Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 02:12 PM EDT

PDB ID	:	5TTR
Title	:	LEU 55 PRO TRANSTHYRETIN CRYSTAL STRUCTURE
Authors	:	Sebastiao, M.P.; Saraiva, M.J.; Damas, A.M.
Deposited on	:	1998-04-30
Resolution	:	2.70 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 (i) symbol.

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

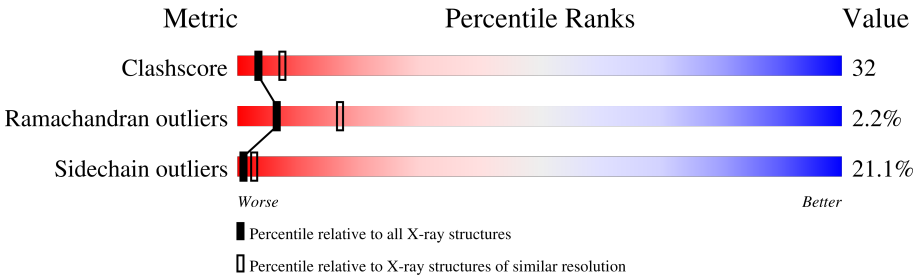
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	24% 47% 17% • 9%
1	B	127	28% 31% 26% 6% 9%
1	C	127	28% 40% 17% 6% 9%
1	D	127	28% 33% 26% 5% 9%
1	E	127	33% 31% 20% 8% 9%
1	F	127	28% 35% 24% 5% 9%
1	G	127	30% 34% 21% 6% 9%
1	H	127	29% 36% 20% 6% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7147 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 TRANSTHYRETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	4	0	0
			895	572	147	174	2			
1	B	116	Total	C	N	O	S	18	0	0
			890	569	145	174	2			
1	C	116	Total	C	N	O	S	7	0	0
			895	572	147	174	2			
1	D	116	Total	C	N	O	S	0	0	0
			891	570	147	172	2			
1	E	116	Total	C	N	O	S	11	0	0
			895	572	147	174	2			
1	F	116	Total	C	N	O	S	0	0	0
			895	572	147	174	2			
1	G	116	Total	C	N	O	S	7	0	0
			891	570	147	172	2			
1	H	116	Total	C	N	O	S	4	0	0
			895	572	147	174	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	PRO	LEU	engineered mutation	UNP P02766
B	55	PRO	LEU	engineered mutation	UNP P02766
C	55	PRO	LEU	engineered mutation	UNP P02766
D	55	PRO	LEU	engineered mutation	UNP P02766
E	55	PRO	LEU	engineered mutation	UNP P02766
F	55	PRO	LEU	engineered mutation	UNP P02766
G	55	PRO	LEU	engineered mutation	UNP P02766
H	55	PRO	LEU	engineered mutation	UNP P02766

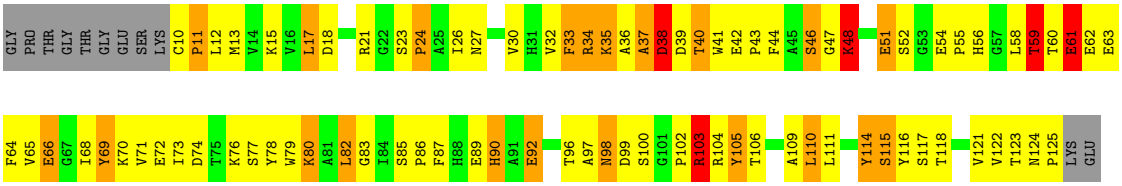
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

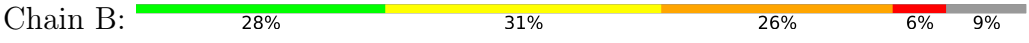
• Molecule 1: TRANSTHYRETIN

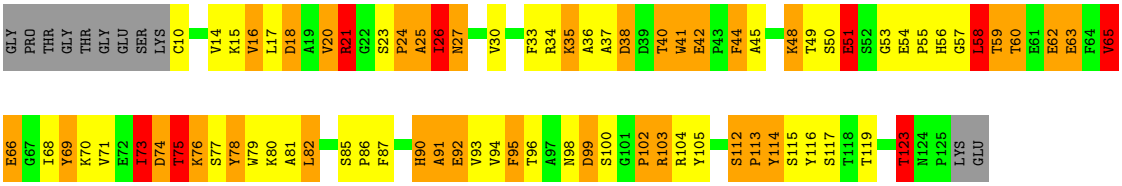
Chain A:



• Molecule 1: TRANSTHYRETIN

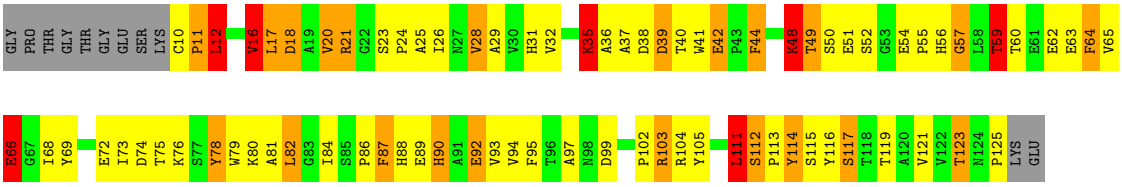
Chain B:





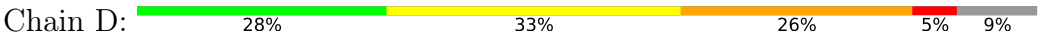
• Molecule 1: TRANSTHYRETIN

Chain C:



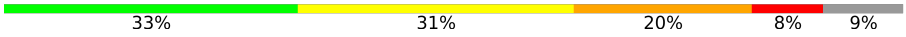
• Molecule 1: TRANSTHYRETIN

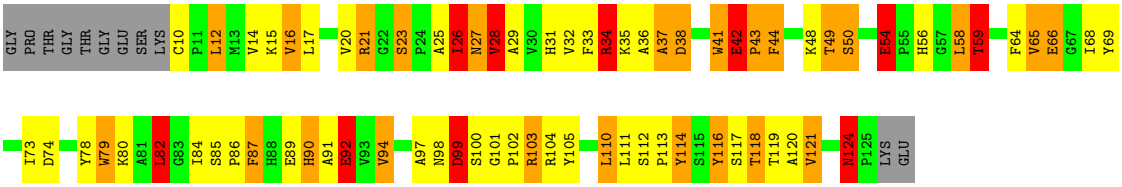
Chain D:



• Molecule 1: TRANSTHYRETIN

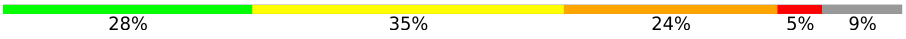
Chain E:

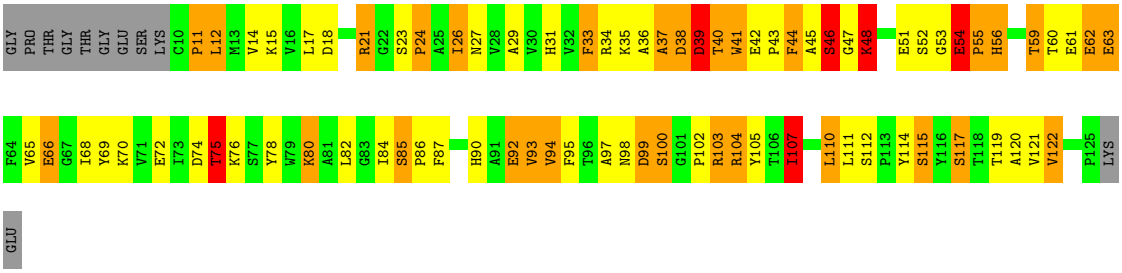




• Molecule 1: TRANSTHYRETIN

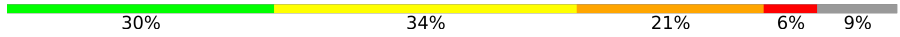
Chain F:

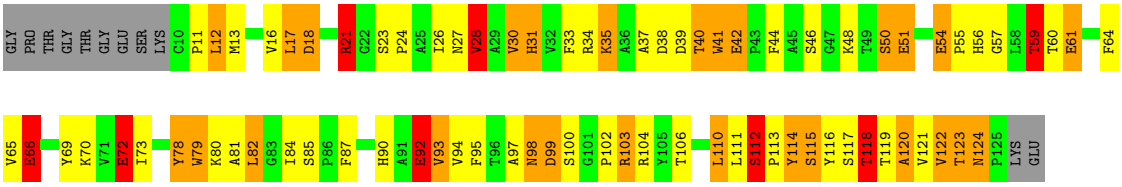




• Molecule 1: TRANSTHYRETIN

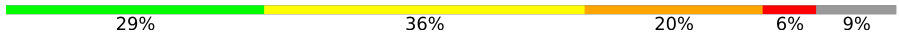
Chain G:

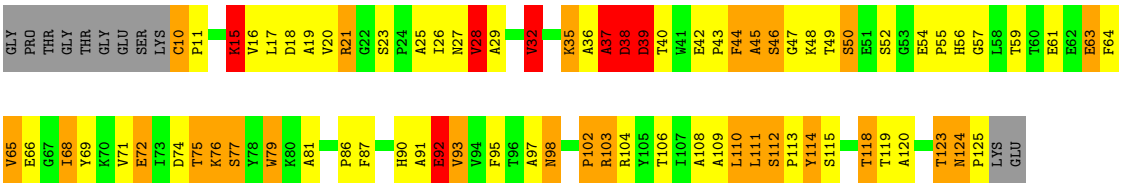




• Molecule 1: TRANSTHYRETIN

Chain H:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.99Å 78.74Å 98.95Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (8.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

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	1.10	0/920	3.12	70/1257 (5.6%)
1	B	1.16	1/914 (0.1%)	2.93	88/1249 (7.0%)
1	C	1.42	1/920 (0.1%)	2.77	87/1257 (6.9%)
1	D	1.07	0/916	3.04	82/1252 (6.5%)
1	E	1.11	1/920 (0.1%)	2.76	75/1257 (6.0%)
1	F	1.06	1/920 (0.1%)	2.87	80/1257 (6.4%)
1	G	1.06	2/916 (0.2%)	3.24	82/1252 (6.5%)
1	H	1.10	1/920 (0.1%)	2.73	80/1257 (6.4%)
All	All	1.14	7/7346 (0.1%)	2.94	644/10038 (6.4%)

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	C	1	0
1	E	0	1
1	G	0	1
All	All	1	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	PRO	CA-C	27.92	2.08	1.52
1	B	123	THR	C-N	15.14	1.68	1.34
1	G	124	ASN	C-N	11.03	1.55	1.34
1	E	92	GLU	CD-OE1	6.22	1.32	1.25
1	G	39	ASP	C-O	5.92	1.34	1.23
1	F	39	ASP	C-O	5.62	1.34	1.23
1	H	42	GLU	CD-OE2	5.50	1.31	1.25

All (644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	124	ASN	O-C-N	-50.10	25.90	121.10
1	A	21	ARG	CD-NE-CZ	40.18	179.85	123.60
1	D	103	ARG	NE-CZ-NH1	29.44	135.02	120.30
1	D	103	ARG	NE-CZ-NH2	-27.97	106.31	120.30
1	E	21	ARG	NE-CZ-NH2	-26.89	106.86	120.30
1	B	34	ARG	NE-CZ-NH1	25.59	133.09	120.30
1	D	21	ARG	NE-CZ-NH2	24.75	132.67	120.30
1	A	74	ASP	CB-CG-OD1	22.34	138.41	118.30
1	D	34	ARG	NE-CZ-NH2	-22.13	109.23	120.30
1	G	35	LYS	CG-CD-CE	21.91	177.63	111.90
1	A	18	ASP	CB-CG-OD1	21.50	137.65	118.30
1	F	103	ARG	NE-CZ-NH1	20.04	130.32	120.30
1	C	21	ARG	NE-CZ-NH1	-20.01	110.30	120.30
1	A	74	ASP	CB-CG-OD2	-20.00	100.30	118.30
1	B	21	ARG	NE-CZ-NH2	18.93	129.76	120.30
1	F	104	ARG	NE-CZ-NH1	18.63	129.62	120.30
1	E	74	ASP	CB-CG-OD1	18.55	135.00	118.30
1	F	21	ARG	NE-CZ-NH1	18.33	129.47	120.30
1	H	114	TYR	CB-CG-CD1	-18.31	110.01	121.00
1	C	54	GLU	CA-CB-CG	17.53	151.96	113.40
1	A	18	ASP	CB-CG-OD2	-16.86	103.12	118.30
1	G	104	ARG	NE-CZ-NH1	-16.62	111.99	120.30
1	B	18	ASP	CB-CG-OD2	-16.42	103.52	118.30
1	F	21	ARG	CD-NE-CZ	16.33	146.47	123.60
1	H	114	TYR	CB-CG-CD2	16.29	130.77	121.00
1	C	125	PRO	CA-C-O	-16.15	81.44	120.20
1	G	114	TYR	CB-CG-CD1	-15.28	111.83	121.00
1	B	21	ARG	NE-CZ-NH1	-15.17	112.72	120.30
1	A	21	ARG	CG-CD-NE	15.02	143.34	111.80
1	A	110	LEU	CA-CB-CG	14.94	149.67	115.30
1	G	78	TYR	CB-CG-CD2	-14.65	112.21	121.00
1	A	34	ARG	NE-CZ-NH2	-13.93	113.33	120.30
1	B	103	ARG	NE-CZ-NH2	13.70	127.15	120.30
1	E	34	ARG	NE-CZ-NH1	13.50	127.05	120.30
1	A	114	TYR	CB-CG-CD1	-13.44	112.94	121.00
1	A	105	TYR	CB-CG-CD2	13.34	129.01	121.00
1	G	114	TYR	CB-CG-CD2	13.26	128.95	121.00
1	H	27	ASN	CA-CB-CG	13.17	142.38	113.40
1	B	103	ARG	NE-CZ-NH1	-13.15	113.73	120.30
1	G	78	TYR	CB-CG-CD1	12.82	128.69	121.00
1	H	21	ARG	CD-NE-CZ	12.79	141.51	123.60
1	D	72	GLU	OE1-CD-OE2	12.71	138.55	123.30
1	F	34	ARG	NE-CZ-NH2	12.45	126.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	72	GLU	OE1-CD-OE2	12.45	138.24	123.30
1	D	18	ASP	CB-CG-OD2	-12.37	107.17	118.30
1	G	34	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	F	107	ILE	CB-CA-C	12.15	135.89	111.60
1	F	18	ASP	CB-CG-OD2	-12.12	107.40	118.30
1	B	34	ARG	NH1-CZ-NH2	-12.05	106.14	119.40
1	C	12	LEU	N-CA-CB	12.05	134.50	110.40
1	G	42	GLU	OE1-CD-OE2	-11.96	108.95	123.30
1	A	105	TYR	CB-CG-CD1	-11.95	113.83	121.00
1	G	18	ASP	CB-CG-OD1	11.76	128.89	118.30
1	H	103	ARG	CD-NE-CZ	11.74	140.03	123.60
1	D	89	GLU	OE1-CD-OE2	11.68	137.31	123.30
1	E	104	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	A	115	SER	CB-CA-C	-11.65	87.96	110.10
1	H	38	ASP	N-CA-CB	11.60	131.48	110.60
1	F	74	ASP	CB-CG-OD1	11.59	128.73	118.30
1	C	125	PRO	CB-CA-C	11.58	140.94	112.00
1	G	34	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	E	59	THR	N-CA-CB	11.47	132.10	110.30
1	B	114	TYR	CB-CG-CD2	11.38	127.83	121.00
1	G	42	GLU	CB-CG-CD	11.26	144.60	114.20
1	B	59	THR	N-CA-CB	11.10	131.38	110.30
1	F	54	GLU	OE1-CD-OE2	-11.05	110.05	123.30
1	F	103	ARG	CD-NE-CZ	11.03	139.04	123.60
1	D	21	ARG	NE-CZ-NH1	-11.00	114.80	120.30
1	H	21	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	G	104	ARG	NH1-CZ-NH2	10.86	131.34	119.40
1	H	38	ASP	CB-CG-OD2	10.78	128.01	118.30
1	C	62	GLU	OE1-CD-OE2	10.66	136.09	123.30
1	D	66	GLU	OE1-CD-OE2	10.62	136.04	123.30
1	E	74	ASP	CB-CG-OD2	-10.55	108.80	118.30
1	B	114	TYR	CB-CG-CD1	-10.54	114.68	121.00
1	B	42	GLU	OE1-CD-OE2	10.53	135.94	123.30
1	F	48	LYS	CA-CB-CG	10.45	136.39	113.40
1	D	114	TYR	CB-CG-CD2	10.45	127.27	121.00
1	G	66	GLU	CB-CG-CD	10.43	142.37	114.20
1	F	54	GLU	CB-CG-CD	10.42	142.33	114.20
1	E	92	GLU	CB-CG-CD	10.25	141.86	114.20
1	B	18	ASP	CB-CG-OD1	10.22	127.50	118.30
1	D	75	THR	N-CA-CB	-10.17	90.98	110.30
1	C	72	GLU	OE1-CD-OE2	9.99	135.29	123.30
1	F	99	ASP	N-CA-CB	-9.98	92.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	37	ALA	C-N-CA	-9.97	96.78	121.70
1	B	20	VAL	CA-CB-CG2	-9.94	95.98	110.90
1	F	18	ASP	CB-CG-OD1	9.91	127.22	118.30
1	G	72	GLU	OE1-CD-OE2	9.88	135.15	123.30
1	B	62	GLU	N-CA-CB	9.85	128.32	110.60
1	C	54	GLU	N-CA-CB	-9.76	93.04	110.60
1	H	61	GLU	OE1-CD-OE2	9.69	134.92	123.30
1	G	38	ASP	CB-CG-OD1	9.54	126.89	118.30
1	H	104	ARG	CD-NE-CZ	9.54	136.96	123.60
1	B	116	TYR	CB-CG-CD2	-9.54	115.28	121.00
1	C	59	THR	N-CA-CB	9.41	128.18	110.30
1	D	93	VAL	CA-CB-CG1	9.37	124.95	110.90
1	E	21	ARG	CD-NE-CZ	9.35	136.69	123.60
1	E	21	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	G	42	GLU	CG-CD-OE1	9.32	136.94	118.30
1	E	42	GLU	CA-CB-CG	9.32	133.90	113.40
1	G	103	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	B	99	ASP	CB-CG-OD1	-9.26	109.97	118.30
1	D	107	ILE	CA-CB-CG1	9.17	128.43	111.00
1	B	73	ILE	CA-CB-CG1	9.16	128.40	111.00
1	C	21	ARG	NH1-CZ-NH2	9.15	129.47	119.40
1	D	51	GLU	OE1-CD-OE2	-9.08	112.40	123.30
1	B	99	ASP	N-CA-CB	-9.04	94.32	110.60
1	D	76	LYS	CD-CE-NZ	8.90	132.17	111.70
1	B	99	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	A	114	TYR	CB-CG-CD2	8.86	126.32	121.00
1	H	110	LEU	CA-CB-CG	8.84	135.62	115.30
1	F	104	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	E	99	ASP	N-CA-CB	-8.79	94.77	110.60
1	E	110	LEU	CB-CA-C	-8.78	93.52	110.20
1	G	104	ARG	CB-CA-C	-8.77	92.86	110.40
1	F	44	PHE	CB-CG-CD2	8.74	126.92	120.80
1	C	117	SER	N-CA-CB	8.72	123.58	110.50
1	A	115	SER	N-CA-CB	8.71	123.56	110.50
1	E	54	GLU	N-CA-CB	-8.66	95.02	110.60
1	B	99	ASP	OD1-CG-OD2	8.65	139.74	123.30
1	G	87	PHE	CB-CG-CD1	-8.65	114.75	120.80
1	A	82	LEU	CA-CB-CG	8.59	135.06	115.30
1	F	115	SER	CA-CB-OG	-8.58	88.03	111.20
1	B	20	VAL	CA-CB-CG1	-8.57	98.05	110.90
1	E	54	GLU	OE1-CD-OE2	8.54	133.55	123.30
1	B	103	ARG	CD-NE-CZ	-8.53	111.66	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	119	THR	N-CA-CB	8.53	126.50	110.30
1	C	28	VAL	CB-CA-C	8.51	127.57	111.40
1	E	92	GLU	OE1-CD-OE2	-8.50	113.10	123.30
1	C	41	TRP	N-CA-CB	8.49	125.88	110.60
1	F	47	GLY	O-C-N	8.46	136.23	122.70
1	D	34	ARG	NH1-CZ-NH2	8.45	128.70	119.40
1	D	75	THR	CA-CB-OG1	-8.41	91.35	109.00
1	D	33	PHE	CB-CA-C	-8.38	93.64	110.40
1	C	116	TYR	CA-CB-CG	8.33	129.23	113.40
1	H	45	ALA	N-CA-CB	8.33	121.76	110.10
1	C	35	LYS	N-CA-CB	8.32	125.57	110.60
1	D	116	TYR	CA-CB-CG	8.23	129.04	113.40
1	G	87	PHE	CB-CG-CD2	8.22	126.56	120.80
1	D	119	THR	CA-CB-CG2	-8.19	100.94	112.40
1	D	35	LYS	CD-CE-NZ	8.16	130.48	111.70
1	H	79	TRP	CB-CG-CD2	8.16	137.20	126.60
1	G	30	VAL	CA-CB-CG1	-8.15	98.67	110.90
1	G	21	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	G	59	THR	C-N-CA	8.12	142.01	121.70
1	D	80	LYS	CA-C-N	8.11	135.05	117.20
1	F	21	ARG	CA-CB-CG	8.09	131.19	113.40
1	C	18	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	H	93	VAL	CA-CB-CG2	-8.06	98.81	110.90
1	G	21	ARG	CD-NE-CZ	8.04	134.86	123.60
1	A	34	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	A	66	GLU	OE1-CD-OE2	8.03	132.94	123.30
1	E	21	ARG	NH1-CZ-NH2	7.98	128.17	119.40
1	B	54	GLU	CA-CB-CG	7.96	130.91	113.40
1	B	20	VAL	CG1-CB-CG2	-7.95	98.18	110.90
1	A	38	ASP	CB-CG-OD2	7.90	125.41	118.30
1	E	23	SER	CB-CA-C	-7.89	95.11	110.10
1	A	116	TYR	CA-CB-CG	7.89	128.39	113.40
1	H	46	SER	CB-CA-C	-7.87	95.15	110.10
1	A	109	ALA	N-CA-CB	7.83	121.06	110.10
1	A	55	PRO	CA-C-N	7.78	134.32	117.20
1	G	112	SER	N-CA-CB	7.77	122.15	110.50
1	G	80	LYS	CD-CE-NZ	7.76	129.55	111.70
1	A	59	THR	N-CA-CB	7.76	125.04	110.30
1	E	87	PHE	CB-CG-CD1	7.73	126.21	120.80
1	F	26	ILE	CB-CG1-CD1	7.73	135.55	113.90
1	G	81	ALA	N-CA-CB	-7.73	99.28	110.10
1	A	21	ARG	NE-CZ-NH1	7.73	124.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	79	TRP	CA-CB-CG	-7.68	99.10	113.70
1	C	56	HIS	CA-CB-CG	-7.67	100.57	113.60
1	E	119	THR	CA-CB-CG2	7.65	123.11	112.40
1	A	98	ASN	N-CA-CB	-7.64	96.85	110.60
1	A	37	ALA	CB-CA-C	7.63	121.55	110.10
1	F	53	GLY	CA-C-O	-7.62	106.88	120.60
1	A	118	THR	CA-CB-OG1	-7.62	93.00	109.00
1	F	48	LYS	CB-CA-C	7.61	125.63	110.40
1	E	44	PHE	N-CA-CB	-7.61	96.91	110.60
1	F	44	PHE	CB-CG-CD1	-7.58	115.49	120.80
1	C	116	TYR	CB-CG-CD2	7.58	125.55	121.00
1	D	109	ALA	CB-CA-C	7.55	121.43	110.10
1	G	18	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	D	75	THR	OG1-CB-CG2	7.53	127.33	110.00
1	E	90	HIS	CA-CB-CG	-7.53	100.80	113.60
1	G	50	SER	CB-CA-C	-7.52	95.81	110.10
1	D	52	SER	N-CA-CB	7.50	121.75	110.50
1	F	33	PHE	CB-CA-C	-7.48	95.44	110.40
1	C	64	PHE	CB-CG-CD2	7.48	126.03	120.80
1	E	44	PHE	CB-CA-C	7.47	125.34	110.40
1	H	63	GLU	OE1-CD-OE2	7.46	132.25	123.30
1	F	117	SER	CB-CA-C	-7.45	95.94	110.10
1	H	112	SER	N-CA-CB	7.44	121.67	110.50
1	B	66	GLU	OE1-CD-OE2	-7.44	114.38	123.30
1	E	65	VAL	CA-CB-CG1	-7.43	99.75	110.90
1	D	72	GLU	CG-CD-OE1	-7.42	103.45	118.30
1	A	69	TYR	CB-CG-CD2	7.42	125.45	121.00
1	C	84	ILE	CA-CB-CG1	7.39	125.04	111.00
1	D	63	GLU	OE1-CD-OE2	7.39	132.16	123.30
1	B	100	SER	N-CA-CB	-7.37	99.45	110.50
1	C	21	ARG	CD-NE-CZ	-7.34	113.33	123.60
1	C	82	LEU	CB-CA-C	-7.34	96.26	110.20
1	C	103	ARG	N-CA-CB	-7.33	97.41	110.60
1	H	106	THR	CA-CB-CG2	-7.33	102.14	112.40
1	H	47	GLY	O-C-N	7.32	134.42	122.70
1	E	29	ALA	N-CA-CB	-7.32	99.86	110.10
1	G	104	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	F	115	SER	CB-CA-C	-7.30	96.23	110.10
1	H	79	TRP	CB-CG-CD1	-7.30	117.51	127.00
1	F	63	GLU	N-CA-CB	-7.29	97.47	110.60
1	D	74	ASP	CB-CG-OD1	7.29	124.86	118.30
1	G	92	GLU	OE1-CD-OE2	7.26	132.02	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	39	ASP	O-C-N	-7.26	111.08	122.70
1	B	21	ARG	CD-NE-CZ	-7.19	113.53	123.60
1	C	42	GLU	OE1-CD-OE2	7.19	131.93	123.30
1	B	78	TYR	CG-CD1-CE1	-7.17	115.56	121.30
1	B	116	TYR	CA-CB-CG	7.17	127.01	113.40
1	D	63	GLU	CB-CG-CD	-7.16	94.88	114.20
1	E	48	LYS	CA-C-N	7.16	132.95	117.20
1	C	28	VAL	CA-CB-CG2	7.15	121.63	110.90
1	E	34	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	G	124	ASN	C-N-CD	7.12	143.36	128.40
1	C	90	HIS	N-CA-CB	7.12	123.42	110.60
1	G	120	ALA	N-CA-CB	7.09	120.02	110.10
1	D	94	VAL	CA-CB-CG2	-7.08	100.28	110.90
1	E	10	CYS	CB-CA-C	7.08	124.56	110.40
1	E	68	ILE	CB-CA-C	-7.07	97.46	111.60
1	H	124	ASN	N-CA-CB	7.06	123.31	110.60
1	D	25	ALA	N-CA-CB	7.05	119.97	110.10
1	A	86	PRO	O-C-N	-7.05	111.42	122.70
1	E	80	LYS	CA-CB-CG	-7.04	97.91	113.40
1	A	80	LYS	O-C-N	-7.04	111.44	122.70
1	D	114	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	F	119	THR	CA-CB-OG1	-7.03	94.25	109.00
1	F	122	VAL	CA-CB-CG1	-7.02	100.36	110.90
1	A	103	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	116	TYR	CB-CG-CD1	7.01	125.21	121.00
1	B	65	VAL	N-CA-CB	6.99	126.87	111.50
1	A	72	GLU	OE1-CD-OE2	6.98	131.68	123.30
1	C	78	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	H	48	LYS	CA-CB-CG	-6.98	98.05	113.40
1	H	63	GLU	CG-CD-OE2	-6.98	104.35	118.30
1	F	34	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	H	92	GLU	OE1-CD-OE2	6.95	131.64	123.30
1	F	45	ALA	N-CA-CB	6.95	119.83	110.10
1	C	48	LYS	CA-CB-CG	6.94	128.67	113.40
1	A	21	ARG	CB-CA-C	6.94	124.28	110.40
1	D	51	GLU	CA-CB-CG	6.94	128.66	113.40
1	F	54	GLU	CG-CD-OE1	6.93	132.16	118.30
1	B	112	SER	N-CA-CB	6.92	120.89	110.50
1	H	61	GLU	CB-CG-CD	-6.92	95.52	114.20
1	E	121	VAL	N-CA-CB	6.91	126.71	111.50
1	H	29	ALA	CB-CA-C	-6.88	99.78	110.10
1	B	62	GLU	OE1-CD-OE2	6.87	131.55	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	23	SER	CA-C-O	-6.87	105.67	120.10
1	D	79	TRP	CA-CB-CG	-6.87	100.65	113.70
1	D	16	VAL	CA-CB-CG2	-6.85	100.62	110.90
1	F	12	LEU	N-CA-CB	6.85	124.10	110.40
1	H	52	SER	CB-CA-C	-6.82	97.14	110.10
1	G	124	ASN	CA-C-O	-6.82	105.78	120.10
1	G	117	SER	CB-CA-C	-6.81	97.16	110.10
1	B	26	ILE	CB-CA-C	6.80	125.20	111.60
1	D	80	LYS	O-C-N	-6.80	111.82	122.70
1	B	60	THR	CA-CB-CG2	-6.79	102.89	112.40
1	C	89	GLU	OE1-CD-OE2	6.79	131.45	123.30
1	G	118	THR	N-CA-CB	6.78	123.18	110.30
1	D	59	THR	N-CA-CB	6.75	123.12	110.30
1	E	92	GLU	CG-CD-OE1	6.73	131.75	118.30
1	F	103	ARG	NH1-CZ-NH2	-6.72	112.00	119.40
1	F	42	GLU	OE1-CD-OE2	6.72	131.36	123.30
1	E	116	TYR	CA-CB-CG	6.71	126.15	113.40
1	C	52	SER	N-CA-CB	-6.71	100.44	110.50
1	F	111	LEU	N-CA-CB	-6.71	96.99	110.40
1	E	118	THR	N-CA-CB	6.70	123.03	110.30
1	B	60	THR	O-C-N	6.69	133.41	122.70
1	C	84	ILE	O-C-N	-6.68	112.01	122.70
1	D	46	SER	CB-CA-C	-6.67	97.42	110.10
1	H	104	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	F	112	SER	N-CA-CB	6.67	120.50	110.50
1	B	76	LYS	CD-CE-NZ	6.66	127.01	111.70
1	D	54	GLU	N-CA-CB	-6.63	98.66	110.60
1	C	81	ALA	O-C-N	-6.63	112.09	122.70
1	B	62	GLU	CB-CG-CD	-6.62	96.32	114.20
1	C	80	LYS	O-C-N	-6.62	112.11	122.70
1	A	51	GLU	CA-CB-CG	6.62	127.95	113.40
1	H	98	ASN	N-CA-CB	-6.60	98.71	110.60
1	B	79	TRP	CA-CB-CG	-6.58	101.19	113.70
1	B	117	SER	CB-CA-C	-6.58	97.60	110.10
1	E	79	TRP	O-C-N	6.57	133.21	122.70
1	G	17	LEU	CB-CG-CD1	-6.57	99.84	111.00
1	F	14	VAL	CA-C-O	-6.54	106.36	120.10
1	B	38	ASP	N-CA-CB	-6.54	98.83	110.60
1	F	59	THR	CA-CB-CG2	-6.53	103.26	112.40
1	D	80	LYS	CB-CA-C	6.52	123.43	110.40
1	A	63	GLU	OE1-CD-OE2	-6.51	115.49	123.30
1	H	81	ALA	CB-CA-C	-6.51	100.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	31	HIS	CB-CA-C	-6.50	97.39	110.40
1	B	79	TRP	N-CA-CB	6.50	122.30	110.60
1	H	38	ASP	CA-CB-CG	-6.50	99.10	113.40
1	B	102	PRO	N-CA-CB	6.49	111.09	103.30
1	B	78	TYR	CD1-CE1-CZ	6.49	125.64	119.80
1	G	110	LEU	CB-CG-CD1	6.49	122.03	111.00
1	A	17	LEU	CB-CG-CD2	-6.47	100.00	111.00
1	C	39	ASP	CA-C-N	6.47	131.44	117.20
1	H	91	ALA	CB-CA-C	6.47	119.80	110.10
1	E	42	GLU	OE1-CD-OE2	-6.46	115.55	123.30
1	G	92	GLU	N-CA-CB	-6.46	98.98	110.60
1	H	118	THR	CA-CB-CG2	6.45	121.42	112.40
1	G	66	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	C	20	VAL	CG1-CB-CG2	-6.42	100.62	110.90
1	G	61	GLU	N-CA-CB	-6.42	99.04	110.60
1	C	57	GLY	N-CA-C	6.41	129.13	113.10
1	C	55	PRO	CA-C-N	6.39	131.25	117.20
1	A	92	GLU	OE1-CD-OE2	6.38	130.96	123.30
1	C	12	LEU	CB-CG-CD2	-6.38	100.15	111.00
1	E	65	VAL	CG1-CB-CG2	6.38	121.11	110.90
1	F	98	ASN	N-CA-CB	-6.38	99.12	110.60
1	C	49	THR	C-N-CA	6.37	137.63	121.70
1	G	21	ARG	CB-CA-C	-6.37	97.66	110.40
1	H	68	ILE	CB-CG1-CD1	-6.37	96.06	113.90
1	B	81	ALA	CB-CA-C	-6.37	100.55	110.10
1	C	69	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	B	91	ALA	CB-CA-C	-6.36	100.56	110.10
1	D	81	ALA	CB-CA-C	-6.36	100.56	110.10
1	C	51	GLU	CA-CB-CG	6.35	127.36	113.40
1	C	12	LEU	O-C-N	6.34	132.85	122.70
1	C	21	ARG	CB-CG-CD	-6.34	95.10	111.60
1	E	15	LYS	CB-CA-C	6.34	123.07	110.40
1	D	34	ARG	CD-NE-CZ	6.33	132.46	123.60
1	G	61	GLU	OE1-CD-OE2	6.31	130.88	123.30
1	G	98	ASN	N-CA-CB	-6.31	99.24	110.60
1	C	59	THR	CB-CA-C	-6.31	94.57	111.60
1	E	79	TRP	N-CA-CB	6.29	121.93	110.60
1	B	96	THR	N-CA-CB	6.29	122.25	110.30
1	A	115	SER	CA-CB-OG	-6.28	94.25	111.20
1	D	21	ARG	NH1-CZ-NH2	-6.28	112.50	119.40
1	C	29	ALA	CB-CA-C	-6.27	100.69	110.10
1	F	24	PRO	CA-C-N	6.27	131.00	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	95	PHE	CB-CG-CD2	6.27	125.19	120.80
1	E	104	ARG	CA-CB-CG	-6.25	99.64	113.40
1	C	92	GLU	CA-CB-CG	6.25	127.16	113.40
1	D	117	SER	CB-CA-C	-6.25	98.22	110.10
1	A	98	ASN	CA-CB-CG	-6.25	99.66	113.40
1	H	18	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	E	26	ILE	CB-CG1-CD1	6.21	131.30	113.90
1	F	55	PRO	N-CA-CB	6.20	110.74	103.30
1	C	66	GLU	CG-CD-OE2	6.20	130.69	118.30
1	A	24	PRO	N-CD-CG	-6.19	93.91	103.20
1	G	124	ASN	C-N-CA	-6.19	96.00	122.00
1	H	56	HIS	CA-CB-CG	-6.18	103.10	113.60
1	H	57	GLY	N-CA-C	6.17	128.53	113.10
1	B	10	CYS	CA-CB-SG	6.17	125.10	114.00
1	C	90	HIS	CA-CB-CG	-6.14	103.16	113.60
1	A	21	ARG	CA-CB-CG	6.14	126.90	113.40
1	A	38	ASP	N-CA-CB	-6.14	99.55	110.60
1	E	16	VAL	CA-CB-CG2	-6.13	101.70	110.90
1	E	28	VAL	CB-CA-C	6.13	123.05	111.40
1	G	12	LEU	CB-CA-C	-6.12	98.56	110.20
1	G	87	PHE	CZ-CE2-CD2	-6.12	112.76	120.10
1	F	74	ASP	N-CA-CB	6.12	121.61	110.60
1	B	78	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	D	69	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	F	75	THR	N-CA-CB	-6.09	98.73	110.30
1	A	46	SER	CB-CA-C	-6.09	98.53	110.10
1	H	56	HIS	CA-C-N	6.08	128.37	116.20
1	F	21	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
1	G	28	VAL	CB-CA-C	6.07	122.93	111.40
1	E	23	SER	O-C-N	6.06	132.62	121.10
1	E	23	SER	N-CA-CB	-6.06	101.42	110.50
1	A	83	GLY	O-C-N	-6.05	113.01	122.70
1	E	82	LEU	N-CA-CB	6.05	122.50	110.40
1	D	122	VAL	CB-CA-C	6.05	122.89	111.40
1	B	45	ALA	N-CA-CB	6.03	118.54	110.10
1	B	24	PRO	N-CA-CB	6.03	110.53	103.30
1	A	117	SER	CB-CA-C	-6.03	98.65	110.10
1	H	76	LYS	CD-CE-NZ	6.02	125.55	111.70
1	F	66	GLU	OE1-CD-OE2	6.02	130.52	123.30
1	B	25	ALA	CB-CA-C	6.01	119.11	110.10
1	C	74	ASP	CB-CA-C	-6.01	98.39	110.40
1	B	21	ARG	CA-C-N	6.00	128.21	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	104	ARG	CD-NE-CZ	6.00	132.00	123.60
1	D	108	ALA	O-C-N	-6.00	113.10	122.70
1	C	88	HIS	CG-ND1-CE1	5.99	116.59	108.20
1	H	108	ALA	CA-C-N	5.99	130.37	117.20
1	B	33	PHE	CB-CA-C	-5.98	98.44	110.40
1	D	98	ASN	CB-CG-OD1	-5.98	109.65	121.60
1	B	38	ASP	CA-CB-CG	5.97	126.55	113.40
1	H	123	THR	N-CA-CB	-5.97	98.95	110.30
1	F	99	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	F	48	LYS	CB-CG-CD	5.95	127.08	111.60
1	H	40	THR	N-CA-CB	-5.95	99.00	110.30
1	A	55	PRO	CA-C-O	-5.94	105.94	120.20
1	C	25	ALA	N-CA-CB	5.94	118.42	110.10
1	A	111	LEU	N-CA-CB	-5.93	98.53	110.40
1	H	92	GLU	CG-CD-OE1	-5.93	106.44	118.30
1	B	62	GLU	CG-CD-OE1	-5.93	106.44	118.30
1	C	54	GLU	CB-CA-C	5.93	122.25	110.40
1	B	56	HIS	CA-C-O	5.92	132.53	120.10
1	E	99	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	D	117	SER	CA-C-O	-5.91	107.68	120.10
1	E	41	TRP	N-CA-CB	-5.91	99.97	110.60
1	C	17	LEU	CB-CG-CD1	-5.90	100.96	111.00
1	D	103	ARG	CA-CB-CG	-5.90	100.42	113.40
1	D	111	LEU	CA-CB-CG	5.90	128.87	115.30
1	F	107	ILE	CA-CB-CG2	5.89	122.68	110.90
1	D	70	LYS	CB-CG-CD	-5.89	96.29	111.60
1	G	111	LEU	N-CA-C	5.89	126.90	111.00
1	F	62	GLU	OE1-CD-OE2	-5.88	116.25	123.30
1	A	80	LYS	CB-CA-C	5.87	122.14	110.40
1	C	113	PRO	O-C-N	-5.87	113.31	122.70
1	D	76	LYS	CG-CD-CE	5.87	129.50	111.90
1	A	48	LYS	CA-C-O	5.87	132.42	120.10
1	G	18	ASP	CB-CA-C	5.87	122.14	110.40
1	G	80	LYS	O-C-N	-5.87	113.31	122.70
1	A	34	ARG	CD-NE-CZ	-5.86	115.39	123.60
1	B	17	LEU	CA-CB-CG	5.85	128.75	115.30
1	C	65	VAL	CA-CB-CG2	5.85	119.67	110.90
1	E	118	THR	CA-CB-CG2	-5.84	104.22	112.40
1	F	12	LEU	CB-CA-C	-5.84	99.10	110.20
1	G	123	THR	CB-CA-C	5.83	127.33	111.60
1	H	20	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	B	40	THR	CB-CA-C	-5.82	95.90	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	110	LEU	CA-C-N	5.81	129.99	117.20
1	B	42	GLU	CB-CA-C	-5.80	98.79	110.40
1	G	94	VAL	O-C-N	-5.79	113.44	122.70
1	D	37	ALA	N-CA-CB	-5.79	102.00	110.10
1	B	63	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	C	16	VAL	CB-CA-C	5.78	122.38	111.40
1	H	75	THR	N-CA-CB	-5.77	99.33	110.30
1	D	27	ASN	OD1-CG-ND2	5.77	135.18	121.90
1	C	112	SER	N-CA-CB	5.77	119.15	110.50
1	B	44	PHE	CB-CA-C	5.76	121.92	110.40
1	D	112	SER	CA-CB-OG	-5.76	95.65	111.20
1	D	107	ILE	CA-CB-CG2	-5.75	99.39	110.90
1	D	110	LEU	CB-CA-C	5.75	121.12	110.20
1	F	65	VAL	CA-CB-CG1	-5.75	102.28	110.90
1	B	35	LYS	N-CA-CB	5.74	120.94	110.60
1	H	77	SER	CB-CA-C	5.74	121.00	110.10
1	A	125	PRO	N-CA-CB	5.73	110.18	103.30
1	A	33	PHE	CB-CA-C	-5.73	98.94	110.40
1	C	93	VAL	CA-C-O	-5.72	108.08	120.10
1	B	41	TRP	N-CA-CB	-5.72	100.30	110.60
1	D	94	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	B	69	TYR	CB-CG-CD1	5.71	124.42	121.00
1	D	74	ASP	CB-CA-C	-5.71	98.99	110.40
1	E	114	TYR	CA-CB-CG	-5.71	102.56	113.40
1	E	49	THR	O-C-N	-5.70	113.58	122.70
1	B	58	LEU	CB-CA-C	5.69	121.02	110.20
1	D	41	TRP	CE3-CZ3-CH2	5.69	127.46	121.20
1	F	11	PRO	N-CA-CB	5.68	110.12	103.30
1	F	41	TRP	CA-CB-CG	-5.68	102.90	113.70
1	H	20	VAL	CA-CB-CG2	5.68	119.43	110.90
1	C	121	VAL	CA-CB-CG1	5.68	119.42	110.90
1	A	59	THR	CB-CA-C	-5.67	96.28	111.60
1	E	104	ARG	CD-NE-CZ	5.67	131.54	123.60
1	G	123	THR	C-N-CA	5.66	135.84	121.70
1	C	31	HIS	CA-CB-CG	-5.65	103.99	113.60
1	B	33	PHE	N-CA-CB	5.65	120.77	110.60
1	D	61	GLU	CA-CB-CG	5.65	125.83	113.40
1	C	103	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	D	123	THR	N-CA-CB	-5.65	99.57	110.30
1	H	64	PHE	O-C-N	-5.65	113.67	122.70
1	E	103	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	61	GLU	CG-CD-OE1	5.64	129.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	10	CYS	CA-CB-SG	-5.64	103.84	114.00
1	A	103	ARG	CD-NE-CZ	5.64	131.50	123.60
1	B	69	TYR	O-C-N	5.64	131.73	122.70
1	F	114	TYR	CG-CD1-CE1	-5.64	116.79	121.30
1	D	103	ARG	CD-NE-CZ	5.63	131.48	123.60
1	H	15	LYS	CA-C-O	-5.62	108.29	120.10
1	G	54	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	C	44	PHE	CA-CB-CG	5.61	127.35	113.90
1	G	13	MET	CB-CG-SD	5.60	129.21	112.40
1	D	33	PHE	CA-C-O	-5.60	108.34	120.10
1	G	122	VAL	CA-CB-CG1	-5.60	102.50	110.90
1	E	34	ARG	CG-CD-NE	-5.60	100.04	111.80
1	E	49	THR	N-CA-CB	-5.59	99.69	110.30
1	D	73	ILE	CA-CB-CG1	5.57	121.58	111.00
1	B	114	TYR	CA-CB-CG	-5.56	102.83	113.40
1	A	121	VAL	CA-CB-CG2	5.56	119.24	110.90
1	C	49	THR	CA-CB-CG2	-5.56	104.62	112.40
1	A	13	MET	CA-CB-CG	-5.56	103.85	113.30
1	C	65	VAL	CA-CB-CG1	-5.55	102.57	110.90
1	B	113	PRO	CA-N-CD	5.55	119.47	111.70
1	G	123	THR	CA-C-N	-5.55	104.99	117.20
1	C	102	PRO	N-CA-CB	5.55	109.96	103.30
1	G	99	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	97	ALA	O-C-N	5.53	131.55	122.70
1	H	69	TYR	CA-CB-CG	5.53	123.91	113.40
1	D	63	GLU	CG-CD-OE2	-5.53	107.24	118.30
1	G	38	ASP	CA-C-N	5.52	129.35	117.20
1	A	78	TYR	CG-CD1-CE1	-5.52	116.88	121.30
1	H	69	TYR	CB-CA-C	5.51	121.42	110.40
1	D	41	TRP	CB-CG-CD2	5.50	133.75	126.60
1	C	20	VAL	CA-CB-CG2	5.49	119.14	110.90
1	H	115	SER	N-CA-CB	-5.49	102.26	110.50
1	H	28	VAL	CB-CA-C	5.49	121.83	111.40
1	E	99	ASP	CB-CA-C	-5.49	99.43	110.40
1	C	84	ILE	CG1-CB-CG2	-5.48	99.34	111.40
1	E	105	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	H	43	PRO	N-CA-CB	5.47	109.87	103.30
1	D	33	PHE	CA-CB-CG	-5.47	100.78	113.90
1	C	62	GLU	CG-CD-OE2	-5.46	107.38	118.30
1	E	79	TRP	CA-C-O	-5.46	108.63	120.10
1	H	75	THR	CA-CB-OG1	-5.46	97.54	109.00
1	G	35	LYS	N-CA-CB	5.45	120.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	69	TYR	CB-CG-CD2	5.44	124.27	121.00
1	H	68	ILE	N-CA-CB	5.44	123.32	110.80
1	C	87	PHE	CB-CG-CD1	5.44	124.61	120.80
1	B	95	PHE	O-C-N	-5.43	114.01	122.70
1	D	56	HIS	C-N-CA	5.43	133.71	122.30
1	D	13	MET	CA-CB-CG	-5.43	104.07	113.30
1	G	69	TYR	CA-CB-CG	-5.42	103.10	113.40
1	C	116	TYR	CB-CA-C	-5.42	99.56	110.40
1	F	119	THR	CA-CB-CG2	5.41	119.98	112.40
1	H	102	PRO	CA-C-O	5.40	133.17	120.20
1	H	108	ALA	CA-C-O	-5.40	108.76	120.10
1	F	46	SER	C-N-CA	-5.40	110.97	122.30
1	E	124	ASN	N-CA-CB	5.40	120.31	110.60
1	F	121	VAL	N-CA-C	-5.39	96.44	111.00
1	H	72	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	E	69	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	D	107	ILE	CB-CG1-CD1	-5.38	98.83	113.90
1	C	111	LEU	CB-CG-CD2	5.38	120.14	111.00
1	G	79	TRP	CA-C-O	-5.38	108.81	120.10
1	G	106	THR	CA-CB-CG2	5.37	119.92	112.40
1	C	32	VAL	CG1-CB-CG2	5.35	119.46	110.90
1	F	68	ILE	CG1-CB-CG2	-5.35	99.63	111.40
1	H	20	VAL	O-C-N	-5.34	114.15	122.70
1	F	97	ALA	CB-CA-C	-5.34	102.09	110.10
1	C	35	LYS	CD-CE-NZ	5.34	123.97	111.70
1	H	21	ARG	CB-CA-C	-5.34	99.73	110.40
1	C	52	SER	O-C-N	-5.33	114.13	123.20
1	A	11	PRO	N-CA-CB	5.33	109.69	103.30
1	C	11	PRO	N-CA-CB	5.33	109.69	103.30
1	F	42	GLU	CB-CG-CD	-5.33	99.81	114.20
1	H	23	SER	CB-CA-C	-5.33	99.98	110.10
1	H	102	PRO	O-C-N	-5.33	114.17	122.70
1	B	87	PHE	N-CA-CB	-5.33	101.01	110.60
1	E	50	SER	O-C-N	-5.33	114.18	122.70
1	G	34	ARG	CB-CG-CD	5.33	125.45	111.60
1	G	104	ARG	CG-CD-NE	-5.32	100.62	111.80
1	H	119	THR	CA-CB-OG1	-5.32	97.84	109.00
1	E	16	VAL	CA-C-O	-5.31	108.94	120.10
1	H	39	ASP	O-C-N	-5.31	114.21	122.70
1	D	65	VAL	O-C-N	-5.30	114.21	122.70
1	E	59	THR	CB-CA-C	-5.30	97.29	111.60
1	F	122	VAL	N-CA-CB	-5.30	99.84	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	44	PHE	CA-C-N	5.29	128.85	117.20
1	C	31	HIS	CA-C-O	-5.29	109.00	120.10
1	E	94	VAL	CA-CB-CG2	5.28	118.82	110.90
1	C	69	TYR	CG-CD2-CE2	-5.27	117.08	121.30
1	G	79	TRP	CB-CA-C	-5.27	99.85	110.40
1	C	94	VAL	CA-CB-CG2	-5.27	103.00	110.90
1	E	118	THR	CB-CA-C	-5.27	97.37	111.60
1	G	93	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	E	34	ARG	CB-CA-C	5.26	120.92	110.40
1	G	16	VAL	CA-CB-CG1	-5.26	103.01	110.90
1	E	48	LYS	CA-C-O	-5.25	109.06	120.10
1	F	103	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	H	40	THR	CA-CB-OG1	-5.25	97.97	109.00
1	C	55	PRO	CA-C-O	-5.24	107.61	120.20
1	G	42	GLU	CA-CB-CG	5.24	124.93	113.40
1	H	65	VAL	CA-CB-CG2	5.24	118.77	110.90
1	H	21	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	124	ASN	CB-CG-OD1	-5.24	111.12	121.60
1	H	56	HIS	N-CA-CB	-5.24	101.17	110.60
1	F	48	LYS	N-CA-C	-5.23	96.87	111.00
1	H	103	ARG	CG-CD-NE	-5.23	100.81	111.80
1	C	119	THR	CA-CB-CG2	5.23	119.72	112.40
1	D	27	ASN	CB-CG-ND2	-5.23	104.15	116.70
1	E	43	PRO	N-CA-CB	5.22	109.56	103.30
1	C	103	ARG	CA-C-O	-5.22	109.14	120.10
1	B	69	TYR	CA-C-O	-5.21	109.15	120.10
1	E	15	LYS	CA-CB-CG	-5.20	101.95	113.40
1	F	62	GLU	CG-CD-OE2	5.20	128.71	118.30
1	B	15	LYS	N-CA-CB	-5.20	101.25	110.60
1	B	90	HIS	CG-ND1-CE1	5.20	115.47	108.20
1	H	103	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	H	109	ALA	CA-C-N	5.19	128.62	117.20
1	A	13	MET	CA-C-O	-5.19	109.20	120.10
1	B	99	ASP	CB-CA-C	-5.19	100.03	110.40
1	H	40	THR	OG1-CB-CG2	5.18	121.92	110.00
1	F	48	LYS	O-C-N	-5.18	114.41	122.70
1	C	114	TYR	CA-CB-CG	-5.18	103.56	113.40
1	F	80	LYS	CD-CE-NZ	5.18	123.61	111.70
1	C	38	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	21	ARG	CD-NE-CZ	-5.17	116.36	123.60
1	B	78	TYR	CA-C-N	5.16	128.56	117.20
1	G	41	TRP	N-CA-CB	5.16	119.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	70	LYS	CA-CB-CG	-5.16	102.06	113.40
1	G	121	VAL	CA-CB-CG1	-5.16	103.17	110.90
1	E	27	ASN	CA-CB-CG	-5.15	102.07	113.40
1	H	120	ALA	CB-CA-C	5.15	117.83	110.10
1	G	21	ARG	CB-CG-CD	5.14	124.97	111.60
1	A	54	GLU	CA-C-O	-5.14	109.30	120.10
1	F	94	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	F	39	ASP	CA-C-N	5.14	128.51	117.20
1	A	90	HIS	CG-ND1-CE1	5.13	115.39	108.20
1	B	38	ASP	CB-CA-C	-5.13	100.14	110.40
1	D	39	ASP	CA-C-N	5.13	128.49	117.20
1	A	79	TRP	CD1-CG-CD2	5.13	110.40	106.30
1	A	103	ARG	N-CA-CB	-5.13	101.37	110.60
1	A	30	VAL	CB-CA-C	-5.12	101.66	111.40
1	D	108	ALA	CA-C-N	5.12	128.46	117.20
1	F	39	ASP	CA-C-O	-5.12	109.36	120.10
1	H	104	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	77	SER	CA-CB-OG	-5.11	97.39	111.20
1	D	36	ALA	CB-CA-C	-5.11	102.43	110.10
1	B	34	ARG	CB-CA-C	5.11	120.61	110.40
1	B	55	PRO	N-CA-CB	5.11	109.43	103.30
1	E	102	PRO	CB-CA-C	-5.10	99.24	112.00
1	B	75	THR	N-CA-CB	-5.10	100.61	110.30
1	B	93	VAL	CG1-CB-CG2	5.10	119.06	110.90
1	F	41	TRP	CB-CA-C	-5.10	100.20	110.40
1	B	21	ARG	N-CA-CB	5.09	119.77	110.60
1	F	42	GLU	CG-CD-OE1	-5.09	108.11	118.30
1	G	69	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	H	32	VAL	CB-CA-C	5.09	121.08	111.40
1	B	82	LEU	CA-CB-CG	5.09	127.01	115.30
1	H	44	PHE	CA-C-N	5.08	128.38	117.20
1	B	74	ASP	N-CA-CB	5.08	119.74	110.60
1	A	12	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	70	LYS	CD-CE-NZ	5.08	123.37	111.70
1	G	119	THR	CA-C-O	-5.07	109.46	120.10
1	F	59	THR	OG1-CB-CG2	5.07	121.65	110.00
1	F	66	GLU	N-CA-CB	-5.06	101.48	110.60
1	A	96	THR	N-CA-CB	5.06	119.91	110.30
1	B	42	GLU	CG-CD-OE2	-5.06	108.19	118.30
1	D	121	VAL	CB-CA-C	5.05	121.00	111.40
1	G	66	GLU	CB-CA-C	5.04	120.48	110.40
1	H	20	VAL	CA-CB-CG1	-5.04	103.34	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	PRO	CA-N-CD	5.04	118.75	111.70
1	C	88	HIS	O-C-N	5.04	130.76	122.70
1	F	93	VAL	CA-C-N	5.04	128.28	117.20
1	A	86	PRO	C-N-CA	5.03	134.28	121.70
1	A	106	THR	N-CA-CB	5.03	119.86	110.30
1	E	17	LEU	N-CA-CB	5.03	120.47	110.40
1	G	98	ASN	CA-CB-CG	-5.03	102.33	113.40
1	H	55	PRO	CB-CA-C	5.03	124.57	112.00
1	C	105	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	E	50	SER	CA-C-O	5.02	130.64	120.10
1	F	54	GLU	CA-CB-CG	5.02	124.44	113.40
1	F	100	SER	CB-CA-C	-5.01	100.57	110.10
1	D	66	GLU	CG-CD-OE1	-5.00	108.30	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	125	PRO	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	124	ASN	Peptide
1	G	124	ASN	Mainchain

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	895	0	865	68	0
1	B	890	0	860	71	0
1	C	895	0	863	50	0
1	D	891	0	861	72	0
1	E	895	0	865	55	0
1	F	895	0	865	49	0
1	G	891	0	859	56	0
1	H	895	0	865	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7147	0	6903	449	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 32.

All (449) 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:D:26:ILE:CD1	1:D:51:GLU:HA	1.24	1.62
1:C:21:ARG:NH2	1:C:82:LEU:HD11	1.29	1.48
1:C:21:ARG:NH2	1:C:82:LEU:CD1	1.82	1.42
1:F:44:PHE:CZ	1:F:59:THR:HG21	1.63	1.33
1:C:44:PHE:CZ	1:C:59:THR:HG21	1.63	1.32
1:B:18:ASP:OD1	1:B:20:VAL:CG2	1.77	1.30
1:C:21:ARG:HH22	1:C:82:LEU:CD2	1.54	1.19
1:C:44:PHE:CZ	1:C:59:THR:CG2	2.26	1.18
1:D:26:ILE:CD1	1:D:51:GLU:CA	2.21	1.17
1:D:26:ILE:HD12	1:D:51:GLU:HA	1.20	1.17
1:A:40:THR:HG22	1:A:42:GLU:OE2	1.42	1.16
1:A:40:THR:CG2	1:A:42:GLU:OE2	1.93	1.15
1:C:21:ARG:HH21	1:C:82:LEU:CD1	1.49	1.14
1:G:44:PHE:CZ	1:G:59:THR:HG21	1.83	1.13
1:G:44:PHE:HZ	1:G:59:THR:HG21	1.01	1.13
1:C:90:HIS:CE1	1:C:92:GLU:OE2	2.01	1.12
1:D:26:ILE:HD13	1:D:51:GLU:HA	1.28	1.10
1:F:15:LYS:HE2	1:F:17:LEU:HD21	1.14	1.10
1:A:103:ARG:HG2	1:A:122:VAL:CG1	1.82	1.08
1:A:34:ARG:HH12	1:A:65:VAL:HG22	1.17	1.08
1:H:123:THR:HG22	1:H:125:PRO:CD	1.82	1.08
1:H:10:CYS:SG	1:H:11:PRO:HD2	1.94	1.07
1:G:44:PHE:CZ	1:G:59:THR:CG2	2.39	1.05
1:C:21:ARG:HH22	1:C:82:LEU:HD21	1.20	1.04
1:D:76:LYS:HZ3	1:D:80:LYS:NZ	1.54	1.03
1:B:18:ASP:OD1	1:B:20:VAL:HG22	1.56	1.02
1:B:20:VAL:HG23	1:B:21:ARG:H	1.24	1.02
1:G:40:THR:HG22	1:G:42:GLU:OE1	1.60	1.02
1:H:123:THR:CG2	1:H:125:PRO:HD3	1.89	1.01
1:D:76:LYS:NZ	1:D:80:LYS:HZ2	1.58	1.01
1:D:26:ILE:HD11	1:D:51:GLU:HA	1.40	1.01
1:G:56:HIS:ND1	1:G:57:GLY:N	2.08	1.00
1:B:36:ALA:HB3	1:B:40:THR:HB	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASP:OD1	1:B:20:VAL:HG23	1.58	0.99
1:E:26:ILE:HG12	1:E:27:ASN:N	1.77	0.99
1:D:44:PHE:CZ	1:D:59:THR:HG21	1.96	0.99
1:H:25:ALA:O	1:H:49:THR:HG21	1.64	0.98
1:H:123:THR:HG22	1:H:125:PRO:HD3	1.00	0.98
1:B:20:VAL:HG23	1:B:21:ARG:N	1.77	0.97
1:B:42:GLU:OE1	1:B:44:PHE:HE2	1.46	0.96
1:D:76:LYS:HZ3	1:D:80:LYS:HZ2	1.07	0.95
1:C:90:HIS:HE1	1:C:92:GLU:OE2	1.40	0.95
1:G:44:PHE:HZ	1:G:59:THR:CG2	1.73	0.95
1:G:70:LYS:HE2	1:G:92:GLU:CD	1.86	0.95
1:A:34:ARG:NH1	1:A:65:VAL:HG22	1.84	0.92
1:C:44:PHE:HZ	1:C:59:THR:HG21	1.12	0.92
1:B:26:ILE:HG21	1:B:51:GLU:HA	1.48	0.92
1:E:66:GLU:OE1	1:E:99:ASP:HA	1.69	0.92
1:H:68:ILE:N	1:H:68:ILE:HD12	1.85	0.91
1:A:103:ARG:HG2	1:A:122:VAL:HG13	1.50	0.91
1:D:11:PRO:HA	1:D:104:ARG:HG2	1.53	0.90
1:D:101:GLY:O	1:D:103:ARG:HD2	1.71	0.90
1:A:89:GLU:HB2	1:B:94:VAL:HG22	1.54	0.90
1:G:11:PRO:HB2	1:G:64:PHE:CD2	2.06	0.89
1:B:98:ASN:OD1	1:B:102:PRO:HA	1.72	0.89
1:D:103:ARG:NH2	1:D:124:ASN:HB3	1.86	0.89
1:D:76:LYS:NZ	1:D:80:LYS:NZ	2.16	0.88
1:F:44:PHE:CE2	1:F:59:THR:HG21	2.09	0.87
1:C:21:ARG:NH2	1:C:82:LEU:HD13	1.89	0.86
1:C:21:ARG:NH2	1:C:82:LEU:CD2	2.36	0.86
1:B:26:ILE:CG2	1:B:51:GLU:HA	2.06	0.86
1:F:102:PRO:O	1:F:103:ARG:HD3	1.76	0.86
1:A:40:THR:HG21	1:A:42:GLU:OE2	1.75	0.85
1:B:21:ARG:HH21	1:D:81:ALA:HA	1.39	0.85
1:G:11:PRO:HB2	1:G:64:PHE:HD2	1.38	0.85
1:B:104:ARG:NH1	1:B:104:ARG:HB3	1.92	0.85
1:H:10:CYS:SG	1:H:11:PRO:CD	2.65	0.85
1:D:26:ILE:HD12	1:D:51:GLU:CA	1.96	0.84
1:G:70:LYS:HE2	1:G:92:GLU:OE1	1.77	0.84
1:A:48:LYS:HD3	1:A:48:LYS:N	1.92	0.84
1:H:16:VAL:O	1:H:17:LEU:HD23	1.77	0.84
1:A:11:PRO:HG3	1:A:61:GLU:HG2	1.57	0.84
1:H:35:LYS:HD3	1:H:39:ASP:HA	1.59	0.84
1:H:25:ALA:O	1:H:49:THR:CG2	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:NH2	1:D:81:ALA:HA	1.93	0.82
1:A:34:ARG:HH12	1:A:65:VAL:CG2	1.91	0.82
1:A:34:ARG:NH1	1:A:65:VAL:CG2	2.42	0.81
1:C:21:ARG:NH2	1:C:82:LEU:CG	2.43	0.81
1:F:15:LYS:CE	1:F:17:LEU:HD21	2.06	0.80
1:A:105:TYR:CD1	1:A:122:VAL:HG22	2.16	0.80
1:D:103:ARG:HH21	1:D:124:ASN:HB3	1.46	0.79
1:C:21:ARG:NH2	1:C:82:LEU:HD21	1.95	0.79
1:H:37:ALA:O	1:H:38:ASP:OD1	1.99	0.79
1:H:123:THR:HG22	1:H:124:ASN:N	2.00	0.76
1:H:123:THR:CG2	1:H:124:ASN:N	2.48	0.76
1:C:44:PHE:CZ	1:C:59:THR:HG23	2.15	0.76
1:C:44:PHE:CE2	1:C:59:THR:HG23	2.20	0.75
1:C:21:ARG:HH22	1:C:82:LEU:CG	2.00	0.75
1:E:79:TRP:HB3	1:E:84:ILE:HB	1.67	0.75
1:G:28:VAL:HG23	1:G:78:TYR:CD1	2.22	0.74
1:C:18:ASP:OD2	1:C:78:TYR:OH	2.05	0.74
1:G:44:PHE:CZ	1:G:59:THR:HG23	2.22	0.74
1:F:44:PHE:HZ	1:F:59:THR:HG21	1.45	0.73
1:D:70:LYS:HG3	1:D:94:VAL:HG22	1.70	0.73
1:F:54:GLU:OE1	1:F:55:PRO:HD2	1.88	0.73
1:G:70:LYS:CE	1:G:92:GLU:CD	2.57	0.72
1:D:24:PRO:HG2	1:D:51:GLU:O	1.89	0.72
1:E:34:ARG:HH21	1:E:65:VAL:HG23	1.54	0.72
1:A:11:PRO:HB2	1:A:64:PHE:CD2	2.25	0.71
1:D:103:ARG:HG3	1:D:105:TYR:OH	1.91	0.71
1:A:36:ALA:HB2	1:A:42:GLU:CG	2.20	0.71
1:F:33:PHE:HD2	1:F:41:TRP:HB3	1.55	0.71
1:G:93:VAL:CG2	1:G:118:THR:HG21	2.21	0.71
1:F:56:HIS:H	1:F:56:HIS:CD2	2.08	0.70
1:H:68:ILE:HD12	1:H:68:ILE:H	1.56	0.70
1:D:103:ARG:HG3	1:D:105:TYR:CZ	2.26	0.70
1:H:28:VAL:H	1:H:49:THR:HB	1.56	0.70
1:B:104:ARG:HB3	1:B:104:ARG:HH11	1.57	0.70
1:F:44:PHE:CZ	1:F:59:THR:CG2	2.59	0.69
1:F:56:HIS:CD2	1:F:56:HIS:N	2.61	0.69
1:C:16:VAL:HG23	1:C:111:LEU:HD23	1.74	0.69
1:C:21:ARG:HH21	1:C:82:LEU:HD11	0.61	0.69
1:A:44:PHE:CZ	1:A:59:THR:HG21	2.29	0.68
1:H:98:ASN:OD1	1:H:102:PRO:HA	1.94	0.68
1:D:26:ILE:HD13	1:D:51:GLU:CA	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:THR:OG1	1:F:63:GLU:HG3	1.93	0.68
1:B:26:ILE:CG2	1:B:51:GLU:CA	2.73	0.67
1:C:48:LYS:O	1:C:48:LYS:HD3	1.94	0.67
1:H:74:ASP:OD2	1:H:77:SER:HB2	1.95	0.67
1:B:42:GLU:OE1	1:B:44:PHE:CE2	2.37	0.67
1:A:26:ILE:N	1:A:26:ILE:HD12	2.10	0.67
1:E:32:VAL:HG21	1:E:58:LEU:HD12	1.77	0.66
1:D:13:MET:CE	1:D:104:ARG:HH12	2.09	0.66
1:E:21:ARG:HG2	1:E:21:ARG:O	1.93	0.66
1:D:44:PHE:CE1	1:D:59:THR:HG21	2.31	0.66
1:F:23:SER:HB2	1:F:24:PRO:HD2	1.78	0.66
1:B:26:ILE:HG23	1:B:50:SER:O	1.96	0.65
1:C:16:VAL:HG23	1:C:111:LEU:CD2	2.26	0.65
1:G:18:ASP:OD2	1:G:21:ARG:CB	2.44	0.65
1:G:18:ASP:OD2	1:G:21:ARG:HB2	1.96	0.65
1:A:44:PHE:HZ	1:A:59:THR:HG21	1.61	0.65
1:G:11:PRO:CB	1:G:64:PHE:HD2	2.10	0.65
1:B:35:LYS:N	1:B:41:TRP:CZ3	2.65	0.65
1:A:70:LYS:HE2	1:A:92:GLU:OE2	1.96	0.64
1:G:40:THR:CG2	1:G:42:GLU:OE1	2.41	0.64
1:A:47:GLY:C	1:A:48:LYS:HD3	2.17	0.64
1:E:14:VAL:O	1:E:54:GLU:HG2	1.97	0.64
1:B:74:ASP:OD2	1:B:77:SER:HB2	1.97	0.64
1:F:29:ALA:HA	1:F:48:LYS:HE3	1.80	0.64
1:A:32:VAL:CG2	1:A:58:LEU:HD13	2.28	0.63
1:A:36:ALA:HB2	1:A:42:GLU:HG2	1.80	0.63
1:C:16:VAL:CG1	1:C:49:THR:HG21	2.28	0.63
1:H:50:SER:OG	1:H:54:GLU:O	2.16	0.63
1:D:103:ARG:HA	1:D:125:PRO:HD3	1.81	0.63
1:G:93:VAL:HG22	1:G:118:THR:HG21	1.80	0.63
1:B:16:VAL:HG13	1:B:49:THR:HG21	1.80	0.63
1:D:79:TRP:HA	1:D:79:TRP:CE3	2.31	0.63
1:C:23:SER:HB2	1:C:24:PRO:HD2	1.80	0.63
1:A:36:ALA:HB2	1:A:42:GLU:HG3	1.80	0.63
1:B:75:THR:HB	1:B:90:HIS:HA	1.79	0.62
1:H:102:PRO:O	1:H:103:ARG:HD3	2.00	0.62
1:B:73:ILE:HB	1:B:91:ALA:HB3	1.81	0.61
1:D:121:VAL:HG21	1:F:17:LEU:HD13	1.82	0.61
1:H:35:LYS:HD3	1:H:39:ASP:CA	2.29	0.61
1:E:32:VAL:CG2	1:E:58:LEU:HD12	2.31	0.61
1:C:11:PRO:HB2	1:C:64:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:CYS:O	1:D:104:ARG:NH1	2.33	0.61
1:B:76:LYS:HG2	1:B:80:LYS:HD2	1.83	0.60
1:A:41:TRP:CH2	1:A:68:ILE:HG22	2.36	0.60
1:C:12:LEU:O	1:C:12:LEU:HD23	2.02	0.60
1:B:41:TRP:HA	1:B:41:TRP:CE3	2.37	0.60
1:G:33:PHE:HB3	1:G:41:TRP:HB3	1.82	0.60
1:D:26:ILE:HG23	1:D:50:SER:C	2.22	0.60
1:A:105:TYR:CE1	1:A:122:VAL:HG22	2.36	0.60
1:E:31:HIS:HB3	1:E:33:PHE:CE1	2.37	0.60
1:G:120:ALA:HB2	1:H:87:PHE:CE2	2.37	0.59
1:G:28:VAL:HG22	1:G:78:TYR:HB2	1.84	0.59
1:E:78:TYR:O	1:E:82:LEU:HD22	2.02	0.59
1:H:10:CYS:CB	1:H:11:PRO:HD2	2.31	0.59
1:B:20:VAL:CG2	1:B:21:ARG:N	2.58	0.59
1:B:36:ALA:CB	1:B:40:THR:HB	2.24	0.59
1:A:24:PRO:O	1:A:26:ILE:HD12	2.02	0.59
1:B:76:LYS:O	1:B:80:LYS:HD3	2.03	0.59
1:F:44:PHE:CE2	1:F:59:THR:CG2	2.83	0.58
1:H:123:THR:CG2	1:H:125:PRO:CD	2.64	0.58
1:G:70:LYS:NZ	1:G:92:GLU:CD	2.57	0.58
1:B:26:ILE:CG2	1:B:51:GLU:N	2.66	0.58
1:C:23:SER:HA	1:E:121:VAL:HG13	1.84	0.58
1:G:70:LYS:NZ	1:G:92:GLU:OE2	2.35	0.58
1:G:84:ILE:HG13	1:G:85:SER:N	2.17	0.58
1:B:65:VAL:O	1:B:69:TYR:OH	2.04	0.58
1:E:28:VAL:O	1:E:49:THR:HG23	2.04	0.58
1:F:33:PHE:CD2	1:F:41:TRP:HB3	2.38	0.58
1:F:66:GLU:OE2	1:F:99:ASP:HA	2.04	0.58
1:E:33:PHE:N	1:E:33:PHE:CD1	2.68	0.58
1:D:79:TRP:HB2	1:D:86:PRO:HG3	1.85	0.58
1:D:44:PHE:CE1	1:D:59:THR:CG2	2.87	0.57
1:A:99:ASP:OD1	1:A:99:ASP:N	2.33	0.57
1:D:70:LYS:HG3	1:D:94:VAL:CG2	2.33	0.57
1:H:38:ASP:OD1	1:H:39:ASP:N	2.38	0.57
1:A:41:TRP:HH2	1:A:68:ILE:HG22	1.70	0.57
1:B:21:ARG:NH2	1:D:81:ALA:CA	2.65	0.57
1:F:102:PRO:O	1:F:103:ARG:CD	2.51	0.57
1:B:26:ILE:HG21	1:B:51:GLU:CA	2.29	0.57
1:B:26:ILE:CG2	1:B:50:SER:C	2.74	0.56
1:E:35:LYS:HE3	1:E:41:TRP:CE2	2.40	0.56
1:A:70:LYS:CE	1:A:92:GLU:OE2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:PHE:CE1	1:G:59:THR:OG1	2.59	0.56
1:H:16:VAL:C	1:H:17:LEU:HD23	2.25	0.56
1:G:114:TYR:N	1:G:114:TYR:CD1	2.73	0.56
1:A:40:THR:HG22	1:A:42:GLU:CD	2.24	0.56
1:C:20:VAL:HG22	1:C:79:TRP:CH2	2.41	0.56
1:H:28:VAL:CG1	1:H:49:THR:HB	2.36	0.56
1:A:23:SER:HB2	1:A:24:PRO:HD2	1.88	0.56
1:E:73:ILE:HB	1:E:91:ALA:HB3	1.87	0.56
1:G:97:ALA:O	1:G:98:ASN:HB2	2.04	0.56
1:B:57:GLY:O	1:B:58:LEU:C	2.43	0.56
1:F:35:LYS:HE2	1:F:39:ASP:O	2.06	0.56
1:G:115:SER:HB2	1:H:118:THR:O	2.06	0.56
1:B:102:PRO:C	1:B:103:ARG:HG2	2.27	0.55
1:F:75:THR:HB	1:F:90:HIS:HA	1.89	0.55
1:C:123:THR:O	1:C:123:THR:HG22	2.06	0.55
1:A:97:ALA:O	1:A:98:ASN:HB2	2.07	0.55
1:E:26:ILE:HG12	1:E:27:ASN:H	1.71	0.55
1:G:72:GLU:O	1:G:72:GLU:HG3	2.06	0.55
1:A:103:ARG:HG2	1:A:122:VAL:HG11	1.84	0.55
1:D:121:VAL:HG13	1:F:23:SER:HA	1.89	0.55
1:E:90:HIS:NE2	1:F:94:VAL:HG21	2.22	0.55
1:H:28:VAL:HG13	1:H:49:THR:CB	2.37	0.55
1:B:66:GLU:HG3	1:B:98:ASN:O	2.07	0.55
1:E:87:PHE:CE2	1:F:120:ALA:HB2	2.42	0.55
1:E:41:TRP:CE3	1:E:41:TRP:HA	2.42	0.54
1:G:66:GLU:HA	1:G:97:ALA:O	2.07	0.54
1:A:34:ARG:HD3	1:A:69:TYR:CE2	2.42	0.54
1:E:26:ILE:HD11	1:E:27:ASN:OD1	2.07	0.54
1:F:105:TYR:CD2	1:F:122:VAL:HG22	2.42	0.54
1:D:76:LYS:NZ	1:D:80:LYS:HZ3	2.03	0.54
1:A:70:LYS:HE2	1:A:92:GLU:CD	2.28	0.54
1:F:27:ASN:ND2	1:F:48:LYS:HG3	2.22	0.54
1:A:23:SER:HB2	1:A:24:PRO:CD	2.38	0.54
1:A:100:SER:O	1:F:103:ARG:NH2	2.41	0.54
1:A:65:VAL:O	1:A:69:TYR:OH	2.21	0.53
1:C:35:LYS:HE3	1:C:35:LYS:N	2.23	0.53
1:E:14:VAL:O	1:E:54:GLU:CG	2.56	0.53
1:G:99:ASP:OD1	1:G:99:ASP:N	2.42	0.53
1:H:123:THR:CG2	1:H:124:ASN:H	2.20	0.53
1:B:35:LYS:HE2	1:B:68:ILE:HD12	1.89	0.53
1:D:20:VAL:HA	1:E:113:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:HIS:HB2	1:G:72:GLU:HG2	1.91	0.53
1:H:16:VAL:CG1	1:H:111:LEU:HD22	2.39	0.53
1:B:27:ASN:O	1:B:48:LYS:NZ	2.42	0.53
1:B:114:TYR:N	1:B:114:TYR:CD1	2.76	0.53
1:D:44:PHE:HZ	1:D:59:THR:HG21	1.63	0.53
1:F:33:PHE:CD1	1:F:33:PHE:N	2.75	0.52
1:C:75:THR:HG21	1:C:111:LEU:HD11	1.91	0.52
1:E:32:VAL:CG2	1:E:58:LEU:CD1	2.87	0.52
1:H:95:PHE:CE2	1:H:97:ALA:HB2	2.45	0.52
1:F:38:ASP:O	1:F:40:THR:N	2.42	0.52
1:G:31:HIS:HB3	1:G:33:PHE:CE1	2.44	0.52
1:C:16:VAL:CG2	1:C:111:LEU:HD23	2.39	0.52
1:E:79:TRP:HZ2	1:E:111:LEU:HB3	1.73	0.52
1:A:26:ILE:HD12	1:A:26:ILE:H	1.75	0.52
1:G:18:ASP:OD2	1:G:21:ARG:HB3	2.09	0.52
1:A:103:ARG:HH22	1:F:100:SER:HB3	1.75	0.52
1:B:21:ARG:HH22	1:D:81:ALA:C	2.13	0.52
1:B:112:SER:HB3	1:B:113:PRO:HD2	1.92	0.52
1:H:95:PHE:HE2	1:H:97:ALA:HB2	1.74	0.52
1:D:20:VAL:HG21	1:D:113:PRO:HD3	1.92	0.52
1:E:66:GLU:CD	1:E:99:ASP:HA	2.28	0.52
1:C:17:LEU:HD23	1:C:24:PRO:HA	1.91	0.51
1:H:26:ILE:HG13	1:H:26:ILE:O	2.10	0.51
1:H:36:ALA:O	1:H:37:ALA:C	2.49	0.51
1:A:11:PRO:HB2	1:A:64:PHE:HD2	1.71	0.51
1:F:104:ARG:HG3	1:F:104:ARG:HH11	1.75	0.51
1:A:73:ILE:O	1:A:90:HIS:HB2	2.11	0.51
1:A:103:ARG:HG3	1:A:123:THR:O	2.11	0.51
1:G:28:VAL:O	1:G:48:LYS:HA	2.10	0.51
1:A:44:PHE:CZ	1:A:59:THR:CG2	2.94	0.51
1:H:15:LYS:CD	1:H:17:LEU:HD21	2.41	0.51
1:E:89:GLU:O	1:E:90:HIS:HB3	2.11	0.50
1:C:99:ASP:N	1:C:99:ASP:OD1	2.45	0.50
1:B:26:ILE:HG23	1:B:50:SER:C	2.31	0.50
1:A:35:LYS:HB2	1:A:41:TRP:CZ3	2.46	0.50
1:F:11:PRO:HA	1:F:104:ARG:HG2	1.94	0.50
1:C:73:ILE:O	1:C:90:HIS:HB2	2.11	0.50
1:D:103:ARG:HH21	1:D:124:ASN:CB	2.22	0.50
1:A:38:ASP:OD1	1:A:40:THR:HB	2.11	0.50
1:B:18:ASP:OD2	1:B:21:ARG:HD3	2.11	0.50
1:G:17:LEU:HB2	1:G:110:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:TYR:N	1:G:114:TYR:HD1	2.09	0.49
1:F:23:SER:HB2	1:F:24:PRO:CD	2.41	0.49
1:G:23:SER:HB2	1:G:24:PRO:CD	2.42	0.49
1:A:32:VAL:HG21	1:A:58:LEU:HD13	1.93	0.49
1:C:48:LYS:HD3	1:C:48:LYS:C	2.33	0.49
1:F:29:ALA:CA	1:F:48:LYS:HE3	2.42	0.49
1:C:16:VAL:HG11	1:C:49:THR:HG21	1.95	0.49
1:E:16:VAL:CG1	1:E:111:LEU:HD22	2.42	0.49
1:E:34:ARG:HD3	1:E:42:GLU:OE2	2.13	0.49
1:E:32:VAL:HG23	1:E:58:LEU:CD1	2.43	0.49
1:A:24:PRO:O	1:A:26:ILE:CD1	2.61	0.49
1:B:77:SER:HA	1:B:80:LYS:HD3	1.94	0.49
1:C:11:PRO:HB2	1:C:64:PHE:HD2	1.78	0.49
1:F:33:PHE:HB2	1:F:70:LYS:HB3	1.95	0.49
1:E:38:ASP:OD1	1:E:38:ASP:N	2.45	0.49
1:A:17:LEU:N	1:A:17:LEU:HD22	2.27	0.48
1:E:36:ALA:O	1:E:37:ALA:C	2.51	0.48
1:G:73:ILE:O	1:G:90:HIS:HB2	2.14	0.48
1:F:93:VAL:HG21	1:F:107:ILE:HD11	1.93	0.48
1:E:32:VAL:C	1:E:33:PHE:HD1	2.17	0.48
1:E:32:VAL:C	1:E:33:PHE:CD1	2.86	0.48
1:E:101:GLY:O	1:E:103:ARG:HD3	2.14	0.48
1:G:44:PHE:HE1	1:G:59:THR:OG1	1.95	0.48
1:A:87:PHE:HE1	1:B:105:TYR:HD2	1.62	0.48
1:C:20:VAL:HG22	1:C:79:TRP:HH2	1.76	0.48
1:E:114:TYR:CD1	1:E:114:TYR:N	2.82	0.48
1:H:28:VAL:HG12	1:H:49:THR:HB	1.95	0.48
1:D:23:SER:HB2	1:D:24:PRO:HD2	1.96	0.47
1:F:11:PRO:HG3	1:F:61:GLU:HG3	1.96	0.47
1:A:32:VAL:HG13	1:A:71:VAL:HG22	1.97	0.47
1:B:36:ALA:HB2	1:B:42:GLU:OE2	2.14	0.47
1:D:13:MET:CE	1:D:104:ARG:NH1	2.75	0.47
1:E:25:ALA:HB1	1:E:28:VAL:HG11	1.96	0.47
1:D:99:ASP:OD1	1:D:99:ASP:N	2.45	0.47
1:E:94:VAL:HG11	1:F:90:HIS:CE1	2.50	0.47
1:B:59:THR:HB	1:B:60:THR:H	1.28	0.47
1:B:104:ARG:HB3	1:B:104:ARG:CZ	2.43	0.47
1:E:79:TRP:CZ2	1:E:111:LEU:HB3	2.49	0.47
1:G:65:VAL:HG22	1:G:66:GLU:H	1.79	0.47
1:A:103:ARG:CG	1:A:122:VAL:CG1	2.74	0.47
1:E:28:VAL:HG13	1:E:49:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:CYS:SG	1:H:11:PRO:N	2.87	0.47
1:H:93:VAL:HG22	1:H:118:THR:HG21	1.96	0.47
1:B:26:ILE:HG23	1:B:51:GLU:HA	1.93	0.47
1:E:35:LYS:N	1:E:41:TRP:CZ3	2.83	0.47
1:E:92:GLU:OE2	1:F:90:HIS:NE2	2.48	0.47
1:D:59:THR:HG22	1:D:63:GLU:OE1	2.15	0.46
1:D:48:LYS:HB3	1:D:48:LYS:HE3	1.54	0.46
1:F:102:PRO:C	1:F:103:ARG:HG2	2.36	0.46
1:H:32:VAL:HG13	1:H:45:ALA:HB3	1.96	0.46
1:A:36:ALA:O	1:A:37:ALA:C	2.53	0.46
1:B:23:SER:HB2	1:B:24:PRO:HD2	1.97	0.46
1:D:98:ASN:HB3	1:D:102:PRO:HA	1.95	0.46
1:E:79:TRP:CD1	1:E:86:PRO:HB3	2.50	0.46
1:E:87:PHE:HB2	1:E:114:TYR:CD2	2.49	0.46
1:G:65:VAL:HG22	1:G:66:GLU:N	2.30	0.46
1:B:26:ILE:HG23	1:B:51:GLU:CA	2.44	0.46
1:A:104:ARG:HH11	1:A:104:ARG:HB3	1.80	0.46
1:B:36:ALA:CB	1:B:42:GLU:OE2	2.63	0.46
1:C:115:SER:HB2	1:D:119:THR:CB	2.46	0.46
1:H:75:THR:HB	1:H:90:HIS:HA	1.97	0.46
1:B:75:THR:HG22	1:B:76:LYS:N	2.29	0.46
1:H:28:VAL:CG1	1:H:49:THR:CB	2.94	0.46
1:B:18:ASP:OD2	1:B:21:ARG:CD	2.64	0.45
1:H:28:VAL:HG13	1:H:49:THR:HB	1.98	0.45
1:B:16:VAL:HG22	1:B:25:ALA:HB3	1.98	0.45
1:A:105:TYR:CE1	1:A:122:VAL:CG2	3.00	0.45
1:D:42:GLU:O	1:D:42:GLU:HG2	2.16	0.45
1:A:97:ALA:O	1:A:98:ASN:CB	2.64	0.45
1:D:21:ARG:HH11	1:D:21:ARG:HD2	1.46	0.45
1:D:13:MET:HE2	1:D:104:ARG:NH1	2.32	0.45
1:F:84:ILE:HG22	1:F:85:SER:N	2.31	0.45
1:H:112:SER:HB3	1:H:113:PRO:HD2	1.99	0.45
1:B:66:GLU:HA	1:B:98:ASN:HB2	1.99	0.45
1:B:105:TYR:N	1:B:105:TYR:CD1	2.85	0.45
1:C:35:LYS:HE3	1:C:35:LYS:CA	2.47	0.45
1:C:68:ILE:HD13	1:D:89:GLU:OE2	2.17	0.45
1:G:21:ARG:O	1:G:21:ARG:HG2	2.16	0.45
1:H:25:ALA:O	1:H:49:THR:HG22	2.11	0.44
1:E:12:LEU:HD12	1:E:64:PHE:CE1	2.53	0.44
1:G:56:HIS:CG	1:G:57:GLY:N	2.85	0.44
1:G:84:ILE:CG1	1:G:85:SER:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:CG2	1:A:124:ASN:N	2.80	0.44
1:C:115:SER:OG	1:D:119:THR:HG22	2.17	0.44
1:D:38:ASP:O	1:D:40:THR:N	2.49	0.44
1:E:44:PHE:CZ	1:E:59:THR:HG21	2.52	0.44
1:A:42:GLU:HA	1:A:43:PRO:HD3	1.72	0.44
1:D:11:PRO:HB2	1:D:64:PHE:HD2	1.82	0.44
1:D:93:VAL:HG13	1:D:118:THR:HG21	1.99	0.44
1:F:78:TYR:O	1:F:82:LEU:HD13	2.18	0.44
1:H:15:LYS:HE3	1:H:15:LYS:HB2	1.42	0.44
1:A:33:PHE:CD1	1:A:33:PHE:N	2.86	0.44
1:D:13:MET:HE1	1:D:104:ARG:HH12	1.83	0.44
1:E:32:VAL:O	1:E:33:PHE:HD1	2.01	0.44
1:E:42:GLU:HA	1:E:43:PRO:HD2	1.84	0.44
1:G:23:SER:HB2	1:G:24:PRO:HD2	1.98	0.43
1:G:26:ILE:HG12	1:G:51:GLU:HA	2.01	0.43
1:B:71:VAL:HG23	1:B:95:PHE:HE1	1.82	0.43
1:D:76:LYS:HZ3	1:D:80:LYS:HZ3	1.51	0.43
1:E:66:GLU:HA	1:E:97:ALA:O	2.19	0.43
1:H:90:HIS:ND1	1:H:90:HIS:C	2.72	0.43
1:B:25:ALA:HB1	1:B:78:TYR:CE1	2.53	0.43
1:D:26:ILE:HD12	1:D:51:GLU:N	2.33	0.43
1:C:66:GLU:OE1	1:C:99:ASP:HA	2.18	0.43
1:B:18:ASP:OD1	1:B:20:VAL:HG21	2.01	0.43
1:D:26:ILE:HD11	1:D:51:GLU:CA	2.24	0.43
1:A:115:SER:OG	1:B:119:THR:HG23	2.19	0.43
1:B:63:GLU:OE1	1:B:63:GLU:HA	2.18	0.43
1:A:70:LYS:HD3	1:A:92:GLU:OE2	2.19	0.43
1:F:23:SER:CB	1:F:24:PRO:CD	2.95	0.43
1:A:41:TRP:HH2	1:A:68:ILE:CG2	2.31	0.43
1:G:28:VAL:CG2	1:G:78:TYR:CD1	2.97	0.43
1:G:102:PRO:C	1:G:103:ARG:HG3	2.37	0.43
1:A:99:ASP:OD1	1:A:100:SER:N	2.51	0.42
1:H:123:THR:HG23	1:H:124:ASN:H	1.84	0.42
1:C:115:SER:HB2	1:D:119:THR:HB	2.01	0.42
1:F:36:ALA:O	1:F:37:ALA:C	2.57	0.42
1:B:24:PRO:HB2	1:B:53:GLY:CA	2.50	0.42
1:D:113:PRO:HD2	1:E:20:VAL:HA	2.02	0.42
1:G:23:SER:CB	1:G:24:PRO:CD	2.95	0.42
1:H:75:THR:HG22	1:H:76:LYS:N	2.35	0.42
1:D:76:LYS:HZ2	1:D:80:LYS:NZ	2.09	0.42
1:E:113:PRO:HB2	1:E:114:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLU:OE2	1:F:92:GLU:HG2	2.18	0.42
1:A:26:ILE:N	1:A:26:ILE:CD1	2.82	0.42
1:D:118:THR:O	1:D:119:THR:HG22	2.19	0.42
1:C:87:PHE:HB2	1:C:114:TYR:CD2	2.55	0.42
1:E:87:PHE:HB2	1:E:114:TYR:CE2	2.55	0.42
1:F:56:HIS:N	1:F:56:HIS:HD2	2.13	0.42
1:C:36:ALA:HB2	1:C:42:GLU:HG2	2.02	0.42
1:G:54:GLU:HA	1:G:55:PRO:HD3	1.86	0.42
1:H:19:ALA:HB2	1:H:110:LEU:HD22	2.01	0.42
1:B:92:GLU:OE2	1:B:94:VAL:HG12	2.20	0.42
1:H:44:PHE:HZ	1:H:59:THR:HG1	1.65	0.42
1:A:38:ASP:O	1:A:40:THR:N	2.54	0.41
1:A:87:PHE:HB2	1:A:114:TYR:CD2	2.54	0.41
1:F:12:LEU:HD21	1:F:95:PHE:HZ	1.85	0.41
1:G:122:VAL:HG12	1:G:123:THR:N	2.35	0.41
1:H:71:VAL:O	1:H:92:GLU:HA	2.19	0.41
1:H:28:VAL:HG13	1:H:49:THR:OG1	2.20	0.41
1:C:95:PHE:CD1	1:C:95:PHE:N	2.88	0.41
1:D:25:ALA:HB1	1:D:28:VAL:CG2	2.50	0.41
1:H:114:TYR:N	1:H:114:TYR:CD1	2.88	0.41
1:D:11:PRO:HB2	1:D:64:PHE:CD2	2.55	0.41
1:D:44:PHE:CZ	1:D:59:THR:CG2	2.84	0.41
1:D:103:ARG:HE	1:D:103:ARG:HB3	1.30	0.41
1:B:36:ALA:HB2	1:B:42:GLU:HG3	2.03	0.41
1:B:92:GLU:OE2	1:B:94:VAL:CG1	2.69	0.41
1:B:102:PRO:C	1:B:103:ARG:CG	2.88	0.41
1:B:104:ARG:CZ	1:B:104:ARG:CB	2.99	0.41
1:D:87:PHE:HB2	1:D:114:TYR:CD2	2.56	0.41
1:B:58:LEU:HA	1:B:58:LEU:HD23	1.78	0.41
1:G:79:TRP:CE3	1:G:82:LEU:HD11	2.56	0.41
1:B:57:GLY:O	1:B:59:THR:N	2.53	0.41
1:C:10:CYS:O	1:C:104:ARG:HD2	2.19	0.41
1:C:87:PHE:CE2	1:D:120:ALA:HB2	2.56	0.41
1:D:58:LEU:HD23	1:D:58:LEU:HA	1.75	0.41
1:F:31:HIS:ND1	1:F:46:SER:OG	2.38	0.41
1:G:70:LYS:CE	1:G:92:GLU:OE2	2.69	0.41
1:H:32:VAL:HG22	1:H:44:PHE:HD1	1.85	0.41
1:A:10:CYS:HA	1:A:11:PRO:HD3	1.92	0.40
1:D:118:THR:C	1:D:119:THR:CG2	2.88	0.40
1:E:31:HIS:HB3	1:E:33:PHE:HE1	1.83	0.40
1:A:36:ALA:CB	1:A:42:GLU:CG	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:PHE:CE2	1:E:98:ASN:ND2	2.88	0.40
1:E:120:ALA:HB2	1:F:87:PHE:CE2	2.56	0.40
1:G:112:SER:O	1:G:113:PRO:C	2.59	0.40
1:B:103:ARG:HB3	1:B:123:THR:O	2.21	0.40
1:D:17:LEU:HD12	1:D:24:PRO:HA	2.04	0.40
1:H:79:TRP:HB2	1:H:86:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	114/127 (90%)	107 (94%)	4 (4%)	3 (3%)	5 13
1	B	114/127 (90%)	105 (92%)	5 (4%)	4 (4%)	3 8
1	C	114/127 (90%)	109 (96%)	2 (2%)	3 (3%)	5 13
1	D	114/127 (90%)	108 (95%)	4 (4%)	2 (2%)	8 21
1	E	114/127 (90%)	103 (90%)	8 (7%)	3 (3%)	5 13
1	F	114/127 (90%)	105 (92%)	7 (6%)	2 (2%)	8 21
1	G	114/127 (90%)	106 (93%)	7 (6%)	1 (1%)	17 40
1	H	114/127 (90%)	109 (96%)	3 (3%)	2 (2%)	8 21
All	All	912/1016 (90%)	852 (93%)	40 (4%)	20 (2%)	6 17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	37	ALA
1	H	37	ALA
1	D	39	ASP
1	E	56	HIS

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Mol	Chain	Res	Type
1	F	37	ALA
1	F	39	ASP
1	A	38	ASP
1	A	39	ASP
1	A	51	GLU
1	B	38	ASP
1	C	39	ASP
1	D	37	ALA
1	B	37	ALA
1	B	58	LEU
1	C	37	ALA
1	B	51	GLU
1	C	57	GLY
1	E	124	ASN
1	H	39	ASP
1	E	37	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	97/105 (92%)	78 (80%)	19 (20%)	1 3
1	B	96/105 (91%)	77 (80%)	19 (20%)	1 3
1	C	97/105 (92%)	78 (80%)	19 (20%)	1 3
1	D	96/105 (91%)	71 (74%)	25 (26%)	0 1
1	E	97/105 (92%)	75 (77%)	22 (23%)	1 2
1	F	97/105 (92%)	75 (77%)	22 (23%)	1 2
1	G	96/105 (91%)	74 (77%)	22 (23%)	1 2
1	H	97/105 (92%)	82 (84%)	15 (16%)	2 7
All	All	773/840 (92%)	610 (79%)	163 (21%)	1 3

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	27	ASN
1	A	35	LYS
1	A	40	THR
1	A	46	SER
1	A	48	LYS
1	A	52	SER
1	A	56	HIS
1	A	59	THR
1	A	60	THR
1	A	61	GLU
1	A	62	GLU
1	A	66	GLU
1	A	76	LYS
1	A	80	LYS
1	A	82	LEU
1	A	85	SER
1	A	103	ARG
1	A	110	LEU
1	B	14	VAL
1	B	16	VAL
1	B	21	ARG
1	B	26	ILE
1	B	27	ASN
1	B	30	VAL
1	B	48	LYS
1	B	51	GLU
1	B	62	GLU
1	B	65	VAL
1	B	73	ILE
1	B	75	THR
1	B	82	LEU
1	B	85	SER
1	B	86	PRO
1	B	92	GLU
1	B	99	ASP
1	B	115	SER
1	B	123	THR
1	C	12	LEU
1	C	16	VAL
1	C	26	ILE
1	C	28	VAL
1	C	35	LYS

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Mol	Chain	Res	Type
1	C	40	THR
1	C	48	LYS
1	C	50	SER
1	C	59	THR
1	C	60	THR
1	C	63	GLU
1	C	66	GLU
1	C	76	LYS
1	C	86	PRO
1	C	103	ARG
1	C	111	LEU
1	C	112	SER
1	C	117	SER
1	C	123	THR
1	D	10	CYS
1	D	17	LEU
1	D	26	ILE
1	D	40	THR
1	D	42	GLU
1	D	48	LYS
1	D	61	GLU
1	D	63	GLU
1	D	65	VAL
1	D	66	GLU
1	D	70	LYS
1	D	75	THR
1	D	76	LYS
1	D	85	SER
1	D	98	ASN
1	D	100	SER
1	D	103	ARG
1	D	104	ARG
1	D	110	LEU
1	D	112	SER
1	D	116	TYR
1	D	118	THR
1	D	122	VAL
1	D	123	THR
1	D	124	ASN
1	E	12	LEU
1	E	23	SER
1	E	26	ILE

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Mol	Chain	Res	Type
1	E	28	VAL
1	E	34	ARG
1	E	38	ASP
1	E	42	GLU
1	E	50	SER
1	E	54	GLU
1	E	58	LEU
1	E	59	THR
1	E	66	GLU
1	E	82	LEU
1	E	85	SER
1	E	92	GLU
1	E	99	ASP
1	E	100	SER
1	E	110	LEU
1	E	112	SER
1	E	116	TYR
1	E	117	SER
1	E	118	THR
1	F	21	ARG
1	F	26	ILE
1	F	38	ASP
1	F	40	THR
1	F	43	PRO
1	F	46	SER
1	F	48	LYS
1	F	51	GLU
1	F	52	SER
1	F	54	GLU
1	F	56	HIS
1	F	62	GLU
1	F	75	THR
1	F	76	LYS
1	F	80	LYS
1	F	85	SER
1	F	86	PRO
1	F	92	GLU
1	F	107	ILE
1	F	110	LEU
1	F	115	SER
1	F	117	SER
1	G	12	LEU

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Mol	Chain	Res	Type
1	G	21	ARG
1	G	27	ASN
1	G	28	VAL
1	G	30	VAL
1	G	35	LYS
1	G	40	THR
1	G	46	SER
1	G	50	SER
1	G	51	GLU
1	G	59	THR
1	G	60	THR
1	G	61	GLU
1	G	66	GLU
1	G	72	GLU
1	G	82	LEU
1	G	92	GLU
1	G	100	SER
1	G	112	SER
1	G	115	SER
1	G	116	TYR
1	G	118	THR
1	H	10	CYS
1	H	15	LYS
1	H	21	ARG
1	H	28	VAL
1	H	32	VAL
1	H	35	LYS
1	H	38	ASP
1	H	46	SER
1	H	50	SER
1	H	63	GLU
1	H	65	VAL
1	H	66	GLU
1	H	72	GLU
1	H	92	GLU
1	H	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	C	90	HIS

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Mol	Chain	Res	Type
1	D	88	HIS
1	D	98	ASN
1	E	124	ASN
1	F	27	ASN
1	F	56	HIS
1	G	27	ASN
1	G	90	HIS
1	H	88	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	123:THR	C	124:ASN	N	1.68

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.