



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:02 AM UTC

PDB ID : 2E2G / pdb_00002e2g
Title : Crystal structure of archaeal peroxiredoxin, thioredoxin peroxidase from *Aeropyrum pernix* K1 (pre-oxidation form)
Authors : Nakamura, T.; Yamamoto, T.; Abe, M.; Matsumura, H.; Hagihara, Y.; Goto, T.; Yamaguchi, T.; Inoue, T.
Deposited on : 2006-11-13
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

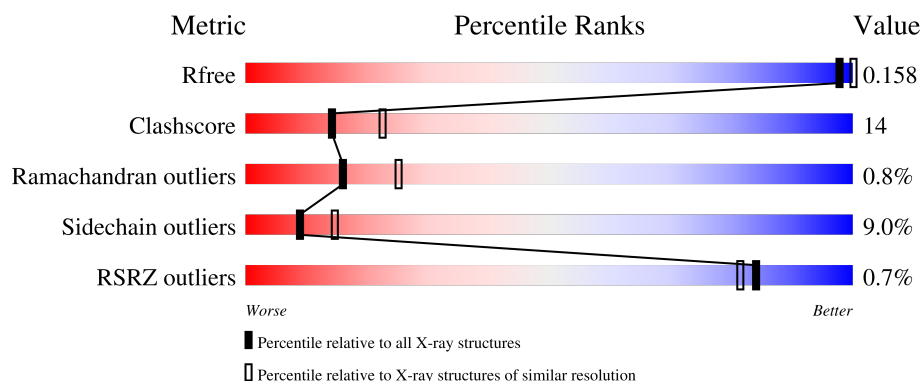
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	% 70% 20% 5% 5%
1	B	250	% 62% 26% 6% . .
1	C	250	62% 29% . . .
1	D	250	67% 22% 5% . 5%
1	E	250	% 64% 24% 7% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	250	66%22%6%5%
1	G	250	% 65%25%5%5%
1	H	250	% 63%25%6%5%
1	I	250	64%26%5%5%
1	J	250	% 65%26%5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19878 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	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	B	239	Total	C	N	O	S	0	0	0
			1942	1250	342	344	6			
1	C	239	Total	C	N	O	S	0	0	0
			1938	1247	340	345	6			
1	D	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	E	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	F	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	G	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	H	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	I	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			
1	J	238	Total	C	N	O	S	0	0	0
			1932	1244	339	343	6			

There are 10 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

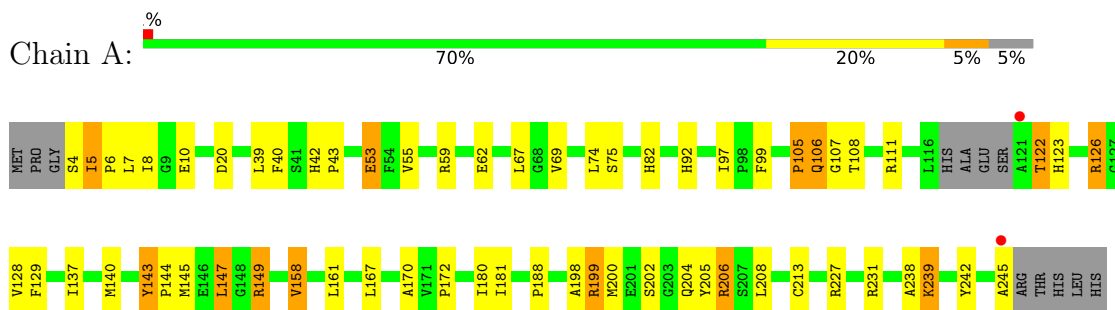
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	60	Total O 60 60	0	0
2	C	39	Total O 39 39	0	0
2	D	57	Total O 57 57	0	0
2	E	65	Total O 65 65	0	0
2	F	59	Total O 59 59	0	0
2	G	61	Total O 61 61	0	0
2	H	65	Total O 65 65	0	0
2	I	30	Total O 30 30	0	0
2	J	49	Total O 49 49	0	0

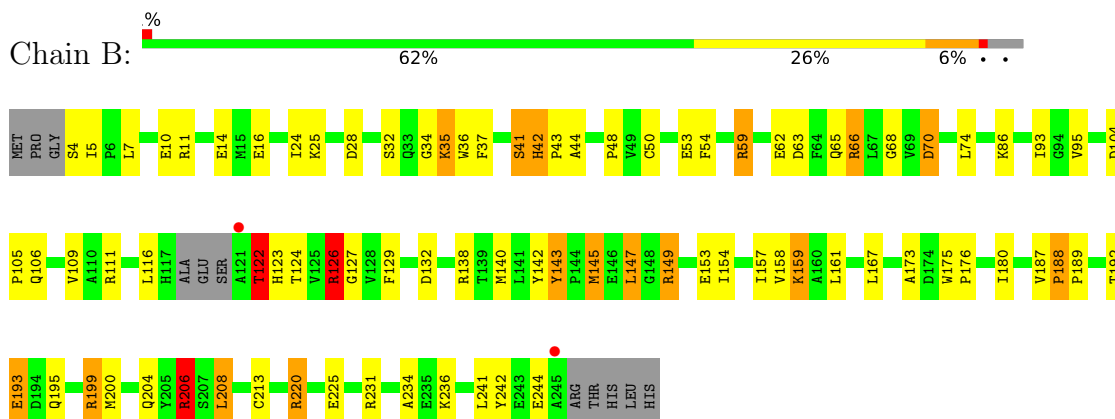
3 Residue-property plots

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

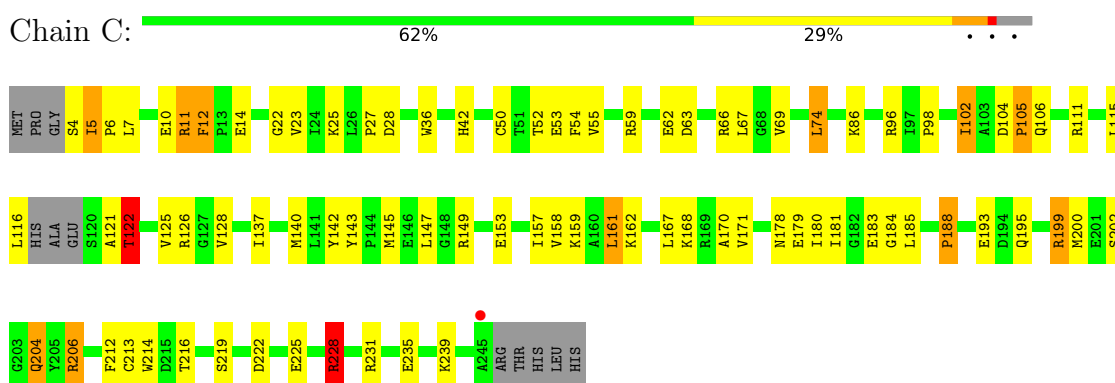
• Molecule 1: Probable peroxiredoxin



• Molecule 1: Probable peroxiredoxin

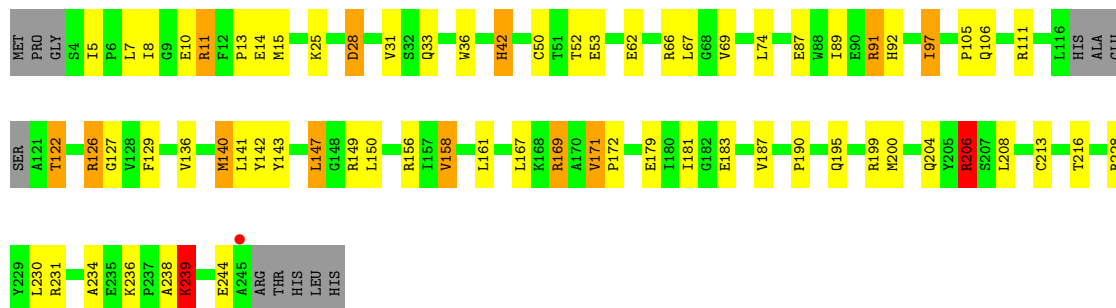


• Molecule 1: Probable peroxiredoxin



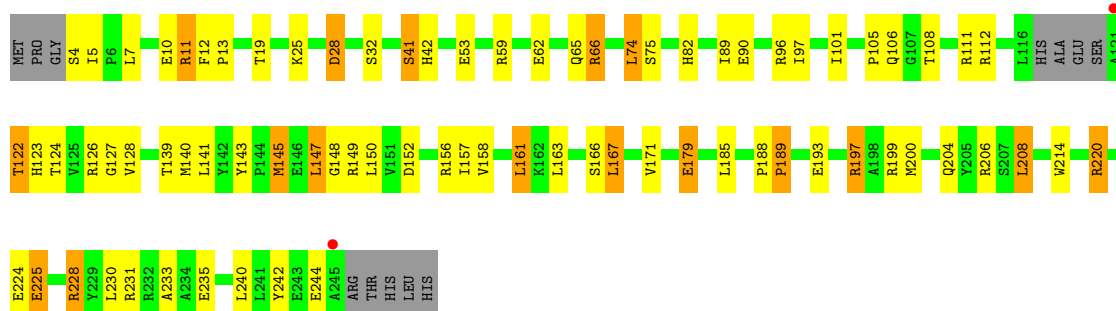
- Molecule 1: Probable peroxiredoxin

Chain D:  67% 22% 5% • 5%



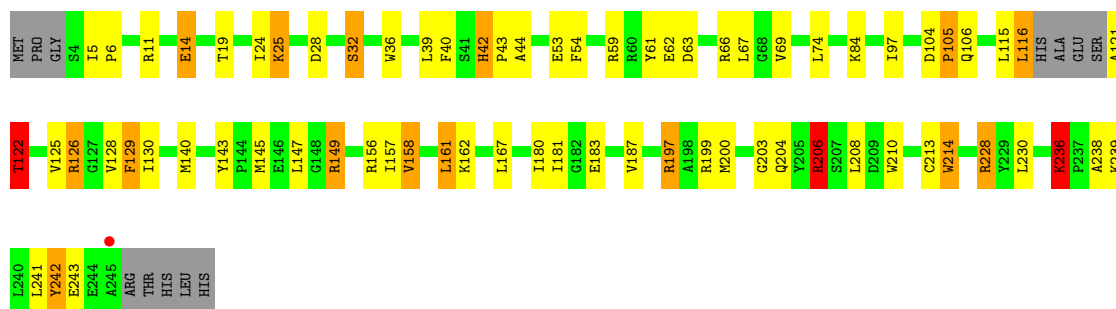
- Molecule 1: Probable peroxiredoxin

Chain E:  64% 24% 7% 5%



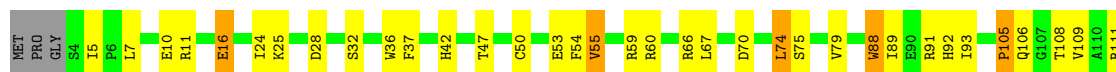
- Molecule 1: Probable peroxiredoxin

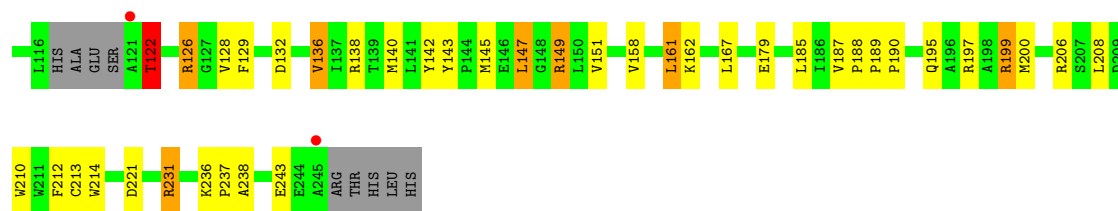
Chain F:  66% 22% 6% • 5%



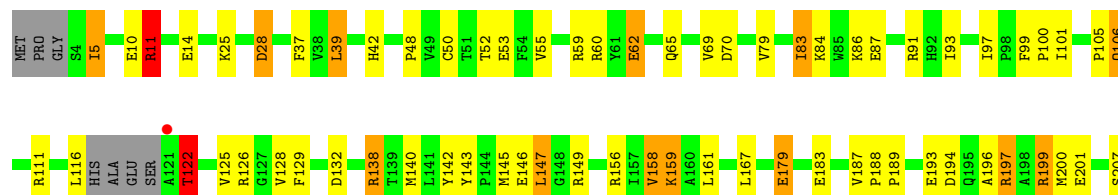
- Molecule 1: Probable peroxiredoxin

Chain G:  65% 25% 5% 5%

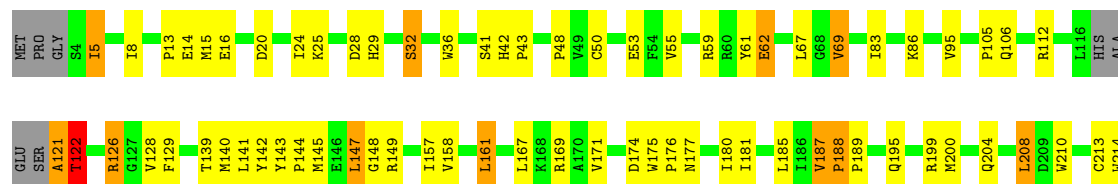




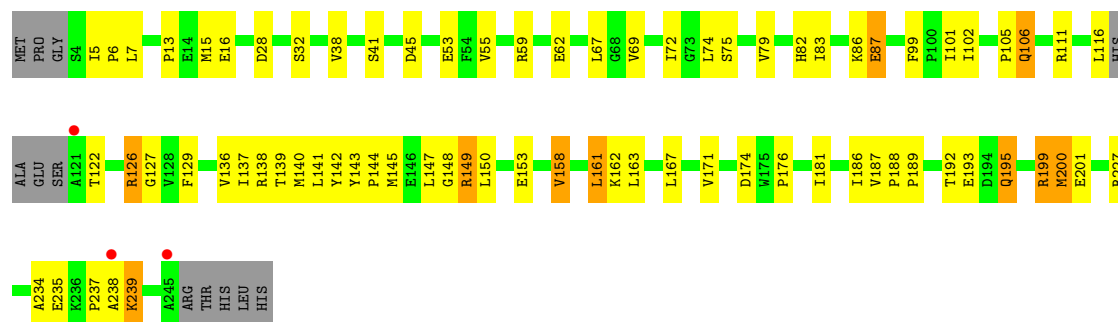
● Molecule 1: Probable peroxiredoxin



● 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	76.20Å 103.35Å 104.63Å 105.79° 105.19° 92.68°	Depositor
Resolution (Å)	19.99 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.99-2.40) 87.2 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.229 0.160 , 0.158	Depositor DCC
R_{free} test set	5083 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19878	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.32	1/1984 (0.1%)	1.35	10/2696 (0.4%)
1	B	1.36	7/1995 (0.4%)	1.36	19/2711 (0.7%)
1	C	1.37	5/1990 (0.3%)	1.38	14/2704 (0.5%)
1	D	1.33	5/1984 (0.3%)	1.37	18/2696 (0.7%)
1	E	1.41	11/1984 (0.6%)	1.36	11/2696 (0.4%)
1	F	1.46	7/1984 (0.4%)	1.42	17/2696 (0.6%)
1	G	1.38	5/1984 (0.3%)	1.35	12/2696 (0.4%)
1	H	1.41	12/1984 (0.6%)	1.33	7/2696 (0.3%)
1	I	1.33	6/1984 (0.3%)	1.34	14/2696 (0.5%)
1	J	1.32	4/1984 (0.2%)	1.31	10/2696 (0.4%)
All	All	1.37	63/19857 (0.3%)	1.36	132/26983 (0.5%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	189	PRO	CA-C	10.86	1.57	1.51
1	B	189	PRO	CA-C	10.43	1.57	1.51
1	E	171	VAL	CA-CB	7.79	1.61	1.54
1	C	102	ILE	CA-CB	-7.58	1.45	1.54
1	I	189	PRO	CA-C	7.53	1.56	1.51
1	F	130	ILE	CA-CB	7.18	1.62	1.54
1	B	124	THR	CA-CB	7.14	1.66	1.53
1	B	149	ARG	CZ-NH1	7.04	1.42	1.32
1	D	122	THR	N-CA	6.95	1.55	1.46
1	G	189	PRO	CA-C	6.90	1.56	1.52
1	C	52	THR	CA-CB	6.69	1.64	1.53
1	F	25	LYS	CA-C	6.63	1.60	1.52
1	J	181	ILE	CA-CB	6.54	1.63	1.54
1	G	136	VAL	CA-CB	6.52	1.62	1.54
1	D	122	THR	CA-CB	6.39	1.64	1.53
1	C	122	THR	CA-CB	6.30	1.64	1.53
1	E	228	ARG	NE-CZ	6.29	1.40	1.33
1	B	122	THR	CA-CB	6.21	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	228	ARG	NE-CZ	6.15	1.39	1.33
1	F	183	GLU	CD-OE2	6.03	1.36	1.25
1	D	97	ILE	CA-CB	6.02	1.61	1.54
1	E	228	ARG	CG-CD	6.01	1.70	1.52
1	G	109	VAL	CA-CB	6.00	1.61	1.54
1	H	122	THR	CA-CB	5.94	1.63	1.53
1	H	228	ARG	CG-CD	5.81	1.69	1.52
1	C	25	LYS	CA-C	5.79	1.59	1.52
1	I	5	ILE	CA-CB	5.68	1.61	1.53
1	H	138	ARG	C-O	-5.59	1.16	1.24
1	I	235	GLU	N-CA	5.56	1.52	1.46
1	E	228	ARG	CA-C	5.54	1.60	1.52
1	D	136	VAL	CA-CB	5.53	1.60	1.54
1	G	122	THR	CA-CB	5.52	1.62	1.53
1	I	5	ILE	CA-C	5.51	1.57	1.52
1	C	171	VAL	CA-CB	5.49	1.58	1.54
1	E	97	ILE	C-O	-5.48	1.18	1.24
1	H	39	LEU	CA-C	5.46	1.59	1.52
1	J	171	VAL	CA-CB	-5.45	1.50	1.54
1	I	69	VAL	CA-CB	5.38	1.60	1.54
1	B	42	HIS	CA-C	-5.37	1.47	1.52
1	D	140	MET	CA-C	-5.35	1.46	1.52
1	H	122	THR	N-CA	5.31	1.53	1.46
1	G	105	PRO	C-O	5.30	1.29	1.23
1	B	34	GLY	C-O	-5.29	1.18	1.24
1	E	225	GLU	N-CA	5.28	1.52	1.46
1	F	54	PHE	CA-C	-5.28	1.46	1.52
1	E	122	THR	CA-CB	5.25	1.62	1.53
1	H	146	GLU	CA-C	5.25	1.61	1.52
1	F	24	ILE	CA-CB	5.22	1.60	1.55
1	J	102	ILE	CA-CB	5.22	1.60	1.54
1	H	5	ILE	CA-CB	5.22	1.61	1.53
1	E	228	ARG	N-CA	5.21	1.52	1.46
1	E	65	GLN	C-O	-5.20	1.17	1.24
1	E	188	PRO	CA-C	5.20	1.56	1.52
1	H	97	ILE	CA-C	5.17	1.57	1.53
1	H	10	GLU	N-CA	5.17	1.52	1.45
1	E	231	ARG	C-O	5.13	1.29	1.24
1	J	163	LEU	C-O	-5.12	1.18	1.24
1	H	225	GLU	CG-CD	5.11	1.64	1.52
1	I	95	VAL	CA-CB	5.08	1.60	1.54
1	B	109	VAL	C-O	-5.04	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	129	PHE	CA-C	-5.03	1.46	1.52
1	H	197	ARG	CG-CD	5.01	1.67	1.52
1	A	205	TYR	CA-C	-5.01	1.46	1.52

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	42	HIS	CA-C-N	9.41	129.63	119.28
1	F	42	HIS	C-N-CA	9.41	129.63	119.28
1	C	204	GLN	N-CA-C	7.89	122.94	113.16
1	B	126	ARG	CA-C-N	-7.53	106.65	121.41
1	B	126	ARG	C-N-CA	-7.53	106.65	121.41
1	E	89	ILE	N-CA-C	7.26	118.02	110.62
1	I	238	ALA	N-CA-C	-7.14	99.96	110.52
1	B	188	PRO	CA-C-N	-7.12	114.46	119.66
1	B	188	PRO	C-N-CA	-7.12	114.46	119.66
1	J	234	ALA	N-CA-C	7.11	119.11	111.36
1	D	171	VAL	CA-C-N	7.00	126.99	119.78
1	D	171	VAL	C-N-CA	7.00	126.99	119.78
1	C	5	ILE	CA-C-N	-6.88	113.22	120.03
1	C	5	ILE	C-N-CA	-6.88	113.22	120.03
1	F	104	ASP	CA-C-N	-6.87	113.58	120.31
1	F	104	ASP	C-N-CA	-6.87	113.58	120.31
1	F	105	PRO	N-CA-C	-6.71	101.37	111.57
1	D	97	ILE	CA-C-N	-6.62	112.89	120.04
1	D	97	ILE	C-N-CA	-6.62	112.89	120.04
1	J	122	THR	N-CA-CB	6.54	121.54	110.49
1	G	122	THR	N-CA-CB	6.47	121.43	110.49
1	F	236	LYS	CA-C-N	-6.42	113.34	119.76
1	F	236	LYS	C-N-CA	-6.42	113.34	119.76
1	J	87	GLU	N-CA-C	-6.42	104.36	111.36
1	E	122	THR	N-CA-CB	6.40	121.31	110.49
1	E	244	GLU	N-CA-C	6.33	120.72	113.19
1	G	238	ALA	N-CA-C	-6.31	99.73	109.76
1	H	122	THR	N-CA-CB	6.29	121.12	110.49
1	B	208	LEU	N-CA-C	-6.23	105.62	113.72
1	C	188	PRO	CA-C-N	-6.21	113.99	120.38
1	C	188	PRO	C-N-CA	-6.21	113.99	120.38
1	B	143	TYR	CA-C-N	-6.17	114.38	120.98
1	B	143	TYR	C-N-CA	-6.17	114.38	120.98
1	G	47	THR	CA-C-N	6.16	125.56	118.85
1	G	47	THR	C-N-CA	6.16	125.56	118.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	ALA	N-CA-C	6.10	118.90	111.82
1	D	206	ARG	N-CA-C	-6.07	102.09	110.35
1	I	189	PRO	N-CA-C	6.06	116.29	110.47
1	F	214	TRP	N-CA-C	6.04	117.95	108.96
1	H	60	ARG	N-CA-C	-6.03	104.03	113.02
1	F	122	THR	N-CA-CB	5.97	120.58	110.49
1	C	105	PRO	N-CA-C	-5.97	101.81	111.19
1	B	234	ALA	N-CA-C	5.97	117.86	111.36
1	H	87	GLU	CB-CA-C	-5.93	100.77	110.85
1	C	170	ALA	N-CA-C	-5.93	101.75	110.52
1	B	44	ALA	N-CA-C	5.90	117.51	108.42
1	F	206	ARG	N-CA-C	-5.89	102.19	110.50
1	F	149	ARG	CB-CG-CD	5.87	124.79	111.30
1	F	187	VAL	N-CA-C	-5.84	103.61	108.63
1	I	121	ALA	CA-C-N	5.82	132.65	121.54
1	I	121	ALA	C-N-CA	5.82	132.65	121.54
1	E	32	SER	CB-CA-C	-5.80	99.21	110.46
1	H	196	ALA	N-CA-C	5.77	117.57	111.28
1	A	149	ARG	CB-CG-CD	5.75	124.54	111.30
1	B	104	ASP	CA-C-N	-5.75	114.05	120.14
1	B	104	ASP	C-N-CA	-5.75	114.05	120.14
1	E	228	ARG	CD-NE-CZ	5.75	132.45	124.40
1	A	97	ILE	CA-C-N	-5.75	113.94	120.89
1	A	97	ILE	C-N-CA	-5.75	113.94	120.89
1	B	41	SER	N-CA-C	5.75	119.05	110.14
1	A	143	TYR	N-CA-C	-5.75	102.81	109.93
1	B	122	THR	N-CA-CB	5.74	120.19	110.49
1	C	12	PHE	CA-C-N	5.72	126.99	119.84
1	C	12	PHE	C-N-CA	5.72	126.99	119.84
1	E	208	LEU	N-CA-C	-5.72	106.94	114.04
1	A	53	GLU	N-CA-C	5.71	117.58	111.36
1	C	228	ARG	N-CA-CB	5.69	118.48	110.12
1	D	187	VAL	CB-CA-C	-5.68	105.66	110.94
1	E	206	ARG	N-CA-C	-5.68	102.08	110.48
1	I	32	SER	CA-C-N	-5.66	113.20	122.54
1	I	32	SER	C-N-CA	-5.66	113.20	122.54
1	I	236	LYS	CB-CA-C	5.66	119.01	109.67
1	D	87	GLU	CB-CA-C	-5.61	101.32	110.85
1	C	122	THR	N-CA-CB	5.61	119.97	110.49
1	I	83	ILE	N-CA-C	5.59	116.33	110.62
1	G	126	ARG	CA-C-N	-5.54	110.55	121.41
1	G	126	ARG	C-N-CA	-5.54	110.55	121.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	LYS	N-CA-C	5.54	117.75	111.11
1	F	97	ILE	CA-C-N	-5.53	114.20	120.89
1	F	97	ILE	C-N-CA	-5.53	114.20	120.89
1	D	213	CYS	N-CA-C	-5.53	100.76	109.50
1	B	193	GLU	N-CA-C	5.51	118.22	111.82
1	J	126	ARG	CA-C-N	-5.49	110.66	121.41
1	J	126	ARG	C-N-CA	-5.49	110.66	121.41
1	I	122	THR	N-CA-CB	5.46	119.72	110.49
1	F	54	PHE	N-CA-C	-5.45	105.33	111.28
1	J	189	PRO	N-CA-C	5.44	117.33	110.70
1	D	87	GLU	CB-CG-CD	-5.43	103.37	112.60
1	G	149	ARG	CB-CG-CD	5.36	123.63	111.30
1	H	11	ARG	N-CA-C	-5.35	102.36	110.28
1	I	187	VAL	CA-C-N	-5.33	114.89	120.38
1	I	187	VAL	C-N-CA	-5.33	114.89	120.38
1	D	122	THR	N-CA-C	5.32	122.12	110.80
1	A	105	PRO	N-CA-C	-5.32	103.49	111.57
1	F	97	ILE	N-CA-C	-5.30	102.30	107.55
1	A	108	THR	CB-CA-C	-5.29	102.34	110.81
1	H	187	VAL	CB-CA-C	-5.28	106.03	110.94
1	F	162	LYS	N-CA-C	-5.26	105.22	111.69
1	G	197	ARG	CA-C-N	5.23	128.07	120.79
1	G	197	ARG	C-N-CA	5.23	128.07	120.79
1	B	206	ARG	N-CA-C	-5.20	103.17	110.50
1	A	204	GLN	CA-C-N	-5.18	114.68	122.81
1	A	204	GLN	C-N-CA	-5.18	114.68	122.81
1	C	22	GLY	CA-C-N	5.17	129.04	122.37
1	C	22	GLY	C-N-CA	5.17	129.04	122.37
1	I	204	GLN	N-CA-C	5.16	119.45	113.20
1	B	126	ARG	O-C-N	-5.16	115.92	122.78
1	D	236	LYS	CA-C-N	-5.15	114.61	119.76
1	D	236	LYS	C-N-CA	-5.15	114.61	119.76
1	J	99	PHE	CA-C-N	-5.15	115.42	120.52
1	J	99	PHE	C-N-CA	-5.15	115.42	120.52
1	H	214	TRP	N-CA-C	5.14	116.66	108.79
1	G	221	ASP	N-CA-C	5.13	116.56	111.07
1	D	183	GLU	CA-C-N	5.13	125.21	120.34
1	D	183	GLU	C-N-CA	5.13	125.21	120.34
1	A	170	ALA	N-CA-C	-5.13	102.47	110.42
1	B	187	VAL	CB-CA-C	-5.13	105.35	110.89
1	E	108	THR	CB-CA-C	-5.12	102.78	110.92
1	I	188	PRO	CA-C-N	5.08	123.36	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	188	PRO	C-N-CA	5.08	123.36	119.66
1	C	23	VAL	CB-CA-C	-5.07	104.62	110.91
1	D	42	HIS	CA-C-N	5.06	124.66	119.05
1	D	42	HIS	C-N-CA	5.06	124.66	119.05
1	J	187	VAL	CA-C-N	-5.06	115.17	120.38
1	J	187	VAL	C-N-CA	-5.06	115.17	120.38
1	G	187	VAL	CB-CA-C	-5.04	106.25	110.94
1	E	188	PRO	CA-C-N	-5.03	115.20	120.38
1	E	188	PRO	C-N-CA	-5.03	115.20	120.38
1	B	70	ASP	N-CA-C	5.02	117.91	110.48
1	E	189	PRO	N-CA-C	5.02	116.82	110.70
1	D	87	GLU	N-CA-C	-5.02	105.89	111.36
1	G	55	VAL	N-CA-C	-5.00	104.84	111.09

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1932	0	1924	60	0
1	B	1942	0	1931	74	0
1	C	1938	0	1929	64	0
1	D	1932	0	1924	51	0
1	E	1932	0	1924	64	0
1	F	1932	0	1924	56	1
1	G	1932	0	1924	67	0
1	H	1932	0	1924	64	1
1	I	1932	0	1924	57	0
1	J	1932	0	1924	47	0
2	A	57	0	0	0	0
2	B	60	0	0	2	0
2	C	39	0	0	4	0
2	D	57	0	0	4	0
2	E	65	0	0	9	0
2	F	59	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	61	0	0	5	0
2	H	65	0	0	6	0
2	I	30	0	0	2	0
2	J	49	0	0	1	0
All	All	19878	0	19252	549	1

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 14.

All (549) 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:F:206:ARG:HG3	1:F:206:ARG:HH11	1.10	1.15
1:H:200:MET:HE3	1:H:210:TRP:HA	1.26	1.12
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.18	1.07
1:F:129:PHE:CE2	1:F:140:MET:HE2	1.90	1.07
1:I:129:PHE:CE2	1:I:140:MET:HE3	1.91	1.06
1:E:220:ARG:HG2	1:E:220:ARG:HH11	0.96	1.06
1:I:105:PRO:O	1:I:106:GLN:HB2	1.54	1.05
1:C:105:PRO:O	1:C:106:GLN:HB3	1.56	1.05
1:F:200:MET:HE3	1:F:210:TRP:HA	1.41	1.02
1:B:59:ARG:HH11	1:B:59:ARG:HG2	1.28	0.98
1:J:105:PRO:O	1:J:106:GLN:HB2	1.58	0.97
1:A:105:PRO:O	1:A:106:GLN:HB2	1.58	0.97
1:G:105:PRO:O	1:G:106:GLN:HB2	1.59	0.97
1:E:220:ARG:HG2	1:E:220:ARG:NH1	1.68	0.96
1:H:235:GLU:HG3	2:H:255:HOH:O	1.65	0.95
1:H:126:ARG:HD2	1:H:145:MET:HA	1.48	0.95
1:H:129:PHE:HE2	1:H:140:MET:CE	1.82	0.93
1:B:111:ARG:HH21	1:F:106:GLN:HE21	1.08	0.93
1:E:220:ARG:HH11	1:E:220:ARG:CG	1.82	0.93
1:B:129:PHE:CE2	1:B:140:MET:HE3	2.04	0.91
1:H:11:ARG:HD3	2:H:280:HOH:O	1.71	0.91
1:F:129:PHE:HE2	1:F:140:MET:HE2	1.33	0.90
1:H:106:GLN:O	1:H:111:ARG:NH2	2.05	0.90
1:A:231:ARG:HG2	2:F:269:HOH:O	1.69	0.90
1:G:129:PHE:CE2	1:G:140:MET:HE3	2.07	0.90
1:A:123:HIS:HA	1:A:145:MET:HE1	1.54	0.89
1:H:105:PRO:O	1:H:106:GLN:HB2	1.74	0.87
1:C:11:ARG:HG2	1:C:11:ARG:HH11	1.38	0.86
1:B:4:SER:HG	1:E:4:SER:N	1.72	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:MET:HE2	1:J:200:MET:HA	1.55	0.86
1:E:126:ARG:HD3	1:E:143:TYR:O	1.76	0.85
1:D:42:HIS:CE1	1:D:149:ARG:NH2	2.43	0.85
1:B:59:ARG:HG2	1:B:59:ARG:NH1	1.87	0.85
1:G:140:MET:HE2	1:G:142:TYR:OH	1.77	0.85
1:D:206:ARG:CG	1:D:206:ARG:HH11	1.90	0.84
1:H:129:PHE:CE2	1:H:140:MET:CE	2.59	0.84
1:H:199:ARG:HD3	2:H:259:HOH:O	1.76	0.84
1:E:11:ARG:HG3	1:E:11:ARG:HH11	1.44	0.83
1:A:200:MET:HE2	1:A:200:MET:HA	1.60	0.83
1:F:206:ARG:HG3	1:F:206:ARG:NH1	1.87	0.83
1:A:111:ARG:HH21	1:D:106:GLN:HE21	1.27	0.82
1:F:11:ARG:NH1	1:F:14:GLU:OE2	2.12	0.82
1:A:180:ILE:HG22	1:A:181:ILE:HG23	1.62	0.82
1:G:42:HIS:NE2	1:G:54:PHE:HE1	1.78	0.81
1:J:129:PHE:CE2	1:J:140:MET:HE3	2.15	0.81
1:F:105:PRO:O	1:F:106:GLN:HB2	1.79	0.81
1:B:43:PRO:CG	1:B:145:MET:HE2	2.11	0.80
1:B:93:ILE:HG22	1:B:95:VAL:HG23	1.61	0.80
1:D:25:LYS:HD3	1:D:28:ASP:OD2	1.82	0.79
1:E:11:ARG:HH11	1:E:11:ARG:CG	1.95	0.79
1:F:129:PHE:CE2	1:F:140:MET:CE	2.65	0.79
1:J:129:PHE:HE2	1:J:140:MET:HE3	1.47	0.78
1:B:59:ARG:HH11	1:B:59:ARG:CG	1.95	0.78
1:C:111:ARG:HH21	1:G:106:GLN:HE21	1.32	0.78
1:F:129:PHE:HE2	1:F:140:MET:CE	1.97	0.77
1:I:129:PHE:CE2	1:I:140:MET:CE	2.67	0.77
1:H:126:ARG:HD3	1:H:143:TYR:O	1.83	0.77
1:H:129:PHE:CE2	1:H:140:MET:HE3	2.18	0.77
1:B:140:MET:HE2	1:B:142:TYR:OH	1.83	0.77
1:H:194:ASP:OD1	1:H:197:ARG:NH2	2.18	0.77
1:B:129:PHE:HE2	1:B:140:MET:HE3	1.47	0.77
1:G:7:LEU:HB2	1:G:10:GLU:OE2	1.83	0.77
1:G:179:GLU:OE1	1:H:59:ARG:HD3	1.85	0.76
1:A:42:HIS:CE1	1:A:149:ARG:NH2	2.52	0.76
1:A:129:PHE:CE2	1:A:140:MET:CE	2.69	0.76
1:F:25:LYS:HD3	1:F:28:ASP:OD2	1.84	0.76
1:B:43:PRO:HG3	1:B:145:MET:HE2	1.67	0.76
1:A:238:ALA:O	1:A:239:LYS:HB2	1.83	0.76
1:E:105:PRO:O	1:E:106:GLN:HB2	1.86	0.76
1:D:169:ARG:HG2	1:D:169:ARG:HH11	1.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ILE:HG12	1:E:5:ILE:CG1	2.16	0.75
1:H:129:PHE:HE2	1:H:140:MET:HE3	1.51	0.75
1:B:111:ARG:NH2	1:F:106:GLN:HE21	1.84	0.75
1:H:129:PHE:CE2	1:H:140:MET:HE2	2.20	0.75
1:D:105:PRO:O	1:D:106:GLN:HB2	1.85	0.75
1:B:220:ARG:HH11	1:B:220:ARG:HB3	1.50	0.75
1:E:200:MET:HE2	1:E:200:MET:HA	1.68	0.75
1:F:42:HIS:CE1	1:F:149:ARG:HH22	2.04	0.74
1:D:228:ARG:HD3	2:D:271:HOH:O	1.87	0.74
1:B:5:ILE:HG12	1:E:5:ILE:HG12	1.70	0.74
1:C:5:ILE:HG12	1:D:5:ILE:HG12	1.68	0.74
1:A:123:HIS:HA	1:A:145:MET:CE	2.18	0.73
1:H:126:ARG:HD2	1:H:145:MET:CA	2.19	0.73
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.52	0.72
1:G:200:MET:HE3	1:G:210:TRP:HA	1.71	0.72
1:C:228:ARG:NE	2:C:287:HOH:O	2.08	0.72
1:H:208:LEU:HD22	1:H:214:TRP:HZ3	1.55	0.72
1:D:42:HIS:CE1	1:D:149:ARG:HH21	2.08	0.72
1:D:200:MET:HE2	1:D:200:MET:HA	1.71	0.72
1:E:62:GLU:HG3	1:E:66:ARG:HH22	1.55	0.71
1:J:149:ARG:NH1	2:J:299:HOH:O	2.23	0.71
1:H:200:MET:CE	1:H:210:TRP:HA	2.12	0.71
1:A:42:HIS:CE1	1:A:149:ARG:HH22	2.09	0.71
1:B:127:GLY:H	1:B:149:ARG:HH12	1.39	0.71
1:D:169:ARG:HG2	1:D:169:ARG:NH1	2.05	0.71
1:J:188:PRO:O	1:J:199:ARG:NH2	2.22	0.71
2:C:260:HOH:O	1:D:231:ARG:HG3	1.90	0.70
1:E:126:ARG:HD2	1:E:145:MET:HA	1.71	0.70
1:H:228:ARG:HD3	2:H:258:HOH:O	1.91	0.70
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.56	0.70
1:B:123:HIS:ND1	1:B:145:MET:HE3	2.06	0.70
1:E:228:ARG:NH1	2:E:308:HOH:O	2.25	0.70
1:B:5:ILE:CD1	1:E:5:ILE:HG12	2.22	0.70
1:F:42:HIS:CE1	1:F:149:ARG:NH2	2.60	0.70
1:F:197:ARG:HH11	1:F:197:ARG:HG3	1.56	0.69
1:A:123:HIS:CA	1:A:145:MET:HE1	2.22	0.69
1:E:41:SER:HB3	1:E:74:LEU:HD12	1.72	0.69
1:G:5:ILE:HG12	1:H:5:ILE:HG12	1.72	0.69
1:H:129:PHE:HE2	1:H:140:MET:HE2	1.57	0.69
1:E:225:GLU:HG3	2:E:293:HOH:O	1.93	0.69
1:G:126:ARG:HD2	1:G:145:MET:HA	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:GLU:OE1	1:G:126:ARG:NH2	2.26	0.69
1:F:206:ARG:HH11	1:F:206:ARG:CG	1.99	0.69
1:G:129:PHE:HE2	1:G:140:MET:HE3	1.56	0.69
1:J:126:ARG:HD3	1:J:143:TYR:O	1.94	0.68
1:A:67:LEU:HD13	1:A:158:VAL:HG22	1.74	0.68
1:C:105:PRO:O	1:C:106:GLN:CB	2.35	0.68
1:C:122:THR:HA	1:C:125:VAL:HG23	1.76	0.68
1:B:53:GLU:OE2	1:B:149:ARG:HG3	1.94	0.68
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.05	0.68
1:C:11:ARG:HH11	1:C:11:ARG:CG	2.05	0.68
1:B:111:ARG:HH21	1:F:106:GLN:NE2	1.89	0.67
1:D:244:GLU:O	1:D:244:GLU:HG2	1.95	0.67
1:I:105:PRO:O	1:I:106:GLN:CB	2.35	0.67
1:C:42:HIS:CE1	1:C:149:ARG:NH2	2.63	0.67
1:E:220:ARG:NH1	1:E:220:ARG:CG	2.46	0.66
1:I:129:PHE:CD2	1:I:140:MET:HE3	2.30	0.66
1:A:206:ARG:HG3	1:A:206:ARG:NH1	1.93	0.66
1:I:42:HIS:CE1	1:I:149:ARG:NH2	2.64	0.66
1:I:121:ALA:O	1:I:122:THR:HG22	1.96	0.66
1:F:126:ARG:HD3	1:F:143:TYR:O	1.96	0.66
1:E:62:GLU:HG3	1:E:66:ARG:NH2	2.11	0.66
1:H:105:PRO:O	1:H:106:GLN:CB	2.44	0.66
1:J:105:PRO:O	1:J:106:GLN:CB	2.36	0.66
1:A:5:ILE:HG12	1:F:5:ILE:HG12	1.77	0.65
1:C:106:GLN:O	1:C:111:ARG:NH2	2.27	0.65
1:A:106:GLN:HE21	1:D:111:ARG:HH21	1.43	0.65
1:C:67:LEU:O	1:C:162:LYS:HE2	1.97	0.65
1:B:105:PRO:O	1:B:106:GLN:HB2	1.95	0.65
1:D:53:GLU:OE1	1:D:126:ARG:NH2	2.29	0.65
1:B:5:ILE:CG1	1:E:5:ILE:HG12	2.27	0.65
1:A:123:HIS:CB	1:A:145:MET:CE	2.74	0.64
1:C:128:VAL:O	1:C:140:MET:HA	1.97	0.64
1:G:16:GLU:OE2	1:G:25:LYS:HD3	1.98	0.64
1:A:126:ARG:HD3	1:A:143:TYR:O	1.97	0.64
1:I:67:LEU:HD13	1:I:158:VAL:HG23	1.79	0.64
1:B:126:ARG:HD3	1:B:143:TYR:O	1.98	0.64
1:C:106:GLN:HE21	1:G:111:ARG:HH21	1.45	0.64
1:G:126:ARG:HD3	1:G:143:TYR:O	1.97	0.64
1:H:62:GLU:OE1	1:H:62:GLU:HA	1.98	0.63
1:F:39:LEU:C	1:F:39:LEU:HD23	2.23	0.63
1:B:159:LYS:NZ	1:B:225:GLU:OE2	2.30	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:CB	1:A:145:MET:HE1	2.29	0.63
1:A:123:HIS:HB3	1:A:145:MET:CE	2.29	0.63
1:D:140:MET:HE2	1:D:142:TYR:OH	1.98	0.63
1:E:143:TYR:HD2	1:E:147:LEU:HD13	1.64	0.62
1:C:225:GLU:HA	1:C:228:ARG:HH11	1.64	0.62
1:D:11:ARG:NH1	1:D:14:GLU:OE2	2.31	0.62
1:G:208:LEU:HD13	1:G:214:TRP:CZ3	2.34	0.62
1:C:200:MET:HE2	1:C:200:MET:HA	1.81	0.62
1:J:140:MET:HE2	1:J:142:TYR:OH	2.00	0.62
1:G:25:LYS:NZ	1:G:28:ASP:OD2	2.32	0.61
1:G:208:LEU:HD13	1:G:214:TRP:HZ3	1.64	0.61
1:J:86:LYS:HE3	1:J:101:ILE:CD1	2.31	0.61
1:D:67:LEU:HD13	1:D:158:VAL:HG22	1.81	0.61
1:G:188:PRO:O	1:G:199:ARG:NH2	2.33	0.61
1:H:208:LEU:CD2	1:H:214:TRP:HZ3	2.12	0.61
1:C:206:ARG:HH11	1:C:206:ARG:HG3	1.64	0.61
1:F:59:ARG:NE	2:F:293:HOH:O	2.34	0.61
1:G:42:HIS:ND1	1:G:50:CYS:SG	2.68	0.61
1:I:14:GLU:OE1	1:I:25:LYS:HE2	2.01	0.61
1:G:55:VAL:O	1:G:59:ARG:HG3	2.01	0.61
1:A:123:HIS:CA	1:A:145:MET:CE	2.79	0.60
1:D:129:PHE:CE2	1:D:140:MET:HE3	2.36	0.60
1:F:59:ARG:NH2	1:F:241:LEU:HD21	2.16	0.60
1:I:200:MET:HE3	1:I:210:TRP:HA	1.82	0.60
1:A:172:PRO:HG3	1:A:181:ILE:HD11	1.82	0.60
1:C:14:GLU:OE1	1:C:28:ASP:OD1	2.20	0.60
1:I:188:PRO:O	1:I:199:ARG:NH2	2.34	0.60
1:C:231:ARG:O	1:C:235:GLU:HG2	2.01	0.60
1:E:235:GLU:CG	2:E:264:HOH:O	2.50	0.60
1:I:42:HIS:ND1	1:I:50:CYS:SG	2.72	0.60
1:D:206:ARG:HH11	1:D:206:ARG:HG2	1.66	0.60
1:G:59:ARG:NH1	1:H:179:GLU:HG2	2.17	0.60
1:B:153:GLU:OE1	1:E:150:LEU:HD22	2.02	0.60
1:G:42:HIS:HB3	1:G:50:CYS:SG	2.41	0.60
1:C:126:ARG:HD2	1:C:145:MET:HA	1.84	0.59
1:E:11:ARG:HD3	2:E:263:HOH:O	2.01	0.59
1:C:42:HIS:CE1	1:C:149:ARG:HH21	2.21	0.59
1:B:7:LEU:O	1:B:10:GLU:HB2	2.03	0.59
1:H:200:MET:HE1	1:H:213:CYS:SG	2.43	0.59
1:I:208:LEU:HD22	1:I:214:TRP:HZ3	1.68	0.59
1:G:7:LEU:HD22	2:H:288:HOH:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:O	1:A:59:ARG:HG3	2.03	0.59
1:F:105:PRO:O	1:F:106:GLN:CB	2.44	0.59
1:I:208:LEU:HD22	1:I:214:TRP:CZ3	2.38	0.59
1:J:129:PHE:CE2	1:J:140:MET:CE	2.85	0.59
1:B:5:ILE:HD11	1:E:5:ILE:HG12	1.84	0.58
1:H:48:PRO:O	1:H:52:THR:HG23	2.03	0.58
1:I:228:ARG:HD3	2:I:259:HOH:O	2.01	0.58
1:J:86:LYS:HE3	1:J:101:ILE:HD12	1.86	0.58
1:B:143:TYR:CD2	1:B:147:LEU:HD13	2.39	0.58
1:D:228:ARG:HD2	2:D:285:HOH:O	2.03	0.58
1:D:42:HIS:CE1	1:D:149:ARG:HH22	2.20	0.58
1:B:7:LEU:HB2	1:B:10:GLU:OE2	2.03	0.58
1:I:13:PRO:HB2	1:I:15:MET:HE3	1.86	0.57
1:A:128:VAL:O	1:A:140:MET:HA	2.03	0.57
1:B:200:MET:HA	1:B:200:MET:HE2	1.86	0.57
1:E:220:ARG:O	1:E:224:GLU:HG3	2.04	0.57
1:B:206:ARG:HG3	1:B:206:ARG:NH1	2.19	0.57
1:B:140:MET:CE	1:B:142:TYR:OH	2.52	0.57
1:E:90:GLU:OE2	1:E:96:ARG:HG3	2.04	0.57
1:A:227:ARG:HH21	1:F:236:LYS:NZ	2.03	0.57
1:J:38:VAL:HG23	1:J:69:VAL:CG1	2.35	0.57
1:A:198:ALA:O	1:A:202:SER:HB3	2.05	0.57
1:G:88:TRP:HZ2	1:H:209:ASP:HB2	1.70	0.56
1:J:200:MET:HA	1:J:200:MET:CE	2.31	0.56
1:J:238:ALA:O	1:J:239:LYS:HB2	2.04	0.56
1:H:132:ASP:OD2	1:H:138:ARG:HD3	2.05	0.56
1:G:105:PRO:O	1:G:106:GLN:CB	2.40	0.56
1:D:91:ARG:HG2	1:D:92:HIS:CD2	2.40	0.56
1:C:115:LEU:HD22	1:C:126:ARG:O	2.06	0.56
1:G:190:PRO:HB3	1:G:195:GLN:HB3	1.87	0.56
1:B:59:ARG:HE	1:E:179:GLU:HG2	1.70	0.56
1:B:53:GLU:OE1	1:B:126:ARG:NH2	2.39	0.56
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.41	0.55
1:B:42:HIS:ND1	1:B:50:CYS:SG	2.79	0.55
1:B:63:ASP:OD1	1:B:66:ARG:NH1	2.39	0.55
1:H:86:LYS:HE3	1:H:101:ILE:HD12	1.88	0.55
1:B:43:PRO:CB	1:B:145:MET:HE2	2.36	0.55
1:D:36:TRP:HB2	1:D:69:VAL:HG22	1.88	0.55
1:G:74:LEU:HD13	1:G:75:SER:N	2.22	0.55
1:J:13:PRO:HB2	1:J:15:MET:HE3	1.87	0.55
1:C:180:ILE:HG22	1:C:181:ILE:HG23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:CD2	1:A:140:MET:HE3	2.42	0.55
1:A:69:VAL:HG21	1:A:158:VAL:HG21	1.87	0.55
1:C:12:PHE:HB3	1:C:27:PRO:HG3	1.87	0.55
1:C:126:ARG:HD3	1:C:143:TYR:O	2.07	0.55
1:B:62:GLU:HG3	1:B:66:ARG:NH2	2.22	0.55
1:G:126:ARG:HD2	1:G:145:MET:CA	2.37	0.55
1:E:11:ARG:CG	1:E:11:ARG:NH1	2.65	0.54
1:E:112:ARG:NE	2:E:267:HOH:O	2.41	0.54
1:H:53:GLU:OE1	1:H:126:ARG:NH2	2.40	0.54
1:J:129:PHE:HE2	1:J:140:MET:CE	2.17	0.54
1:I:55:VAL:O	1:I:59:ARG:HG3	2.08	0.54
1:J:192:THR:OG1	1:J:195:GLN:HB2	2.07	0.54
1:E:228:ARG:HD3	2:E:259:HOH:O	2.06	0.54
1:F:67:LEU:HD13	1:F:158:VAL:CG2	2.37	0.54
1:G:66:ARG:HD3	2:G:271:HOH:O	2.07	0.54
1:G:143:TYR:HD2	1:G:147:LEU:HD13	1.73	0.54
1:B:220:ARG:HB3	1:B:220:ARG:NH1	2.21	0.54
1:C:212:PHE:C	1:C:212:PHE:HD2	2.15	0.54
1:C:7:LEU:HB2	1:C:10:GLU:OE2	2.08	0.54
1:E:53:GLU:OE2	1:E:148:GLY:HA2	2.08	0.54
1:I:224:GLU:O	1:I:228:ARG:HB2	2.08	0.54
1:A:123:HIS:CG	1:A:145:MET:HE1	2.44	0.53
1:C:212:PHE:C	1:C:212:PHE:CD2	2.86	0.53
1:J:126:ARG:HD2	1:J:145:MET:HA	1.91	0.53
1:B:14:GLU:OE1	1:B:28:ASP:OD1	2.27	0.53
1:B:200:MET:HE1	1:B:213:CYS:SG	2.49	0.53
1:I:200:MET:HA	1:I:200:MET:HE2	1.89	0.53
1:B:11:ARG:HG2	1:B:11:ARG:HH11	1.74	0.53
1:G:42:HIS:CE1	1:G:149:ARG:NH2	2.77	0.53
1:H:199:ARG:CD	2:H:259:HOH:O	2.45	0.53
1:I:53:GLU:OE1	1:I:126:ARG:NH2	2.40	0.53
1:D:13:PRO:HB2	1:D:15:MET:HE3	1.89	0.53
1:I:140:MET:HE2	1:I:142:TYR:OH	2.08	0.53
1:A:39:LEU:C	1:A:39:LEU:HD23	2.34	0.53
1:B:65:GLN:HG3	2:B:305:HOH:O	2.08	0.52
1:I:8:ILE:HD11	1:J:142:TYR:O	2.10	0.52
1:J:75:SER:HB3	1:J:82:HIS:CE1	2.44	0.52
1:F:36:TRP:HB2	1:F:69:VAL:HG22	1.92	0.52
1:H:225:GLU:O	1:H:228:ARG:HG3	2.09	0.52
1:I:141:LEU:HD22	1:J:141:LEU:HD22	1.90	0.52
1:H:42:HIS:ND1	1:H:50:CYS:SG	2.78	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LEU:HA	1:B:244:GLU:OE2	2.08	0.52
1:G:59:ARG:HH11	1:H:179:GLU:HG2	1.75	0.52
1:F:203:GLY:HA2	2:F:299:HOH:O	2.10	0.52
1:E:143:TYR:CD2	1:E:147:LEU:HD13	2.43	0.52
1:A:53:GLU:CD	1:A:126:ARG:HH22	2.17	0.52
1:A:227:ARG:NH2	1:F:236:LYS:NZ	2.58	0.52
1:D:129:PHE:HE2	1:D:140:MET:HE3	1.74	0.52
1:C:55:VAL:O	1:C:59:ARG:HG3	2.09	0.51
1:D:89:ILE:HG21	1:D:97:ILE:HD11	1.91	0.51
1:G:42:HIS:CG	1:G:50:CYS:HG	2.27	0.51
1:E:25:LYS:HD3	1:E:28:ASP:OD2	2.10	0.51
1:B:192:THR:OG1	1:B:195:GLN:HB2	2.10	0.51
1:D:14:GLU:OE1	1:D:25:LYS:HE2	2.11	0.51
1:F:238:ALA:O	1:F:239:LYS:CB	2.58	0.51
1:B:220:ARG:HH11	1:B:220:ARG:CB	2.21	0.51
1:A:123:HIS:HB3	1:A:145:MET:HE3	1.93	0.51
1:G:200:MET:HE1	1:G:213:CYS:SG	2.51	0.51
1:B:5:ILE:HG12	1:E:5:ILE:HG13	1.89	0.51
1:C:4:SER:N	2:C:288:HOH:O	2.43	0.51
1:G:74:LEU:CD1	1:G:74:LEU:C	2.83	0.51
1:H:208:LEU:CD2	1:H:214:TRP:CZ3	2.94	0.51
1:I:147:LEU:HG	1:J:161:LEU:HD13	1.92	0.51
1:J:55:VAL:O	1:J:59:ARG:HG3	2.11	0.51
1:I:28:ASP:O	1:I:29:HIS:C	2.53	0.51
1:B:143:TYR:HD2	1:B:147:LEU:HD13	1.74	0.50
1:B:123:HIS:HE1	2:B:293:HOH:O	1.94	0.50
1:B:132:ASP:OD2	1:B:138:ARG:HD3	2.11	0.50
1:G:74:LEU:HD13	1:G:74:LEU:C	2.36	0.50
1:G:92:HIS:CE1	2:G:259:HOH:O	2.64	0.50
1:H:140:MET:HE2	1:H:142:TYR:OH	2.12	0.50
1:I:53:GLU:OE2	1:I:148:GLY:HA2	2.11	0.50
1:C:74:LEU:C	1:C:74:LEU:HD13	2.37	0.50
1:G:25:LYS:HG2	1:G:28:ASP:OD2	2.11	0.50
1:C:42:HIS:ND1	1:C:50:CYS:SG	2.84	0.50
1:C:206:ARG:HG3	1:C:206:ARG:NH1	2.26	0.50
1:E:111:ARG:HH21	1:I:106:GLN:HE21	1.59	0.50
1:H:69:VAL:HG21	1:H:158:VAL:HG21	1.93	0.50
1:J:69:VAL:HG21	1:J:158:VAL:HG21	1.93	0.50
1:A:5:ILE:O	1:A:5:ILE:HG13	2.12	0.49
1:A:227:ARG:NH2	1:F:236:LYS:HZ3	2.10	0.49
1:B:180:ILE:O	1:E:240:LEU:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:PRO:HG3	1:D:181:ILE:HD11	1.94	0.49
1:J:176:PRO:HG2	1:J:227:ARG:HG3	1.94	0.49
1:A:92:HIS:O	1:A:245:ALA:HB1	2.12	0.49
1:B:48:PRO:CD	1:E:189:PRO:HG3	2.43	0.49
1:C:53:GLU:CD	1:C:126:ARG:HH22	2.21	0.49
1:D:169:ARG:HH11	1:D:169:ARG:CG	2.20	0.49
1:G:42:HIS:HE2	1:G:54:PHE:HE1	1.59	0.49
1:C:106:GLN:HA	1:G:106:GLN:C	2.38	0.49
1:H:159:LYS:HD3	1:H:225:GLU:HG2	1.94	0.49
1:I:187:VAL:HG23	1:I:213:CYS:O	2.13	0.49
1:B:37:PHE:HA	1:B:70:ASP:O	2.12	0.49
1:C:225:GLU:HA	1:C:228:ARG:HD2	1.95	0.49
1:F:180:ILE:HG22	1:F:181:ILE:HG23	1.95	0.49
1:A:200:MET:HA	1:A:200:MET:CE	2.40	0.49
1:A:227:ARG:HH21	1:F:236:LYS:HZ3	1.61	0.49
1:B:188:PRO:O	1:B:199:ARG:NH2	2.44	0.49
1:G:91:ARG:HG2	1:G:92:HIS:CD2	2.47	0.49
1:C:53:GLU:OE1	1:C:126:ARG:NH2	2.46	0.49
1:J:5:ILE:HD12	1:J:140:MET:CE	2.43	0.49
1:B:126:ARG:CD	1:B:143:TYR:O	2.61	0.49
1:C:185:LEU:O	1:C:214:TRP:HB2	2.12	0.49
1:H:143:TYR:HD2	1:H:147:LEU:HD13	1.78	0.49
1:A:123:HIS:ND1	1:A:145:MET:HE1	2.27	0.48
1:F:122:THR:HA	1:F:125:VAL:HG23	1.94	0.48
1:G:210:TRP:NE1	1:J:87:GLU:OE1	2.45	0.48
1:H:42:HIS:CE1	1:H:149:ARG:NH2	2.81	0.48
1:D:238:ALA:O	1:D:239:LYS:HB2	2.13	0.48
1:C:161:LEU:HD13	1:D:147:LEU:HD12	1.95	0.48
1:A:129:PHE:CE2	1:A:140:MET:HE2	2.48	0.48
1:D:25:LYS:CD	1:D:28:ASP:OD2	2.58	0.48
1:E:7:LEU:O	1:E:10:GLU:HB2	2.12	0.48
1:H:125:VAL:O	1:H:125:VAL:HG12	2.13	0.48
1:I:62:GLU:HB2	2:I:258:HOH:O	2.12	0.48
1:A:40:PHE:HZ	1:A:99:PHE:CE1	2.32	0.48
1:G:128:VAL:HG21	1:G:149:ARG:HD2	1.96	0.48
1:C:142:TYR:O	1:D:8:ILE:HD11	2.13	0.48
1:G:136:VAL:O	1:G:138:ARG:HG2	2.14	0.48
1:D:129:PHE:CE2	1:D:140:MET:CE	2.97	0.48
1:I:175:TRP:CG	1:I:176:PRO:HA	2.49	0.48
1:F:53:GLU:OE1	1:F:126:ARG:NH2	2.41	0.48
1:J:136:VAL:O	1:J:138:ARG:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TYR:O	1:E:139:THR:HG23	2.14	0.48
1:F:128:VAL:HG21	1:F:149:ARG:HD2	1.96	0.48
1:I:126:ARG:HD3	1:I:143:TYR:O	2.13	0.48
1:C:36:TRP:HB2	1:C:69:VAL:HG22	1.96	0.48
1:C:200:MET:HE1	1:C:213:CYS:SG	2.54	0.48
1:H:86:LYS:HE3	1:H:101:ILE:CD1	2.44	0.48
1:B:42:HIS:NE2	1:B:54:PHE:HE1	2.11	0.47
1:C:159:LYS:HD3	1:C:225:GLU:HG2	1.95	0.47
1:F:238:ALA:O	1:F:239:LYS:HB2	2.13	0.47
1:I:144:PRO:HD3	1:J:139:THR:OG1	2.14	0.47
1:A:126:ARG:HD2	1:A:144:PRO:C	2.38	0.47
1:A:129:PHE:CE2	1:A:140:MET:HE3	2.49	0.47
1:E:123:HIS:CG	1:E:145:MET:HE1	2.49	0.47
1:A:53:GLU:OE1	1:A:126:ARG:NH2	2.48	0.47
1:J:79:VAL:O	1:J:83:ILE:HG13	2.15	0.47
1:E:235:GLU:HG3	2:E:264:HOH:O	2.11	0.47
1:G:88:TRP:CZ2	1:H:209:ASP:HB2	2.50	0.47
1:G:60:ARG:HG3	1:G:60:ARG:HH11	1.80	0.47
1:G:67:LEU:HD13	1:G:158:VAL:HG23	1.95	0.47
1:A:106:GLN:NE2	1:D:111:ARG:HH21	2.11	0.47
1:F:67:LEU:HD13	1:F:158:VAL:HG22	1.95	0.47
1:G:53:GLU:CD	1:G:126:ARG:HH22	2.22	0.47
1:I:36:TRP:HB2	1:I:69:VAL:HG22	1.97	0.47
1:I:157:ILE:O	1:I:161:LEU:HB2	2.14	0.47
1:A:180:ILE:HG22	1:A:181:ILE:CG2	2.39	0.47
1:E:228:ARG:CD	2:E:259:HOH:O	2.62	0.47
1:G:190:PRO:HD3	2:G:311:HOH:O	2.14	0.47
1:C:6:PRO:HB2	1:C:137:ILE:HD12	1.97	0.47
1:H:159:LYS:CE	1:H:222:ASP:OD1	2.62	0.47
1:I:48:PRO:HG2	1:J:186:ILE:HG21	1.96	0.47
1:D:171:VAL:HG12	2:D:251:HOH:O	2.14	0.47
1:I:42:HIS:CE1	1:I:149:ARG:HH21	2.30	0.47
1:G:37:PHE:HA	1:G:70:ASP:O	2.15	0.46
1:I:15:MET:CE	1:I:112:ARG:HG2	2.45	0.46
1:I:180:ILE:HG22	1:I:181:ILE:HG23	1.96	0.46
1:F:126:ARG:CD	1:F:143:TYR:O	2.61	0.46
1:H:55:VAL:O	1:H:59:ARG:HG3	2.15	0.46
1:A:143:TYR:HD2	1:A:147:LEU:HD13	1.79	0.46
1:C:42:HIS:NE2	1:C:54:PHE:HE1	2.13	0.46
1:E:75:SER:HB3	1:E:82:HIS:CE1	2.50	0.46
1:E:12:PHE:HA	1:E:13:PRO:HD2	1.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:THR:HA	1:E:101:ILE:O	2.16	0.46
1:F:128:VAL:CG2	1:F:149:ARG:HD2	2.46	0.46
1:A:105:PRO:C	1:A:107:GLY:H	2.23	0.46
1:E:156:ARG:HD3	1:E:230:LEU:HD21	1.97	0.46
1:I:43:PRO:HG2	1:I:145:MET:HG3	1.98	0.46
1:I:139:THR:OG1	1:J:144:PRO:HD3	2.15	0.46
1:I:67:LEU:CD1	1:I:158:VAL:HG23	2.44	0.46
1:D:127:GLY:HA2	1:D:141:LEU:O	2.16	0.46
1:G:42:HIS:CD2	1:G:54:PHE:HE1	2.32	0.46
1:A:188:PRO:O	1:A:199:ARG:NH2	2.40	0.46
1:G:11:ARG:HD2	2:G:302:HOH:O	2.14	0.46
1:G:236:LYS:HD2	1:G:237:PRO:HD2	1.98	0.46
1:J:6:PRO:O	1:J:140:MET:HE1	2.15	0.46
1:A:67:LEU:HD13	1:A:158:VAL:CG2	2.42	0.46
1:B:147:LEU:HG	1:E:161:LEU:HD13	1.98	0.46
1:F:214:TRP:NE1	2:F:295:HOH:O	2.33	0.46
1:H:128:VAL:HG21	1:H:149:ARG:HD2	1.97	0.46
1:H:159:LYS:HE2	1:H:222:ASP:OD1	2.15	0.46
1:B:41:SER:O	1:B:149:ARG:NH2	2.50	0.45
1:C:74:LEU:CD2	1:C:104:ASP:HB2	2.46	0.45
1:C:157:ILE:O	1:C:161:LEU:HB2	2.16	0.45
1:D:7:LEU:H	1:D:10:GLU:CD	2.23	0.45
1:D:31:VAL:C	1:D:33:GLN:H	2.24	0.45
1:F:84:LYS:HE3	1:F:84:LYS:HB3	1.77	0.45
1:I:126:ARG:HD2	1:I:144:PRO:C	2.42	0.45
1:C:62:GLU:OE2	1:C:62:GLU:HA	2.15	0.45
1:C:231:ARG:NH1	2:C:273:HOH:O	2.40	0.45
1:F:156:ARG:HD3	1:F:230:LEU:HD21	1.98	0.45
1:H:53:GLU:CD	1:H:126:ARG:HH22	2.23	0.45
1:J:45:ASP:OD2	1:J:82:HIS:ND1	2.38	0.45
1:A:6:PRO:HB2	1:A:137:ILE:HD13	1.98	0.45
1:B:154:ILE:O	1:B:158:VAL:HG22	2.17	0.45
1:F:43:PRO:O	1:F:44:ALA:HB2	2.16	0.45
1:G:67:LEU:O	1:G:162:LYS:HE3	2.16	0.45
1:C:157:ILE:HG23	1:D:147:LEU:HD11	1.99	0.45
1:A:75:SER:HB3	1:A:82:HIS:CE1	2.52	0.45
1:F:228:ARG:HD3	2:F:284:HOH:O	2.15	0.45
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.52	0.45
1:E:11:ARG:HG3	1:E:11:ARG:NH1	2.23	0.45
1:H:156:ARG:HD3	1:H:230:LEU:HD21	1.99	0.45
1:J:53:GLU:OE2	1:J:148:GLY:HA2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:106:GLN:O	1:J:111:ARG:NH2	2.47	0.45
1:F:39:LEU:C	1:F:39:LEU:CD2	2.90	0.44
1:B:147:LEU:HD11	1:E:157:ILE:HG23	1.98	0.44
1:C:188:PRO:O	1:C:199:ARG:NH2	2.50	0.44
1:D:42:HIS:HE1	1:D:149:ARG:HH21	1.62	0.44
1:B:93:ILE:HG22	1:B:95:VAL:CG2	2.41	0.44
1:I:171:VAL:HG22	1:I:185:LEU:HD22	1.99	0.44
1:F:116:LEU:CD2	1:F:121:ALA:HB3	2.47	0.44
1:G:5:ILE:HD12	1:G:140:MET:HE1	1.99	0.44
1:J:53:GLU:CD	1:J:126:ARG:HH22	2.26	0.44
1:G:231:ARG:HG3	2:G:268:HOH:O	2.16	0.44
1:A:105:PRO:O	1:A:106:GLN:CB	2.39	0.44
1:B:35:LYS:HE2	1:B:68:GLY:HA2	1.98	0.44
1:H:37:PHE:HA	1:H:70:ASP:O	2.18	0.44
1:C:67:LEU:HD13	1:C:158:VAL:HG23	1.99	0.44
1:E:111:ARG:NH2	1:I:106:GLN:HE21	2.16	0.44
1:E:124:THR:O	1:E:126:ARG:N	2.51	0.44
1:F:200:MET:HE1	1:F:213:CYS:SG	2.58	0.44
1:H:129:PHE:CD2	1:H:140:MET:HE3	2.51	0.44
1:B:11:ARG:HG2	1:B:11:ARG:NH1	2.33	0.43
1:C:206:ARG:HH11	1:C:206:ARG:CG	2.31	0.43
1:I:200:MET:HE1	1:I:213:CYS:SG	2.58	0.43
1:B:105:PRO:O	1:B:106:GLN:CB	2.61	0.43
1:C:5:ILE:HD12	1:C:140:MET:HE1	2.00	0.43
1:G:88:TRP:CE3	1:G:88:TRP:C	2.96	0.43
1:I:129:PHE:N	1:I:129:PHE:CD1	2.87	0.43
1:H:11:ARG:NH1	1:H:14:GLU:OE2	2.51	0.43
1:I:128:VAL:HB	1:I:141:LEU:HB2	2.00	0.43
1:D:126:ARG:HD3	1:D:143:TYR:O	2.19	0.43
1:F:157:ILE:O	1:F:161:LEU:HB2	2.18	0.43
1:F:200:MET:CE	1:F:210:TRP:HA	2.30	0.43
1:G:143:TYR:CD2	1:G:147:LEU:HD13	2.53	0.43
1:B:16:GLU:HG2	1:B:25:LYS:HG3	2.01	0.43
1:B:173:ALA:HB2	1:E:53:GLU:HG3	2.01	0.43
1:F:61:TYR:HE1	2:F:273:HOH:O	2.01	0.43
1:J:5:ILE:HD12	1:J:140:MET:HE1	2.00	0.43
1:J:67:LEU:HD13	1:J:158:VAL:CG2	2.48	0.43
1:A:206:ARG:O	1:A:213:CYS:HA	2.18	0.43
1:G:161:LEU:HD13	1:H:147:LEU:HG	2.00	0.43
1:I:42:HIS:CE1	1:I:149:ARG:HH22	2.36	0.42
1:J:150:LEU:HD23	1:J:153:GLU:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HB2	1:C:102:ILE:HD12	2.02	0.42
1:E:42:HIS:CE1	1:E:149:ARG:NH2	2.87	0.42
1:E:149:ARG:HD3	2:E:251:HOH:O	2.19	0.42
1:A:7:LEU:HB2	1:A:10:GLU:OE2	2.20	0.42
1:B:7:LEU:H	1:B:10:GLU:CD	2.28	0.42
1:H:84:LYS:HD2	1:I:210:TRP:HE1	1.83	0.42
1:G:60:ARG:HD3	1:G:151:VAL:HG12	2.00	0.42
1:H:14:GLU:OE1	1:H:25:LYS:HE2	2.20	0.42
1:H:28:ASP:OD1	1:H:28:ASP:N	2.53	0.42
1:I:15:MET:HE2	1:I:112:ARG:HG2	2.00	0.42
1:I:169:ARG:HB3	1:I:185:LEU:HB3	2.02	0.42
1:A:238:ALA:O	1:A:239:LYS:CB	2.61	0.42
1:C:202:SER:OG	1:C:204:GLN:HG2	2.20	0.42
1:D:42:HIS:ND1	1:D:50:CYS:SG	2.89	0.42
1:F:115:LEU:HD22	1:F:126:ARG:O	2.20	0.42
1:J:38:VAL:HG23	1:J:69:VAL:HG11	2.00	0.42
1:C:86:LYS:NZ	1:H:193:GLU:OE1	2.41	0.42
1:I:145:MET:HE2	1:I:145:MET:HB3	1.89	0.42
1:G:185:LEU:O	1:G:214:TRP:HB2	2.20	0.42
1:J:67:LEU:HD13	1:J:158:VAL:HG22	2.00	0.42
1:B:43:PRO:HB3	1:B:122:THR:O	2.20	0.41
1:C:7:LEU:O	1:C:10:GLU:HB2	2.20	0.41
1:C:184:GLY:HA2	1:C:216:THR:HG22	2.01	0.41
1:H:79:VAL:O	1:H:83:ILE:HG13	2.20	0.41
1:A:231:ARG:HH11	1:A:231:ARG:HD2	1.71	0.41
1:B:175:TRP:CG	1:B:176:PRO:HA	2.54	0.41
1:D:156:ARG:HD3	1:D:230:LEU:HD21	2.01	0.41
1:E:127:GLY:HA2	1:E:141:LEU:O	2.20	0.41
1:E:185:LEU:O	1:E:214:TRP:HB2	2.20	0.41
1:H:99:PHE:HB2	1:H:100:PRO:HD2	2.02	0.41
1:I:20:ASP:OD2	1:I:86:LYS:NZ	2.50	0.41
1:J:53:GLU:OE1	1:J:126:ARG:NH2	2.53	0.41
1:C:178:ASN:HD21	1:D:52:THR:HB	1.84	0.41
1:E:90:GLU:CD	1:E:96:ARG:HG3	2.45	0.41
1:I:128:VAL:O	1:I:140:MET:HA	2.21	0.41
1:J:127:GLY:HA2	1:J:141:LEU:O	2.20	0.41
1:C:7:LEU:HD23	1:C:7:LEU:HA	1.86	0.41
1:C:96:ARG:NH2	1:C:98:PRO:HB3	2.35	0.41
1:F:63:ASP:OD1	1:F:66:ARG:NH1	2.38	0.41
1:G:128:VAL:O	1:G:140:MET:HA	2.20	0.41
1:B:43:PRO:HG3	1:B:145:MET:CE	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:THR:O	2:D:306:HOH:O	2.22	0.41
1:E:163:LEU:HD22	1:E:167:LEU:HD22	2.02	0.41
1:F:6:PRO:O	1:F:140:MET:HE1	2.21	0.41
1:F:40:PHE:HD1	1:F:42:HIS:HE2	1.69	0.41
1:D:190:PRO:HB3	1:D:195:GLN:HB3	2.03	0.41
1:G:60:ARG:HG3	1:G:60:ARG:NH1	2.35	0.41
1:G:89:ILE:HG23	1:G:93:ILE:HD12	2.03	0.41
1:H:188:PRO:O	1:H:199:ARG:NH2	2.49	0.41
1:B:153:GLU:O	1:B:157:ILE:HG13	2.21	0.41
1:H:39:LEU:O	1:H:128:VAL:HA	2.21	0.41
1:C:63:ASP:OD1	1:C:66:ARG:NH1	2.53	0.40
1:G:212:PHE:HD2	1:G:212:PHE:C	2.29	0.40
1:A:180:ILE:HA	1:F:241:LEU:HB2	2.03	0.40
1:E:28:ASP:OD1	1:E:28:ASP:N	2.55	0.40
1:E:128:VAL:O	1:E:140:MET:HA	2.21	0.40
1:H:231:ARG:O	1:H:235:GLU:HG2	2.20	0.40
1:A:42:HIS:HA	1:A:43:PRO:HD3	1.87	0.40
1:F:242:TYR:CE2	1:F:243:GLU:HG3	2.56	0.40
1:H:105:PRO:O	1:H:105:PRO:HG2	2.22	0.40
1:I:61:TYR:CD2	1:I:61:TYR:C	3.00	0.40
1:I:112:ARG:O	1:I:112:ARG:HG3	2.20	0.40
1:E:197:ARG:HH11	1:E:197:ARG:HG3	1.86	0.40
1:I:177:ASN:HB3	1:J:237:PRO:HD3	2.03	0.40
1:C:153:GLU:OE1	1:D:150:LEU:HD22	2.19	0.40
1:C:219:SER:O	1:C:222:ASP:HB2	2.21	0.40
1:E:53:GLU:OE1	1:E:126:ARG:NH2	2.55	0.40
1:E:152:ASP:HB2	1:E:233:ALA:HB2	2.03	0.40
1:J:28:ASP:OD1	1:J:28:ASP:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ARG:NH1	1:H:228:ARG:CB[1_544]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/250 (94%)	224 (96%)	7 (3%)	3 (1%)	9	14
1	B	235/250 (94%)	228 (97%)	6 (3%)	1 (0%)	30	43
1	C	235/250 (94%)	219 (93%)	15 (6%)	1 (0%)	30	43
1	D	234/250 (94%)	219 (94%)	13 (6%)	2 (1%)	14	22
1	E	234/250 (94%)	223 (95%)	11 (5%)	0	100	100
1	F	234/250 (94%)	224 (96%)	8 (3%)	2 (1%)	14	22
1	G	234/250 (94%)	217 (93%)	15 (6%)	2 (1%)	14	22
1	H	234/250 (94%)	221 (94%)	10 (4%)	3 (1%)	9	14
1	I	234/250 (94%)	221 (94%)	10 (4%)	3 (1%)	9	14
1	J	234/250 (94%)	211 (90%)	21 (9%)	2 (1%)	14	22
All	All	2342/2500 (94%)	2207 (94%)	116 (5%)	19 (1%)	16	25

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	C	121	ALA
1	F	32	SER
1	F	122	THR
1	I	122	THR
1	J	32	SER
1	J	106	GLN
1	H	106	GLN
1	H	122	THR
1	I	32	SER
1	I	239	LYS
1	A	20	ASP
1	B	122	THR
1	D	122	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	239	LYS
1	G	243	GLU
1	A	239	LYS
1	G	122	THR
1	H	239	LYS

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	206/216 (95%)	190 (92%)	16 (8%)	11	20
1	B	207/216 (96%)	184 (89%)	23 (11%)	6	9
1	C	207/216 (96%)	191 (92%)	16 (8%)	12	20
1	D	206/216 (95%)	188 (91%)	18 (9%)	9	16
1	E	206/216 (95%)	185 (90%)	21 (10%)	7	11
1	F	206/216 (95%)	187 (91%)	19 (9%)	8	14
1	G	206/216 (95%)	192 (93%)	14 (7%)	14	25
1	H	206/216 (95%)	185 (90%)	21 (10%)	7	11
1	I	206/216 (95%)	190 (92%)	16 (8%)	11	20
1	J	206/216 (95%)	184 (89%)	22 (11%)	6	10
All	All	2062/2160 (96%)	1876 (91%)	186 (9%)	9	15

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	5	ILE
1	A	8	ILE
1	A	62	GLU
1	A	74	LEU
1	A	106	GLN
1	A	122	THR
1	A	126	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	147	LEU
1	A	158	VAL
1	A	161	LEU
1	A	167	LEU
1	A	199	ARG
1	A	206	ARG
1	A	208	LEU
1	A	242	TYR
1	B	24	ILE
1	B	32	SER
1	B	35	LYS
1	B	59	ARG
1	B	66	ARG
1	B	74	LEU
1	B	116	LEU
1	B	122	THR
1	B	126	ARG
1	B	145	MET
1	B	147	LEU
1	B	159	LYS
1	B	161	LEU
1	B	167	LEU
1	B	193	GLU
1	B	199	ARG
1	B	204	GLN
1	B	206	ARG
1	B	208	LEU
1	B	220	ARG
1	B	231	ARG
1	B	236	LYS
1	B	242	TYR
1	C	11	ARG
1	C	74	LEU
1	C	116	LEU
1	C	122	THR
1	C	147	LEU
1	C	161	LEU
1	C	167	LEU
1	C	168	LYS
1	C	179	GLU
1	C	183	GLU
1	C	193	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	195	GLN
1	C	199	ARG
1	C	206	ARG
1	C	228	ARG
1	C	239	LYS
1	D	11	ARG
1	D	28	ASP
1	D	62	GLU
1	D	66	ARG
1	D	74	LEU
1	D	91	ARG
1	D	126	ARG
1	D	147	LEU
1	D	158	VAL
1	D	161	LEU
1	D	167	LEU
1	D	169	ARG
1	D	179	GLU
1	D	199	ARG
1	D	204	GLN
1	D	206	ARG
1	D	208	LEU
1	D	239	LYS
1	E	11	ARG
1	E	28	ASP
1	E	41	SER
1	E	59	ARG
1	E	66	ARG
1	E	74	LEU
1	E	122	THR
1	E	145	MET
1	E	147	LEU
1	E	158	VAL
1	E	161	LEU
1	E	166	SER
1	E	167	LEU
1	E	179	GLU
1	E	193	GLU
1	E	197	ARG
1	E	199	ARG
1	E	204	GLN
1	E	208	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	220	ARG
1	E	242	TYR
1	F	14	GLU
1	F	19	THR
1	F	32	SER
1	F	62	GLU
1	F	74	LEU
1	F	116	LEU
1	F	126	ARG
1	F	145	MET
1	F	147	LEU
1	F	158	VAL
1	F	161	LEU
1	F	167	LEU
1	F	197	ARG
1	F	199	ARG
1	F	204	GLN
1	F	206	ARG
1	F	208	LEU
1	F	236	LYS
1	F	242	TYR
1	G	16	GLU
1	G	24	ILE
1	G	32	SER
1	G	74	LEU
1	G	79	VAL
1	G	88	TRP
1	G	108	THR
1	G	122	THR
1	G	147	LEU
1	G	161	LEU
1	G	167	LEU
1	G	199	ARG
1	G	206	ARG
1	G	231	ARG
1	H	11	ARG
1	H	28	ASP
1	H	62	GLU
1	H	65	GLN
1	H	83	ILE
1	H	91	ARG
1	H	93	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	116	LEU
1	H	122	THR
1	H	147	LEU
1	H	158	VAL
1	H	159	LYS
1	H	161	LEU
1	H	167	LEU
1	H	179	GLU
1	H	183	GLU
1	H	199	ARG
1	H	201	GLU
1	H	207	SER
1	H	228	ARG
1	H	242	TYR
1	I	5	ILE
1	I	16	GLU
1	I	24	ILE
1	I	41	SER
1	I	62	GLU
1	I	126	ARG
1	I	147	LEU
1	I	161	LEU
1	I	167	LEU
1	I	174	ASP
1	I	195	GLN
1	I	208	LEU
1	I	220	ARG
1	I	236	LYS
1	I	243	GLU
1	I	244	GLU
1	J	7	LEU
1	J	16	GLU
1	J	41	SER
1	J	62	GLU
1	J	72	ILE
1	J	74	LEU
1	J	116	LEU
1	J	137	ILE
1	J	147	LEU
1	J	149	ARG
1	J	158	VAL
1	J	161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	162	LYS
1	J	167	LEU
1	J	174	ASP
1	J	193	GLU
1	J	195	GLN
1	J	199	ARG
1	J	200	MET
1	J	201	GLU
1	J	235	GLU
1	J	239	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	B	106	GLN
1	B	123	HIS
1	C	106	GLN
1	D	65	GLN
1	D	106	GLN
1	D	123	HIS
1	E	106	GLN
1	F	106	GLN
1	F	204	GLN
1	G	92	HIS
1	G	106	GLN
1	I	21	HIS
1	I	29	HIS
1	I	106	GLN
1	I	123	HIS
1	I	195	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	238/250 (95%)	-0.78	2 (0%) 82 80	12, 22, 45, 72	0
1	B	239/250 (95%)	-0.68	2 (0%) 82 80	14, 24, 44, 62	0
1	C	239/250 (95%)	-0.68	1 (0%) 88 86	15, 25, 44, 71	0
1	D	238/250 (95%)	-0.68	1 (0%) 88 86	13, 25, 46, 76	0
1	E	238/250 (95%)	-0.65	2 (0%) 82 80	13, 25, 44, 65	0
1	F	238/250 (95%)	-0.71	1 (0%) 88 86	11, 22, 41, 65	0
1	G	238/250 (95%)	-0.67	2 (0%) 82 80	14, 24, 44, 59	0
1	H	238/250 (95%)	-0.65	2 (0%) 82 80	13, 24, 45, 63	0
1	I	238/250 (95%)	-0.56	1 (0%) 88 86	18, 30, 49, 68	0
1	J	238/250 (95%)	-0.62	3 (1%) 75 71	15, 27, 48, 63	0
All	All	2382/2500 (95%)	-0.67	17 (0%) 84 81	11, 25, 46, 76	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	245	ALA	3.5
1	F	245	ALA	3.3
1	H	121	ALA	3.2
1	H	245	ALA	3.1
1	J	238	ALA	3.0
1	J	121	ALA	2.9
1	B	245	ALA	2.7
1	A	245	ALA	2.6
1	C	245	ALA	2.3
1	J	245	ALA	2.3
1	B	121	ALA	2.3
1	E	121	ALA	2.3
1	D	245	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	245	ALA	2.2
1	G	121	ALA	2.2
1	G	245	ALA	2.1
1	A	121	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.