:O	1:E:168:LYS:CD	2.43	0.63
1:C:172:PRO:HG3	1:C:181:ILE:HD11	1.80	0.63
1:E:168:LYS:HE3	1:E:188:PRO:HD2	1.79	0.63
1:F:42:HIS:NE2	1:F:54:PHE:HE1	1.97	0.63
1:A:126:ARG:NH1	1:A:145:MET:C	2.50	0.63
1:D:42:HIS:NE2	1:D:54:PHE:HE1	1.97	0.62
1:I:161:LEU:HD11	1:J:144:PRO:HG3	1.81	0.62
1:H:105:PRO:O	1:H:106:GLN:CB	2.45	0.62
1:G:220:ARG:O	1:G:224:GLU:HG3	1.99	0.62
1:F:194:ASP:OD1	1:F:197:ARG:NH2	2.31	0.62
1:G:42:HIS:NE2	1:G:54:PHE:HE1	1.97	0.62
1:I:125:VAL:HA	1:I:145:MET:CE	2.29	0.62
1:I:115:LEU:HD21	1:I:129:PHE:HE1	1.64	0.62
1:G:193:GLU:OE2	1:I:86:LYS:HD2	1.99	0.61
1:B:145:MET:O	1:B:145:MET:HG2	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ARG:CG	1:D:206:ARG:HH11	2.04	0.61
1:A:14:GLU:OE1	1:A:28:ASP:OD1	2.18	0.61
1:F:86:LYS:HE3	1:F:101:ILE:CD1	2.30	0.61
1:A:7:LEU:HD22	1:B:117:HIS:CD2	2.35	0.61
1:H:125:VAL:HA	1:H:145:MET:CE	2.31	0.61
1:J:111:ARG:HG3	1:J:116:LEU:HD12	1.83	0.61
1:G:59:ARG:HG2	1:G:59:ARG:HH11	1.65	0.61
1:B:115:LEU:HB3	1:B:124:THR:HG23	1.82	0.61
1:D:14:GLU:OE1	1:D:28:ASP:OD1	2.19	0.61
1:A:208:LEU:CD1	1:A:214:TRP:HZ3	2.13	0.60
1:E:146:GLU:HG3	2:F:287:HOH:O	2.01	0.60
1:F:40:PHE:HD1	1:F:42:HIS:NE2	1.94	0.60
1:B:126:ARG:HH12	1:B:145:MET:HG2	1.66	0.60
1:A:117:HIS:O	1:A:120:SER:HB2	2.00	0.60
1:G:202:SER:OG	1:G:204:GLN:HG2	2.02	0.60
1:D:154:ILE:O	1:D:158:VAL:HG23	2.01	0.60
1:D:228:ARG:HH11	1:D:228:ARG:CG	2.15	0.60
1:E:129:PHE:HE2	1:E:140:MET:CE	2.15	0.60
1:A:120:SER:C	1:A:121:ALA:O	2.39	0.60
1:F:62:GLU:CG	1:F:66:ARG:NH2	2.64	0.60
1:E:134:ARG:NH1	2:E:306:HOH:O	2.31	0.60
1:A:4:SER:HA	1:B:4:SER:HB2	1.84	0.60
1:H:106:GLN:HG3	1:I:121:ALA:O	2.02	0.60
1:E:5:ILE:HD13	1:F:5:ILE:HD13	1.83	0.60
1:I:40:PHE:HD1	1:I:42:HIS:NE2	2.00	0.60
1:B:206:ARG:HG3	1:B:206:ARG:NH1	2.14	0.60
1:E:242:TYR:CE1	1:F:214:TRP:HH2	2.19	0.59
1:H:59:ARG:NH1	1:H:59:ARG:HG3	2.14	0.59
1:C:50:OCS:OD1	1:C:126:ARG:NH2	2.36	0.59
1:J:206:ARG:CG	1:J:206:ARG:NH1	2.53	0.59
1:I:5:ILE:HG12	1:J:5:ILE:HG12	1.83	0.59
1:E:42:HIS:NE2	1:E:54:PHE:HE1	2.01	0.59
1:A:122:THR:HG22	1:A:123:HIS:CD2	2.38	0.59
1:F:62:GLU:HG3	1:F:66:ARG:CZ	2.32	0.59
1:B:140:MET:HE1	1:B:142:TYR:OH	2.02	0.59
1:J:200:MET:HA	1:J:200:MET:HE2	1.85	0.59
1:F:167:LEU:N	1:F:167:LEU:HD12	2.18	0.59
1:I:59:ARG:HH12	1:J:179:GLU:CG	2.13	0.59
1:D:126:ARG:HD2	1:D:144:PRO:O	2.03	0.59
1:B:40:PHE:HD1	1:B:42:HIS:NE2	2.00	0.59
1:I:200:MET:HA	1:I:200:MET:HE2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PRO:HB3	1:C:123:HIS:HB3	1.84	0.59
1:I:126:ARG:HH12	1:I:145:MET:C	2.05	0.59
1:I:11:ARG:NH2	2:I:302:HOH:O	2.35	0.59
1:B:43:PRO:HG2	1:B:145:MET:HG3	1.84	0.59
1:J:67:LEU:HD21	1:J:159:LYS:HD3	1.85	0.58
1:B:190:PRO:HB3	1:B:195:GLN:HB3	1.86	0.58
1:A:105:PRO:O	1:A:106:GLN:HB2	2.03	0.58
1:G:104:ASP:OD2	1:G:107:GLY:HA2	2.04	0.58
1:D:69:VAL:CG2	1:D:158:VAL:HG11	2.32	0.58
1:J:14:GLU:OE1	1:J:28:ASP:OD1	2.21	0.58
1:I:120:SER:HB3	1:I:123:HIS:O	2.04	0.57
1:F:129:PHE:CE2	1:F:140:MET:HE2	2.37	0.57
1:H:159:LYS:NZ	1:H:225:GLU:OE2	2.33	0.57
1:A:163:LEU:O	1:A:167:LEU:HB2	2.04	0.57
1:G:172:PRO:HG3	1:G:181:ILE:HD11	1.85	0.57
1:I:144:PRO:HB3	2:J:326:HOH:O	2.03	0.57
1:G:144:PRO:HG3	1:H:161:LEU:HD11	1.86	0.57
1:F:167:LEU:N	1:F:167:LEU:CD1	2.67	0.57
1:E:4:SER:HA	1:F:4:SER:HA	1.85	0.57
1:A:62:GLU:HG3	1:A:66:ARG:NH1	2.18	0.57
1:C:236:LYS:NZ	2:C:270:HOH:O	2.36	0.57
1:C:244:GLU:HG3	1:C:245:ALA:N	2.19	0.57
1:D:117:HIS:HB2	1:D:125:VAL:HG11	1.87	0.57
1:G:183:GLU:OE1	1:H:236:LYS:NZ	2.27	0.57
1:E:238:ALA:O	1:E:239:LYS:CB	2.52	0.57
1:D:75:SER:HB3	1:D:82:HIS:CE1	2.39	0.57
1:C:214:TRP:HH2	1:D:242:TYR:CG	2.23	0.56
1:A:188:PRO:O	1:A:199:ARG:NH2	2.38	0.56
1:B:86:LYS:HE3	1:B:101:ILE:HD12	1.87	0.56
1:I:125:VAL:HA	1:I:145:MET:HE3	1.86	0.56
1:C:105:PRO:O	1:C:106:GLN:CB	2.48	0.56
1:A:129:PHE:HE2	1:A:140:MET:HE3	1.70	0.56
1:E:105:PRO:O	1:E:106:GLN:CB	2.54	0.56
1:B:206:ARG:CG	1:B:206:ARG:HH11	2.17	0.56
1:A:118:ALA:CB	1:B:10:GLU:HG3	2.35	0.56
1:I:89:ILE:HG21	1:I:97:ILE:HD11	1.86	0.56
1:E:118:ALA:HB2	1:F:10:GLU:HG3	1.87	0.56
1:F:163:LEU:O	1:F:167:LEU:HD13	2.06	0.56
1:D:28:ASP:OD1	1:D:28:ASP:N	2.39	0.56
1:D:110:ALA:HB1	1:D:124:THR:HG22	1.86	0.56
1:D:146:GLU:OE2	1:D:146:GLU:N	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:CD1	1:D:5:ILE:HD13	2.35	0.56
1:E:118:ALA:CB	1:F:10:GLU:HG3	2.35	0.56
1:E:206:ARG:HG3	1:E:206:ARG:HH11	1.71	0.56
1:E:50:OCS:SG	1:E:126:ARG:NH2	2.79	0.56
1:A:129:PHE:CE2	1:A:140:MET:HE3	2.41	0.56
1:E:117:HIS:HB2	1:E:125:VAL:CG2	2.36	0.56
1:E:144:PRO:HD3	1:F:139:THR:OG1	2.06	0.56
1:J:40:PHE:CD1	1:J:42:HIS:NE2	2.72	0.56
1:F:124:THR:CG2	1:F:125:VAL:O	2.54	0.55
1:D:200:MET:CE	1:D:210:TRP:HA	2.36	0.55
1:C:126:ARG:HD2	1:C:144:PRO:O	2.07	0.55
1:A:193:GLU:OE2	1:C:86:LYS:HD2	2.06	0.55
1:F:190:PRO:HB3	1:F:195:GLN:HB3	1.88	0.55
1:F:67:LEU:HD21	1:F:159:LYS:HD2	1.89	0.55
1:D:228:ARG:HH11	1:D:228:ARG:HG2	1.71	0.55
1:F:67:LEU:HD13	1:F:158:VAL:HG23	1.89	0.55
1:H:40:PHE:HD1	1:H:42:HIS:NE2	2.04	0.55
1:A:139:THR:HG1	1:B:144:PRO:HD3	1.72	0.55
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.06	0.55
1:I:126:ARG:HG3	1:I:149:ARG:CZ	2.36	0.55
1:H:190:PRO:HB3	1:H:195:GLN:HB3	1.89	0.55
1:F:220:ARG:NH1	1:F:224:GLU:OE2	2.40	0.55
1:D:144:PRO:HG2	1:D:147:LEU:HB2	1.89	0.54
1:H:228:ARG:HD3	2:H:266:HOH:O	2.07	0.54
1:H:11:ARG:NH2	2:H:271:HOH:O	2.40	0.54
1:C:134:ARG:NH1	2:C:308:HOH:O	2.26	0.54
1:C:146:GLU:HG3	2:D:258:HOH:O	2.06	0.54
1:I:140:MET:HE1	1:I:142:TYR:OH	2.07	0.54
1:H:238:ALA:O	1:H:239:LYS:HB3	2.08	0.54
1:I:140:MET:CE	1:I:142:TYR:OH	2.56	0.54
1:H:67:LEU:HD21	1:H:159:LYS:HD3	1.90	0.54
1:B:225:GLU:HB2	1:B:228:ARG:HH22	1.73	0.54
1:H:14:GLU:OE1	1:H:28:ASP:OD1	2.24	0.54
1:I:59:ARG:HH12	1:J:179:GLU:HB3	1.72	0.53
1:F:215:ASP:OD1	1:F:217:PRO:HD3	2.08	0.53
1:G:129:PHE:CE2	1:G:140:MET:HE2	2.44	0.53
1:D:16:GLU:OE1	1:D:23:VAL:CG1	2.56	0.53
1:A:117:HIS:HB2	1:A:125:VAL:HG13	1.90	0.53
1:H:35:LYS:NZ	2:H:308:HOH:O	2.40	0.53
1:F:239:LYS:HE2	1:F:244:GLU:OE1	2.08	0.53
1:C:220:ARG:NH1	1:C:224:GLU:OE2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LEU:HB3	1:E:124:THR:CG2	2.39	0.53
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.43	0.53
1:B:50:OCS:OD1	1:B:126:ARG:NH2	2.42	0.53
1:H:106:GLN:NE2	1:I:111:ARG:HE	2.07	0.53
2:C:259:HOH:O	1:D:146:GLU:HG3	2.07	0.53
1:J:126:ARG:HD2	1:J:144:PRO:O	2.08	0.53
1:A:5:ILE:HD12	1:A:140:MET:HE1	1.91	0.53
1:I:11:ARG:NH1	1:I:14:GLU:OE2	2.40	0.53
1:E:122:THR:HG23	1:E:123:HIS:CD2	2.44	0.53
1:A:62:GLU:HG3	1:A:66:ARG:HH11	1.74	0.53
1:E:11:ARG:HG3	1:E:11:ARG:HH11	1.71	0.53
1:G:146:GLU:HG3	2:H:267:HOH:O	2.08	0.53
1:C:200:MET:HE3	1:C:210:TRP:HA	1.91	0.53
1:B:126:ARG:NH1	1:B:145:MET:O	2.42	0.52
1:D:66:ARG:NH1	1:D:66:ARG:HG3	2.24	0.52
1:D:122:THR:HG23	1:D:123:HIS:CD2	2.45	0.52
1:H:124:THR:HG23	1:H:125:VAL:O	2.08	0.52
1:I:236:LYS:HD2	1:I:237:PRO:HD2	1.91	0.52
1:I:5:ILE:CD1	1:I:6:PRO:O	2.48	0.52
1:D:228:ARG:HG2	1:D:228:ARG:NH1	2.25	0.52
1:E:129:PHE:CE2	1:E:140:MET:HE3	2.45	0.52
1:G:129:PHE:CE2	1:G:140:MET:CE	2.92	0.52
1:I:63:ASP:HA	1:I:66:ARG:NH1	2.24	0.52
1:D:16:GLU:OE1	1:D:23:VAL:HG12	2.10	0.52
1:B:200:MET:HE3	1:B:210:TRP:HA	1.91	0.52
2:G:268:HOH:O	1:H:146:GLU:HG3	2.10	0.52
1:I:144:PRO:HG3	1:J:161:LEU:HD11	1.90	0.52
1:C:104:ASP:OD2	1:C:107:GLY:HA2	2.10	0.52
1:A:128:VAL:O	1:A:140:MET:HA	2.10	0.52
1:I:36:TRP:HB2	1:I:69:VAL:HG22	1.91	0.52
1:D:122:THR:CG2	1:D:123:HIS:CD2	2.93	0.51
1:I:117:HIS:CB	1:I:125:VAL:HG11	2.40	0.51
1:E:117:HIS:HB2	1:E:125:VAL:HG22	1.92	0.51
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.44	0.51
1:A:239:LYS:HG2	1:A:244:GLU:OE1	2.10	0.51
1:I:147:LEU:HG	1:J:161:LEU:HD13	1.93	0.51
1:A:129:PHE:CE2	1:A:140:MET:CE	2.93	0.51
1:D:117:HIS:CG	1:D:125:VAL:HG11	2.46	0.51
1:E:188:PRO:O	1:E:199:ARG:NH2	2.43	0.51
1:E:242:TYR:HD1	1:F:208:LEU:HD11	1.76	0.51
1:E:5:ILE:CD1	1:F:5:ILE:HD13	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:OG1	1:B:144:PRO:HD3	2.11	0.51
1:I:115:LEU:HD21	1:I:129:PHE:CE1	2.44	0.51
1:E:144:PRO:HB3	2:E:286:HOH:O	2.09	0.51
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.46	0.51
1:I:178:ASN:HD21	1:J:52:THR:HB	1.76	0.51
1:B:126:ARG:NH1	1:B:145:MET:CG	2.73	0.51
1:B:134:ARG:NH1	2:B:297:HOH:O	2.44	0.51
1:I:190:PRO:HB3	1:I:195:GLN:HB3	1.91	0.51
1:F:42:HIS:CD2	1:F:54:PHE:HE1	2.29	0.51
1:E:122:THR:HG23	1:E:123:HIS:CG	2.46	0.51
1:E:220:ARG:HG3	2:E:264:HOH:O	2.11	0.51
1:E:238:ALA:O	1:E:239:LYS:HB2	2.11	0.51
1:E:200:MET:HA	1:E:200:MET:CE	2.37	0.51
1:J:63:ASP:OD1	1:J:228:ARG:NH2	2.43	0.51
1:F:126:ARG:HG2	1:F:143:TYR:O	2.10	0.51
1:I:37:PHE:HA	1:I:70:ASP:O	2.11	0.51
1:A:122:THR:HG22	1:A:123:HIS:CG	2.46	0.50
1:F:75:SER:HB3	1:F:82:HIS:CE1	2.46	0.50
1:J:120:SER:CB	1:J:123:HIS:O	2.60	0.50
1:D:76:VAL:O	1:D:105:PRO:HA	2.11	0.50
1:D:120:SER:C	1:D:122:THR:N	2.64	0.50
1:F:220:ARG:HH11	1:F:220:ARG:HG3	1.76	0.50
1:D:66:ARG:HH11	1:D:66:ARG:HG3	1.75	0.50
1:G:163:LEU:HD11	1:G:222:ASP:HB3	1.93	0.50
1:H:104:ASP:OD2	1:H:107:GLY:HA2	2.12	0.50
1:C:206:ARG:HH12	1:C:215:ASP:HA	1.75	0.50
1:G:7:LEU:HB2	1:G:10:GLU:OE2	2.12	0.50
1:G:63:ASP:OD1	1:G:228:ARG:NH1	2.45	0.50
1:C:86:LYS:HE2	1:C:101:ILE:HD11	1.93	0.50
1:E:7:LEU:HD12	1:E:10:GLU:OE2	2.11	0.50
1:E:43:PRO:CG	1:E:145:MET:HG2	2.39	0.50
1:A:43:PRO:HD2	1:A:50:OCS:OD3	2.11	0.50
1:J:190:PRO:HB3	1:J:195:GLN:HB3	1.94	0.50
1:J:120:SER:HB2	1:J:123:HIS:O	2.11	0.50
1:H:122:THR:CG2	1:H:123:HIS:CD2	2.95	0.50
1:I:59:ARG:HH12	1:J:179:GLU:CB	2.24	0.50
1:I:60:ARG:HG3	1:I:60:ARG:NH1	2.27	0.50
1:D:14:GLU:OE1	1:D:25:LYS:HE3	2.12	0.50
1:C:40:PHE:CD1	1:C:42:HIS:NE2	2.79	0.50
1:A:191:THR:H	1:A:195:GLN:NE2	2.10	0.50
1:J:63:ASP:OD2	1:J:228:ARG:NH2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:207:SER:HB3	1:J:213:CYS:SG	2.52	0.49
1:A:9:GLY:HA3	1:B:119:GLU:HG2	1.94	0.49
1:C:214:TRP:CH2	1:D:242:TYR:CG	3.00	0.49
1:I:43:PRO:CB	1:I:123:HIS:HB3	2.42	0.49
1:A:126:ARG:NH1	1:A:145:MET:HA	2.27	0.49
1:C:8:ILE:HD11	1:D:142:TYR:HB3	1.94	0.49
1:B:67:LEU:HD13	1:B:158:VAL:CG2	2.42	0.49
1:I:236:LYS:HD3	1:J:227:ARG:NH2	2.27	0.49
1:E:7:LEU:O	1:E:10:GLU:HB2	2.12	0.49
1:E:105:PRO:O	1:E:106:GLN:HB2	2.12	0.49
1:F:14:GLU:OE1	1:F:28:ASP:OD1	2.30	0.49
1:I:146:GLU:HG3	2:J:263:HOH:O	2.13	0.49
1:D:16:GLU:OE2	1:D:25:LYS:HB2	2.13	0.49
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.77	0.49
1:A:144:PRO:HB3	2:A:333:HOH:O	2.12	0.49
1:J:140:MET:CE	1:J:142:TYR:OH	2.60	0.49
1:H:126:ARG:HG3	1:H:143:TYR:O	2.13	0.49
1:B:208:LEU:HD22	1:B:214:TRP:HZ3	1.77	0.49
1:B:117:HIS:NE2	1:B:125:VAL:HG21	2.27	0.49
1:I:120:SER:C	1:I:122:THR:H	2.16	0.49
1:G:14:GLU:O	1:G:15:MET:HB3	2.13	0.49
1:A:105:PRO:HG2	1:J:122:THR:CG2	2.34	0.49
1:B:124:THR:HG22	1:B:125:VAL:O	2.12	0.49
1:F:238:ALA:O	1:F:239:LYS:CB	2.52	0.49
1:B:200:MET:CE	1:B:210:TRP:HA	2.42	0.49
1:G:14:GLU:CG	1:G:25:LYS:NZ	2.61	0.49
1:J:41:SER:HB2	1:J:124:THR:HG21	1.94	0.49
1:G:54:PHE:CE2	1:G:101:ILE:HD11	2.48	0.49
1:E:4:SER:HA	1:F:4:SER:N	2.27	0.49
1:A:142:TYR:HB3	1:B:8:ILE:HD11	1.95	0.49
1:F:200:MET:HA	1:F:200:MET:HE2	1.94	0.49
1:C:206:ARG:NH1	1:C:215:ASP:HA	2.28	0.48
1:C:42:HIS:NE2	1:C:54:PHE:HE1	2.12	0.48
1:C:157:ILE:O	1:C:161:LEU:HB2	2.13	0.48
1:F:41:SER:HB2	1:F:124:THR:HG21	1.95	0.48
1:G:117:HIS:CD2	1:H:8:ILE:H	2.25	0.48
1:J:117:HIS:HB2	1:J:125:VAL:HG22	1.95	0.48
1:I:43:PRO:HB2	1:I:123:HIS:HB3	1.94	0.48
1:C:4:SER:HA	1:D:4:SER:HA	1.96	0.48
1:E:11:ARG:NH1	1:E:11:ARG:CG	2.50	0.48
1:J:115:LEU:HD11	1:J:129:PHE:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:ARG:HH12	1:F:145:MET:C	2.14	0.48
1:H:120:SER:HA	2:H:279:HOH:O	2.14	0.48
1:B:228:ARG:CD	2:B:271:HOH:O	2.44	0.48
1:A:40:PHE:HZ	1:A:99:PHE:CE1	2.31	0.48
1:A:204:GLN:HB2	2:A:324:HOH:O	2.12	0.48
1:I:7:LEU:HB2	1:I:10:GLU:CD	2.34	0.48
1:G:129:PHE:HE2	1:G:140:MET:HE3	1.78	0.48
1:G:79:VAL:O	1:G:83:ILE:HG13	2.13	0.48
1:C:214:TRP:CH2	1:D:242:TYR:CE1	2.96	0.47
1:I:154:ILE:O	1:I:158:VAL:HG13	2.14	0.47
1:A:202:SER:C	1:A:204:GLN:N	2.65	0.47
1:G:200:MET:CE	1:G:200:MET:HA	2.44	0.47
1:I:59:ARG:NH1	1:J:179:GLU:CG	2.73	0.47
1:C:40:PHE:HD1	1:C:42:HIS:NE2	2.12	0.47
1:A:156:ARG:HD3	1:A:230:LEU:HD21	1.96	0.47
1:I:41:SER:HB2	1:I:124:THR:HG21	1.95	0.47
1:F:228:ARG:HD3	2:F:268:HOH:O	2.15	0.47
1:I:126:ARG:NH1	1:I:145:MET:O	2.31	0.47
1:H:146:GLU:N	1:H:146:GLU:OE2	2.42	0.47
1:E:4:SER:HA	1:F:4:SER:CA	2.44	0.47
1:E:144:PRO:HG2	1:E:147:LEU:HB2	1.97	0.47
1:C:153:GLU:O	1:C:157:ILE:HG13	2.14	0.47
1:D:172:PRO:HG3	1:D:181:ILE:HD11	1.95	0.47
1:C:140:MET:HE1	1:C:142:TYR:OH	2.15	0.47
1:H:122:THR:HG23	1:I:105:PRO:HG2	1.97	0.47
1:F:86:LYS:HE3	1:F:101:ILE:HD11	1.95	0.47
1:H:111:ARG:HH21	1:I:106:GLN:HE21	1.61	0.47
1:B:115:LEU:HB3	1:B:124:THR:CG2	2.45	0.47
1:H:44:ALA:O	1:H:47:THR:OG1	2.30	0.47
1:I:104:ASP:OD2	1:I:107:GLY:HA2	2.14	0.47
1:F:167:LEU:HD23	1:F:217:PRO:HG2	1.97	0.47
1:G:128:VAL:O	1:G:140:MET:HA	2.15	0.47
1:C:7:LEU:O	1:C:10:GLU:HB2	2.15	0.47
1:J:128:VAL:O	1:J:140:MET:HA	2.15	0.46
1:I:125:VAL:HA	1:I:145:MET:HE2	1.95	0.46
1:D:110:ALA:HB2	1:D:124:THR:HG21	1.97	0.46
1:J:63:ASP:CG	1:J:228:ARG:NH2	2.68	0.46
1:C:125:VAL:HA	1:C:145:MET:HE1	1.98	0.46
1:E:220:ARG:O	1:E:224:GLU:HG3	2.15	0.46
1:B:208:LEU:HD22	1:B:214:TRP:CZ3	2.50	0.46
1:J:124:THR:HG23	1:J:125:VAL:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLN:NE2	1:C:107:GLY:HA3	2.29	0.46
1:B:105:PRO:O	1:B:106:GLN:CB	2.53	0.46
1:G:146:GLU:OE2	1:G:146:GLU:N	2.45	0.46
1:F:146:GLU:OE2	1:F:146:GLU:N	2.36	0.46
1:I:118:ALA:HB2	1:J:10:GLU:CG	2.46	0.46
1:D:110:ALA:CB	1:D:124:THR:CG2	2.93	0.46
1:J:40:PHE:HD1	1:J:42:HIS:NE2	2.13	0.46
1:A:174:ASP:HB3	2:B:279:HOH:O	2.15	0.46
1:E:39:LEU:HD23	1:E:39:LEU:C	2.36	0.46
1:E:242:TYR:CE1	1:F:214:TRP:CH2	3.02	0.46
1:A:115:LEU:O	1:A:125:VAL:HG22	2.16	0.46
1:G:157:ILE:O	1:G:161:LEU:HB2	2.16	0.46
1:G:106:GLN:O	1:G:111:ARG:NH2	2.49	0.46
1:I:128:VAL:HG23	1:I:149:ARG:HH11	1.80	0.46
1:D:228:ARG:CG	1:D:228:ARG:NH1	2.79	0.46
1:E:203:GLY:HA2	2:E:269:HOH:O	2.16	0.46
1:D:45:ASP:HA	1:D:85:TRP:CE3	2.51	0.46
1:J:11:ARG:CG	1:J:11:ARG:HH11	2.12	0.46
1:A:124:THR:HG23	1:A:125:VAL:O	2.15	0.46
1:D:45:ASP:HA	1:D:85:TRP:CZ3	2.51	0.46
1:G:16:GLU:HG2	1:G:25:LYS:CD	2.45	0.46
1:I:117:HIS:CG	1:I:125:VAL:HG11	2.51	0.46
1:A:126:ARG:HB3	1:A:143:TYR:O	2.16	0.46
1:D:110:ALA:HB1	1:D:124:THR:CG2	2.44	0.46
1:E:128:VAL:O	1:E:140:MET:HA	2.16	0.46
1:H:126:ARG:NH1	1:H:145:MET:O	2.49	0.45
1:A:43:PRO:HB3	1:A:123:HIS:HB3	1.98	0.45
1:C:200:MET:HG2	1:C:210:TRP:HB3	1.97	0.45
1:A:5:ILE:HD13	1:B:5:ILE:HG12	1.97	0.45
1:F:67:LEU:O	1:F:162:LYS:HE2	2.16	0.45
1:I:69:VAL:HG21	1:I:158:VAL:HG21	1.97	0.45
1:F:99:PHE:HB2	1:F:100:PRO:HD2	1.98	0.45
1:A:77:ASP:OD2	1:J:77:ASP:OD2	2.33	0.45
1:H:74:LEU:HD13	1:H:75:SER:N	2.32	0.45
1:B:43:PRO:CB	1:B:123:HIS:HB3	2.44	0.45
1:F:239:LYS:CE	1:F:244:GLU:OE1	2.65	0.45
1:I:75:SER:HB3	1:I:82:HIS:CE1	2.52	0.45
1:A:67:LEU:CD1	1:A:158:VAL:HG23	2.46	0.45
1:A:117:HIS:O	1:A:120:SER:CB	2.63	0.45
1:C:86:LYS:HE3	1:C:101:ILE:HD12	1.97	0.45
1:C:160:ALA:HB1	1:C:171:VAL:HG11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:LYS:HD2	1:E:87:GLU:OE1	2.16	0.45
1:F:126:ARG:O	1:F:126:ARG:HG3	2.16	0.45
1:C:67:LEU:HD13	1:C:158:VAL:CG2	2.46	0.45
1:I:200:MET:HA	1:I:200:MET:CE	2.46	0.45
1:J:66:ARG:NH1	1:J:66:ARG:CG	2.65	0.45
1:F:124:THR:HG22	1:F:124:THR:O	2.17	0.45
1:D:220:ARG:O	1:D:224:GLU:HG3	2.16	0.45
1:A:11:ARG:NH1	1:A:14:GLU:OE2	2.50	0.45
1:C:40:PHE:HZ	1:C:99:PHE:CE1	2.35	0.45
1:H:111:ARG:HG3	1:H:116:LEU:HD12	1.99	0.45
1:C:144:PRO:HG3	1:D:161:LEU:HD11	1.99	0.45
1:A:5:ILE:HG13	1:A:6:PRO:O	2.17	0.45
1:H:244:GLU:HG2	2:H:296:HOH:O	2.16	0.45
1:D:43:PRO:HB3	1:D:123:HIS:HB3	1.99	0.45
1:C:43:PRO:CB	1:C:123:HIS:HB3	2.45	0.45
1:C:54:PHE:CE2	1:C:101:ILE:HD13	2.52	0.45
1:F:105:PRO:O	1:F:106:GLN:CB	2.38	0.45
1:D:122:THR:HA	1:E:106:GLN:CG	2.47	0.45
1:A:231:ARG:NH2	1:B:234:ALA:HB1	2.32	0.45
1:A:117:HIS:CD2	1:A:125:VAL:HG21	2.52	0.45
2:I:251:HOH:O	1:J:183:GLU:HG2	2.16	0.45
1:J:43:PRO:HG3	1:J:145:MET:HE2	1.99	0.44
1:B:59:ARG:HG2	1:B:59:ARG:NH1	2.28	0.44
1:G:36:TRP:HB2	1:G:69:VAL:HG22	1.98	0.44
1:E:207:SER:HB2	1:E:213:CYS:SG	2.57	0.44
1:E:171:VAL:HB	1:F:147:LEU:HD23	1.98	0.44
1:G:37:PHE:HA	1:G:70:ASP:O	2.17	0.44
1:D:106:GLN:CD	1:E:111:ARG:HH21	2.19	0.44
1:A:67:LEU:HD13	1:A:158:VAL:CG2	2.45	0.44
1:H:238:ALA:O	1:H:239:LYS:CB	2.62	0.44
1:C:188:PRO:O	1:C:199:ARG:NH2	2.50	0.44
1:C:60:ARG:HA	2:C:273:HOH:O	2.18	0.44
1:G:16:GLU:HG2	1:G:25:LYS:HD2	1.98	0.44
1:E:126:ARG:NH1	1:E:145:MET:HA	2.33	0.44
1:J:43:PRO:CB	1:J:123:HIS:HB3	2.48	0.44
1:D:167:LEU:N	1:D:167:LEU:HD12	2.32	0.44
1:A:183:GLU:HG2	2:A:286:HOH:O	2.17	0.44
1:A:190:PRO:HG2	1:A:196:ALA:HA	2.00	0.44
1:I:172:PRO:HG3	1:I:181:ILE:HD11	2.00	0.44
1:E:156:ARG:HD3	1:E:230:LEU:HD21	1.99	0.44
1:A:96:ARG:NH2	1:A:98:PRO:HB3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ILE:HG22	1:B:95:VAL:HG23	1.99	0.44
1:C:150:LEU:HD22	1:D:153:GLU:OE1	2.17	0.44
1:G:203:GLY:HA2	2:G:289:HOH:O	2.18	0.44
1:C:5:ILE:HD12	1:C:140:MET:HE1	2.00	0.44
1:A:40:PHE:HD1	1:A:42:HIS:HE2	1.65	0.44
1:G:175:TRP:CG	1:G:176:PRO:HA	2.53	0.44
1:H:111:ARG:HE	1:I:106:GLN:HE21	1.57	0.44
1:E:42:HIS:CD2	1:E:54:PHE:HE1	2.36	0.44
1:I:118:ALA:HB2	1:J:10:GLU:HG3	2.00	0.44
1:D:228:ARG:HH11	1:D:228:ARG:CB	2.31	0.44
1:E:163:LEU:HD11	1:E:222:ASP:HB3	2.00	0.44
1:C:124:THR:CG2	1:C:124:THR:O	2.66	0.44
1:F:116:LEU:HD13	1:G:106:GLN:NE2	2.33	0.43
1:D:224:GLU:O	1:D:228:ARG:HD3	2.17	0.43
1:E:206:ARG:HG3	1:E:206:ARG:NH1	2.31	0.43
1:F:159:LYS:HD3	1:F:225:GLU:OE2	2.17	0.43
1:E:59:ARG:HH11	1:E:59:ARG:CG	2.13	0.43
1:B:175:TRP:CG	1:B:176:PRO:HA	2.54	0.43
1:E:45:ASP:HA	1:E:85:TRP:CZ3	2.53	0.43
1:F:112:ARG:HG2	2:F:264:HOH:O	2.17	0.43
1:F:106:GLN:NE2	1:G:116:LEU:HD11	2.33	0.43
1:J:140:MET:HE2	1:J:142:TYR:OH	2.17	0.43
1:E:157:ILE:O	1:E:161:LEU:HB2	2.18	0.43
1:G:225:GLU:HG2	2:G:266:HOH:O	2.18	0.43
1:H:45:ASP:HA	1:H:85:TRP:CZ3	2.52	0.43
1:D:122:THR:HA	1:E:106:GLN:HG3	1.99	0.43
1:A:208:LEU:HD12	1:A:214:TRP:CZ3	2.52	0.43
1:A:117:HIS:HB2	1:A:125:VAL:CG1	2.49	0.43
1:I:74:LEU:HD13	1:I:75:SER:N	2.34	0.43
1:C:239:LYS:HE2	1:C:239:LYS:HB3	1.56	0.43
1:J:106:GLN:O	1:J:111:ARG:NH2	2.52	0.43
1:C:140:MET:CE	1:C:142:TYR:OH	2.67	0.43
1:A:208:LEU:HD12	1:A:214:TRP:HZ3	1.80	0.43
1:H:50:OCS:OD1	1:H:126:ARG:NH2	2.50	0.43
1:E:4:SER:CA	1:F:4:SER:HA	2.49	0.43
1:H:157:ILE:O	1:H:161:LEU:HB2	2.19	0.43
1:H:59:ARG:CG	1:H:59:ARG:NH1	2.66	0.43
1:A:206:ARG:NH1	2:A:309:HOH:O	2.51	0.43
1:I:124:THR:HG22	1:I:124:THR:O	2.18	0.43
1:D:120:SER:O	1:D:122:THR:N	2.52	0.43
1:C:208:LEU:HD13	1:D:242:TYR:HD1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:GLU:HG3	1:C:25:LYS:HE2	2.00	0.43
1:C:120:SER:OG	1:C:125:VAL:CG1	2.67	0.43
1:I:126:ARG:HD2	1:I:126:ARG:HH11	1.51	0.43
1:A:99:PHE:HB2	1:A:100:PRO:HD2	2.01	0.43
1:B:225:GLU:CG	1:B:228:ARG:HH12	2.32	0.42
1:J:129:PHE:CE2	1:J:140:MET:CE	3.01	0.42
1:A:117:HIS:C	1:A:120:SER:HB2	2.39	0.42
1:J:198:ALA:O	1:J:199:ARG:C	2.56	0.42
1:D:189:PRO:HA	1:D:190:PRO:HD3	1.96	0.42
1:D:106:GLN:HB2	1:D:106:GLN:HE21	1.50	0.42
1:J:11:ARG:HG3	1:J:135:GLY:O	2.19	0.42
1:J:129:PHE:HE2	1:J:140:MET:HE3	1.83	0.42
1:C:236:LYS:HD2	1:D:227:ARG:NH2	2.33	0.42
1:A:121:ALA:O	1:A:123:HIS:N	2.50	0.42
1:B:50:OCS:SG	1:B:126:ARG:NH2	2.93	0.42
1:C:214:TRP:NE1	2:C:302:HOH:O	2.07	0.42
1:D:117:HIS:CB	1:D:125:VAL:HG11	2.49	0.42
1:A:11:ARG:NH2	1:A:14:GLU:OE2	2.52	0.42
1:F:50:OCS:OD1	1:F:126:ARG:NH2	2.50	0.42
1:D:106:GLN:HG3	1:D:106:GLN:O	2.18	0.42
1:G:228:ARG:NH2	2:G:292:HOH:O	2.47	0.42
1:B:39:LEU:HA	1:B:72:ILE:O	2.20	0.42
1:C:59:ARG:HH11	1:D:179:GLU:HG2	1.85	0.42
1:G:54:PHE:CE2	1:G:101:ILE:CD1	3.02	0.42
1:F:220:ARG:NH1	1:F:220:ARG:HG3	2.34	0.42
1:J:168:LYS:HE3	1:J:168:LYS:HB3	1.83	0.42
1:B:79:VAL:O	1:B:83:ILE:HG13	2.19	0.42
1:E:107:GLY:O	1:E:111:ARG:HB2	2.20	0.42
1:A:41:SER:HB2	1:A:124:THR:HG21	2.00	0.42
1:G:172:PRO:HB3	1:G:186:ILE:HD11	2.00	0.42
1:A:143:TYR:CD2	1:A:147:LEU:HD13	2.54	0.42
1:I:188:PRO:O	1:I:199:ARG:NH2	2.53	0.42
1:D:40:PHE:HZ	1:D:99:PHE:CE1	2.38	0.42
1:F:122:THR:HA	1:G:106:GLN:OE1	2.19	0.42
1:G:63:ASP:CG	1:G:228:ARG:NH1	2.71	0.42
1:A:150:LEU:HD23	1:A:153:GLU:HB2	2.01	0.42
1:E:119:GLU:HB3	1:F:9:GLY:HA3	2.01	0.42
1:D:185:LEU:O	1:D:214:TRP:HB2	2.19	0.42
1:C:192:THR:OG1	1:C:195:GLN:HB2	2.20	0.42
1:F:153:GLU:HA	1:F:153:GLU:OE1	2.20	0.42
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:HG2	1:A:227:ARG:HG2	2.02	0.42
1:I:128:VAL:O	1:I:140:MET:HA	2.19	0.42
1:C:128:VAL:O	1:C:140:MET:HA	2.20	0.42
1:B:128:VAL:O	1:B:140:MET:HA	2.19	0.42
1:J:48:PRO:O	1:J:52:THR:HG23	2.19	0.42
1:C:136:VAL:O	1:C:138:ARG:HG2	2.20	0.42
1:E:69:VAL:HG21	1:E:158:VAL:HG11	2.02	0.42
1:B:220:ARG:HG3	2:B:288:HOH:O	2.19	0.42
1:E:168:LYS:O	1:E:168:LYS:CG	2.68	0.41
1:B:7:LEU:HD12	1:B:10:GLU:OE2	2.20	0.41
1:H:40:PHE:HZ	1:H:99:PHE:CE1	2.37	0.41
1:D:91:ARG:O	1:D:91:ARG:HG3	2.17	0.41
1:B:126:ARG:NH1	1:B:145:MET:HG3	2.34	0.41
1:F:11:ARG:NH2	1:F:14:GLU:OE2	2.44	0.41
1:C:139:THR:OG1	1:D:144:PRO:HD3	2.20	0.41
1:A:120:SER:O	1:A:121:ALA:O	2.39	0.41
1:H:120:SER:O	1:H:121:ALA:HB3	2.19	0.41
1:I:231:ARG:HH11	1:I:231:ARG:HG2	1.85	0.41
1:D:43:PRO:CB	1:D:123:HIS:HB3	2.50	0.41
1:J:144:PRO:HB2	1:J:146:GLU:OE1	2.20	0.41
1:G:8:ILE:H	1:H:117:HIS:CD2	2.27	0.41
1:A:208:LEU:HD13	1:A:214:TRP:CZ3	2.54	0.41
1:I:36:TRP:CD2	1:I:132:ASP:HA	2.55	0.41
1:H:120:SER:O	1:H:121:ALA:CB	2.68	0.41
1:J:207:SER:CB	1:J:213:CYS:SG	3.09	0.41
1:F:61:TYR:HB3	2:F:325:HOH:O	2.21	0.41
1:F:122:THR:HB	1:G:105:PRO:HG2	2.03	0.41
1:J:140:MET:HE1	1:J:142:TYR:OH	2.20	0.41
1:C:179:GLU:CB	1:D:59:ARG:HH12	2.33	0.41
1:H:54:PHE:CZ	1:H:101:ILE:HD13	2.55	0.41
1:F:116:LEU:HD23	1:F:116:LEU:HA	1.78	0.41
1:F:208:LEU:HD13	1:F:214:TRP:HZ3	1.86	0.41
1:A:126:ARG:NH1	1:A:145:MET:CA	2.84	0.41
1:E:24:ILE:HD11	1:E:72:ILE:CD1	2.51	0.41
1:C:173:ALA:HB2	1:D:53:GLU:HG2	2.02	0.41
1:J:129:PHE:CE2	1:J:140:MET:HE3	2.55	0.41
1:H:43:PRO:HB3	1:H:123:HIS:HB3	2.03	0.41
1:A:231:ARG:HA	1:A:231:ARG:HD3	1.89	0.41
1:I:139:THR:HG1	1:J:144:PRO:HD3	1.85	0.41
1:D:29:HIS:O	1:D:33:GLN:NE2	2.46	0.41
1:I:67:LEU:HD23	1:I:67:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:HG2	1:B:25:LYS:HD3	2.01	0.41
1:C:43:PRO:CG	1:C:145:MET:HG2	2.51	0.41
1:I:59:ARG:NH1	1:J:179:GLU:HB3	2.36	0.40
1:E:126:ARG:HG3	1:E:143:TYR:O	2.21	0.40
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.56	0.40
1:A:8:ILE:HD11	1:A:139:THR:HA	2.02	0.40
1:A:8:ILE:HG21	1:A:8:ILE:HD13	1.72	0.40
1:F:126:ARG:NH1	1:F:145:MET:HA	2.36	0.40
1:C:190:PRO:HB3	1:C:195:GLN:HB3	2.03	0.40
1:D:159:LYS:HE2	1:D:225:GLU:OE2	2.21	0.40
1:J:39:LEU:HD23	1:J:39:LEU:C	2.41	0.40
1:D:183:GLU:HG2	1:D:227:ARG:HH22	1.85	0.40
1:E:144:PRO:HD3	1:F:139:THR:HG1	1.86	0.40
1:A:8:ILE:O	1:B:118:ALA:HB3	2.21	0.40
1:G:129:PHE:CE2	1:G:140:MET:HE3	2.54	0.40
1:C:179:GLU:CG	1:D:59:ARG:HH12	2.34	0.40
1:J:143:TYR:CD2	1:J:147:LEU:HD13	2.56	0.40
1:G:61:TYR:O	1:G:65:GLN:HG2	2.21	0.40
1:J:115:LEU:HD11	1:J:129:PHE:HE1	1.85	0.40
1:E:125:VAL:HG11	1:F:8:ILE:HD12	2.01	0.40
1:D:167:LEU:H	1:D:167:LEU:HD12	1.86	0.40
1:E:84:LYS:HD2	1:E:84:LYS:HA	1.78	0.40
1:G:185:LEU:O	1:G:214:TRP:HB2	2.21	0.40
1:E:122:THR:CG2	1:E:123:HIS:CD2	3.04	0.40
1:D:86:LYS:HE3	1:D:101:ILE:HD12	2.03	0.40
1:E:150:LEU:HD22	1:F:153:GLU:OE1	2.20	0.40
1:G:41:SER:HB2	1:G:74:LEU:HD12	2.03	0.40
1:H:39:LEU:HD23	1:H:39:LEU:C	2.41	0.40
1:A:37:PHE:HA	1:A:70:ASP:O	2.21	0.40
1:F:42:HIS:HA	1:F:43:PRO:HD3	1.92	0.40
1:J:126:ARG:NH1	1:J:145:MET:O	2.53	0.40
1:G:53:GLU:OE1	1:G:126:ARG:NH2	2.53	0.40
1:E:241:LEU:HD23	1:E:241:LEU:HA	1.88	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	239/250 (96%)	221 (92%)	16 (7%)	2 (1%)	24	26
1	B	235/250 (94%)	223 (95%)	9 (4%)	3 (1%)	15	13
1	C	235/250 (94%)	224 (95%)	8 (3%)	3 (1%)	15	13
1	D	239/250 (96%)	226 (95%)	10 (4%)	3 (1%)	15	13
1	E	239/250 (96%)	220 (92%)	15 (6%)	4 (2%)	11	9
1	F	239/250 (96%)	228 (95%)	10 (4%)	1 (0%)	39	46
1	G	239/250 (96%)	227 (95%)	10 (4%)	2 (1%)	24	26
1	H	239/250 (96%)	226 (95%)	8 (3%)	5 (2%)	9	6
1	I	239/250 (96%)	226 (95%)	10 (4%)	3 (1%)	15	13
1	J	239/250 (96%)	223 (93%)	14 (6%)	2 (1%)	24	26
All	All	2382/2500 (95%)	2244 (94%)	110 (5%)	28 (1%)	16	15

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	B	118	ALA
1	C	121	ALA
1	E	239	LYS
1	G	239	LYS
1	H	120	SER
1	H	125	VAL
1	E	203	GLY
1	E	244	GLU
1	H	121	ALA
1	I	119	GLU
1	C	239	LYS
1	I	121	ALA
1	B	239	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	121	ALA
1	G	32	SER
1	A	239	LYS
1	B	124	THR
1	D	239	LYS
1	H	124	THR
1	H	243	GLU
1	J	106	GLN
1	I	125	VAL
1	D	184	GLY
1	E	125	VAL
1	C	125	VAL
1	J	125	VAL
1	F	125	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	208/215 (97%)	188 (90%)	20 (10%)	10	10
1	B	207/215 (96%)	189 (91%)	18 (9%)	13	13
1	C	207/215 (96%)	186 (90%)	21 (10%)	9	9
1	D	208/215 (97%)	188 (90%)	20 (10%)	10	10
1	E	208/215 (97%)	192 (92%)	16 (8%)	16	17
1	F	208/215 (97%)	190 (91%)	18 (9%)	13	13
1	G	208/215 (97%)	192 (92%)	16 (8%)	16	17
1	H	208/215 (97%)	187 (90%)	21 (10%)	9	9
1	I	208/215 (97%)	187 (90%)	21 (10%)	9	9
1	J	208/215 (97%)	188 (90%)	20 (10%)	10	10
All	All	2078/2150 (97%)	1887 (91%)	191 (9%)	11	11

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	74	LEU
1	A	77	ASP
1	A	106	GLN
1	A	120	SER
1	A	124	THR
1	A	125	VAL
1	A	147	LEU
1	A	161	LEU
1	A	162	LYS
1	A	167	LEU
1	A	193	GLU
1	A	199	ARG
1	A	204	GLN
1	A	206	ARG
1	A	212	PHE
1	A	220	ARG
1	A	231	ARG
1	A	239	LYS
1	A	242	TYR
1	B	5	ILE
1	B	28	ASP
1	B	59	ARG
1	B	62	GLU
1	B	66	ARG
1	B	74	LEU
1	B	119	GLU
1	B	120	SER
1	B	125	VAL
1	B	147	LEU
1	B	161	LEU
1	B	167	LEU
1	B	168	LYS
1	B	206	ARG
1	B	208	LEU
1	B	212	PHE
1	B	225	GLU
1	B	239	LYS
1	C	28	ASP
1	C	59	ARG
1	C	74	LEU
1	C	82	HIS
1	C	91	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	119	GLU
1	C	122	THR
1	C	124	THR
1	C	126	ARG
1	C	147	LEU
1	C	161	LEU
1	C	167	LEU
1	C	168	LYS
1	C	197	ARG
1	C	199	ARG
1	C	208	LEU
1	C	220	ARG
1	C	235	GLU
1	C	239	LYS
1	C	243	GLU
1	C	244	GLU
1	D	8	ILE
1	D	11	ARG
1	D	24	ILE
1	D	28	ASP
1	D	59	ARG
1	D	62	GLU
1	D	74	LEU
1	D	91	ARG
1	D	106	GLN
1	D	120	SER
1	D	122	THR
1	D	147	LEU
1	D	168	LYS
1	D	193	GLU
1	D	199	ARG
1	D	206	ARG
1	D	208	LEU
1	D	212	PHE
1	D	228	ARG
1	D	244	GLU
1	E	11	ARG
1	E	28	ASP
1	E	59	ARG
1	E	62	GLU
1	E	79	VAL
1	E	91	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	122	THR
1	E	145	MET
1	E	147	LEU
1	E	167	LEU
1	E	168	LYS
1	E	193	GLU
1	E	199	ARG
1	E	212	PHE
1	E	225	GLU
1	E	228	ARG
1	F	28	ASP
1	F	59	ARG
1	F	74	LEU
1	F	77	ASP
1	F	119	GLU
1	F	124	THR
1	F	125	VAL
1	F	126	ARG
1	F	145	MET
1	F	147	LEU
1	F	161	LEU
1	F	193	GLU
1	F	199	ARG
1	F	206	ARG
1	F	208	LEU
1	F	212	PHE
1	F	228	ARG
1	F	242	TYR
1	G	8	ILE
1	G	28	ASP
1	G	59	ARG
1	G	62	GLU
1	G	77	ASP
1	G	122	THR
1	G	125	VAL
1	G	147	LEU
1	G	167	LEU
1	G	183	GLU
1	G	193	GLU
1	G	199	ARG
1	G	206	ARG
1	G	212	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	225	GLU
1	G	244	GLU
1	H	28	ASP
1	H	59	ARG
1	H	62	GLU
1	H	74	LEU
1	H	77	ASP
1	H	96	ARG
1	H	106	GLN
1	H	119	GLU
1	H	122	THR
1	H	124	THR
1	H	145	MET
1	H	147	LEU
1	H	158	VAL
1	H	161	LEU
1	H	167	LEU
1	H	199	ARG
1	H	206	ARG
1	H	208	LEU
1	H	212	PHE
1	H	228	ARG
1	H	239	LYS
1	I	28	ASP
1	I	59	ARG
1	I	62	GLU
1	I	74	LEU
1	I	77	ASP
1	I	106	GLN
1	I	120	SER
1	I	122	THR
1	I	124	THR
1	I	147	LEU
1	I	158	VAL
1	I	161	LEU
1	I	167	LEU
1	I	168	LYS
1	I	199	ARG
1	I	206	ARG
1	I	212	PHE
1	I	228	ARG
1	I	231	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	242	TYR
1	I	244	GLU
1	J	11	ARG
1	J	28	ASP
1	J	59	ARG
1	J	66	ARG
1	J	74	LEU
1	J	77	ASP
1	J	91	ARG
1	J	122	THR
1	J	124	THR
1	J	125	VAL
1	J	147	LEU
1	J	161	LEU
1	J	167	LEU
1	J	183	GLU
1	J	193	GLU
1	J	199	ARG
1	J	206	ARG
1	J	212	PHE
1	J	239	LYS
1	J	242	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	195	GLN
1	B	123	HIS
1	D	117	HIS
1	D	123	HIS
1	F	117	HIS
1	F	195	GLN
1	G	92	HIS
1	G	117	HIS
1	G	123	HIS
1	H	106	GLN
1	H	117	HIS
1	I	92	HIS
1	I	106	GLN
1	I	117	HIS
1	I	123	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	117	HIS
1	J	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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
1	OCS	A	50	1	7,8,9	2.92	3 (42%)	7,11,13	1.55	1 (14%)
1	OCS	B	50	1	7,8,9	2.27	3 (42%)	7,11,13	3.80	3 (42%)
1	OCS	C	50	1	7,8,9	2.50	2 (28%)	7,11,13	3.83	4 (57%)
1	OCS	D	50	1	7,8,9	2.91	3 (42%)	7,11,13	2.30	2 (28%)
1	OCS	E	50	1	7,8,9	2.82	2 (28%)	7,11,13	2.60	4 (57%)
1	OCS	F	50	1	7,8,9	2.34	3 (42%)	7,11,13	1.46	1 (14%)
1	OCS	G	50	1	7,8,9	2.46	2 (28%)	7,11,13	1.97	2 (28%)
1	OCS	H	50	1	7,8,9	2.65	2 (28%)	7,11,13	2.48	3 (42%)
1	OCS	I	50	1	7,8,9	3.14	2 (28%)	7,11,13	2.09	4 (57%)
1	OCS	J	50	1	7,8,9	2.77	2 (28%)	7,11,13	2.62	3 (42%)

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
1	OCS	A	50	1	-	0/4/7/9	0/0/0/0
1	OCS	B	50	1	-	0/4/7/9	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	C	50	1	-	0/4/7/9	0/0/0/0
1	OCS	D	50	1	-	0/4/7/9	0/0/0/0
1	OCS	E	50	1	-	0/4/7/9	0/0/0/0
1	OCS	F	50	1	-	0/4/7/9	0/0/0/0
1	OCS	G	50	1	-	0/4/7/9	0/0/0/0
1	OCS	H	50	1	-	0/4/7/9	0/0/0/0
1	OCS	I	50	1	-	0/4/7/9	0/0/0/0
1	OCS	J	50	1	-	0/4/7/9	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	50	OCS	CB-SG	-6.86	1.67	1.77
1	H	50	OCS	CB-SG	-6.15	1.68	1.77
1	A	50	OCS	CB-SG	-5.98	1.69	1.77
1	D	50	OCS	CB-SG	-5.94	1.69	1.77
1	E	50	OCS	CB-SG	-5.82	1.69	1.77
1	J	50	OCS	CB-SG	-5.49	1.69	1.77
1	G	50	OCS	CB-SG	-4.57	1.71	1.77
1	C	50	OCS	CB-SG	-4.43	1.71	1.77
1	F	50	OCS	CB-SG	-3.70	1.72	1.77
1	B	50	OCS	CB-SG	-3.46	1.72	1.77
1	D	50	OCS	OD3-SG	2.06	1.51	1.45
1	A	50	OCS	OD3-SG	2.16	1.52	1.45
1	F	50	OCS	OD2-SG	2.27	1.52	1.46
1	B	50	OCS	OD2-SG	2.35	1.52	1.46
1	H	50	OCS	O-C	2.69	1.32	1.19
1	B	50	OCS	O-C	3.62	1.36	1.19
1	E	50	OCS	O-C	3.93	1.38	1.19
1	G	50	OCS	O-C	3.94	1.38	1.19
1	F	50	OCS	O-C	3.94	1.38	1.19
1	C	50	OCS	O-C	3.95	1.38	1.19
1	I	50	OCS	O-C	4.08	1.38	1.19
1	A	50	OCS	O-C	4.08	1.38	1.19
1	D	50	OCS	O-C	4.12	1.38	1.19
1	J	50	OCS	O-C	4.56	1.40	1.19

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	OCS	O-C-CA	-4.82	112.94	125.49
1	J	50	OCS	OD1-SG-CB	-4.81	102.89	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	OCS	O-C-CA	-4.48	113.83	125.49
1	E	50	OCS	O-C-CA	-4.31	114.25	125.49
1	C	50	OCS	O-C-CA	-4.31	114.28	125.49
1	J	50	OCS	O-C-CA	-3.86	115.44	125.49
1	G	50	OCS	OD1-SG-CB	-3.78	103.76	106.94
1	H	50	OCS	O-C-CA	-3.72	115.81	125.49
1	A	50	OCS	O-C-CA	-3.38	116.70	125.49
1	F	50	OCS	O-C-CA	-3.25	117.03	125.49
1	C	50	OCS	OD1-SG-CB	-3.20	104.24	106.94
1	I	50	OCS	OD3-SG-CB	-3.13	104.30	106.94
1	H	50	OCS	OD3-SG-CB	-3.03	104.38	106.94
1	G	50	OCS	O-C-CA	-2.99	117.69	125.49
1	I	50	OCS	O-C-CA	-2.70	118.44	125.49
1	B	50	OCS	OD3-SG-OD1	-2.33	104.99	113.48
1	C	50	OCS	OD2-SG-OD3	-2.24	106.39	111.61
1	E	50	OCS	OD2-SG-OD3	-2.14	106.62	111.61
1	D	50	OCS	OD3-SG-CB	-2.14	105.14	106.94
1	I	50	OCS	OD3-SG-OD1	-2.03	106.08	113.48
1	J	50	OCS	OD2-SG-OD1	2.03	116.34	111.61
1	E	50	OCS	OD2-SG-OD1	2.05	116.38	111.61
1	I	50	OCS	OD2-SG-OD1	2.32	117.00	111.61
1	E	50	OCS	OD3-SG-CB	3.69	110.05	106.94
1	H	50	OCS	OD1-SG-CB	3.88	110.21	106.94
1	C	50	OCS	OD3-SG-CB	8.22	113.87	106.94
1	B	50	OCS	OD1-SG-CB	8.33	113.97	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	50	OCS	1	0
1	B	50	OCS	2	0
1	C	50	OCS	2	0
1	D	50	OCS	1	0
1	E	50	OCS	2	0
1	F	50	OCS	1	0
1	G	50	OCS	1	0
1	H	50	OCS	1	0
1	J	50	OCS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	241/250 (96%)	-0.25	8 (3%)	50	63	19, 30, 60, 79	0
1	B	239/250 (95%)	-0.29	3 (1%)	79	87	21, 31, 59, 79	0
1	C	239/250 (95%)	-0.33	5 (2%)	67	79	22, 33, 61, 74	0
1	D	241/250 (96%)	-0.18	4 (1%)	73	83	25, 38, 63, 79	0
1	E	241/250 (96%)	-0.13	5 (2%)	67	79	19, 33, 62, 78	0
1	F	241/250 (96%)	-0.25	7 (2%)	55	67	20, 29, 57, 72	0
1	G	241/250 (96%)	-0.31	2 (0%)	87	93	18, 28, 54, 73	0
1	H	241/250 (96%)	-0.27	5 (2%)	67	79	19, 28, 59, 78	0
1	I	241/250 (96%)	-0.20	11 (4%)	36	51	20, 31, 63, 83	0
1	J	241/250 (96%)	-0.16	6 (2%)	61	73	22, 32, 59, 76	0
All	All	2406/2500 (96%)	-0.24	56 (2%)	64	76	18, 32, 61, 83	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	118	ALA	7.0
1	I	118	ALA	5.4
1	E	4	SER	5.2
1	H	245	ALA	4.2
1	I	4	SER	4.1
1	A	245	ALA	3.9
1	A	118	ALA	3.7
1	D	238	ALA	3.7
1	I	244	GLU	3.7
1	D	118	ALA	3.6
1	J	122	THR	3.5
1	F	4	SER	3.5
1	B	117	HIS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	118	ALA	3.4
1	J	4	SER	3.4
1	E	118	ALA	3.3
1	H	244	GLU	3.2
1	A	5	ILE	3.2
1	C	238	ALA	3.2
1	E	117	HIS	3.1
1	I	5	ILE	3.1
1	C	239	LYS	3.0
1	F	201	GLU	3.0
1	I	117	HIS	3.0
1	G	245	ALA	3.0
1	D	4	SER	2.9
1	I	121	ALA	2.8
1	C	4	SER	2.8
1	I	201	GLU	2.8
1	I	245	ALA	2.8
1	C	242	TYR	2.8
1	H	118	ALA	2.8
1	I	242	TYR	2.7
1	D	220	ARG	2.6
1	A	117	HIS	2.6
1	F	202	SER	2.5
1	H	242	TYR	2.4
1	H	4	SER	2.4
1	J	242	TYR	2.3
1	A	121	ALA	2.3
1	C	5	ILE	2.2
1	B	4	SER	2.2
1	F	200	MET	2.2
1	I	220	ARG	2.2
1	J	134	ARG	2.2
1	F	245	ALA	2.1
1	E	5	ILE	2.1
1	F	5	ILE	2.1
1	A	203	GLY	2.1
1	A	4	SER	2.1
1	J	120	SER	2.1
1	A	122	THR	2.1
1	E	32	SER	2.0
1	I	243	GLU	2.0
1	J	243	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	242	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OCS	J	50	9/10	0.98	0.12	-	27,29,35,35	0
1	OCS	I	50	9/10	0.98	0.10	-	25,26,33,34	0
1	OCS	F	50	9/10	0.97	0.13	-	25,27,33,34	0
1	OCS	E	50	9/10	0.98	0.11	-	27,28,38,38	0
1	OCS	H	50	9/10	0.98	0.10	-	20,21,31,31	0
1	OCS	G	50	9/10	0.98	0.10	-	23,25,29,31	0
1	OCS	B	50	9/10	0.98	0.10	-	23,24,33,33	0
1	OCS	A	50	9/10	0.98	0.10	-	26,28,35,35	0
1	OCS	D	50	9/10	0.98	0.08	-	28,30,36,41	0
1	OCS	C	50	9/10	0.98	0.09	-	26,27,33,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.