



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:34 PM GMT

PDB ID : 1XTC  
Title : CHOLERA TOXIN  
Authors : Zhang, R.-G.; Westbrook, E.  
Deposited on : 1996-01-10  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

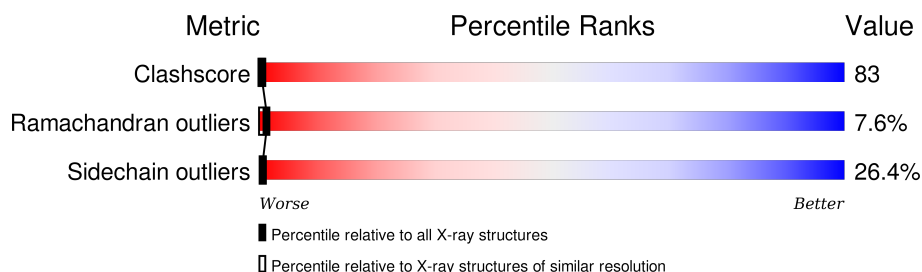
# 1 Overall quality at a glance

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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	<div> <div>26%</div> <div>45%</div> <div>18%</div> <div>10%</div> <div>.</div> </div>
2	C	46	<div> <div>20%</div> <div>48%</div> <div>24%</div> <div>7%</div> <div>.</div> </div>
3	D	103	<div> <div>16%</div> <div>52%</div> <div>23%</div> <div>9%</div> </div>
3	E	103	<div> <div>13%</div> <div>59%</div> <div>22%</div> <div>6%</div> </div>
3	F	103	<div> <div>20%</div> <div>47%</div> <div>29%</div> <div>.</div> </div>
3	G	103	<div> <div>16%</div> <div>61%</div> <div>17%</div> <div>7%</div> </div>
3	H	103	<div> <div>12%</div> <div>45%</div> <div>32%</div> <div>12%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6135 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 CHOLERA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1532	961	279	288	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	LEU	ILE	CONFLICT	UNP P01555
A	88	LEU	ILE	CONFLICT	UNP P01555

- Molecule 2 is a protein called CHOLERA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	45	Total	C	N	O	S	0	0	0
			370	227	64	78	1			

- Molecule 3 is a protein called CHOLERA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	E	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	F	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	G	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			
3	H	103	Total	C	N	O	S	0	0	0
			819	516	140	158	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	54	SER	GLY	CONFLICT	UNP P01556
D	87	THR	VAL	CONFLICT	UNP P01556
E	54	SER	GLY	CONFLICT	UNP P01556
E	87	THR	VAL	CONFLICT	UNP P01556
F	54	SER	GLY	CONFLICT	UNP P01556
F	87	THR	VAL	CONFLICT	UNP P01556
G	54	SER	GLY	CONFLICT	UNP P01556
G	87	THR	VAL	CONFLICT	UNP P01556
H	54	SER	GLY	CONFLICT	UNP P01556
H	87	THR	VAL	CONFLICT	UNP P01556

- Molecule 4 is water.

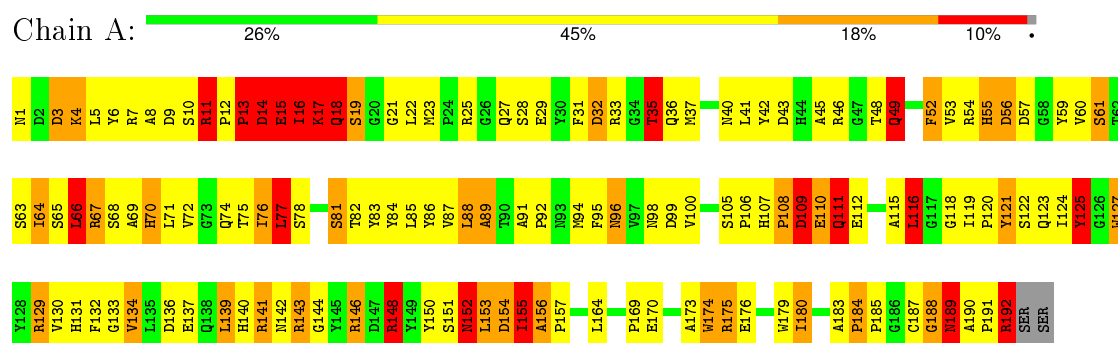
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	C	4	Total O 4 4	0	0
4	D	24	Total O 24 24	0	0
4	E	19	Total O 19 19	0	0
4	F	19	Total O 19 19	0	0
4	G	19	Total O 19 19	0	0
4	H	18	Total O 18 18	0	0

### 3 Residue-property plots

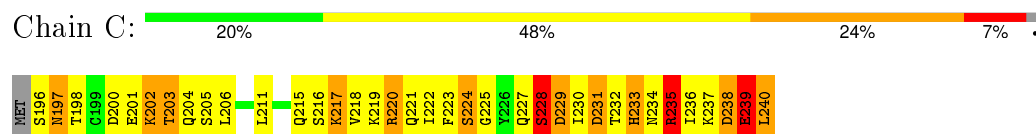
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

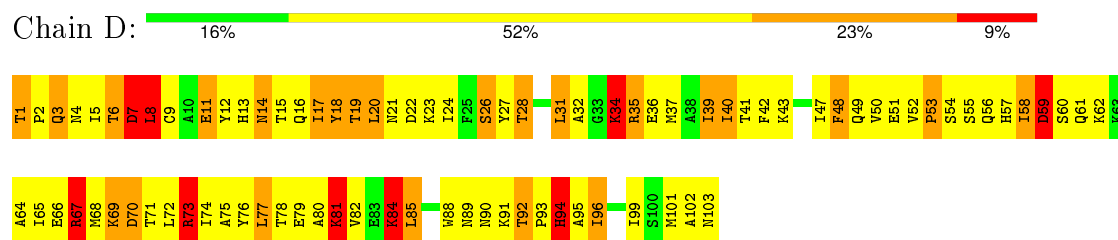
#### • Molecule 1: CHOLERA TOXIN



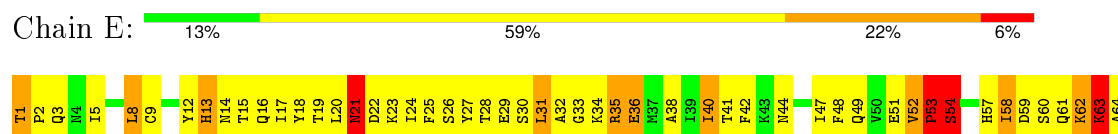
#### • Molecule 2: CHOLERA TOXIN

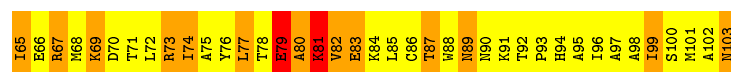


#### • Molecule 3: CHOLERA TOXIN

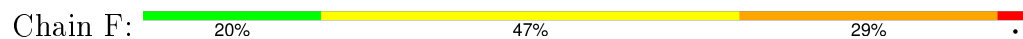


#### • Molecule 3: CHOLERA TOXIN

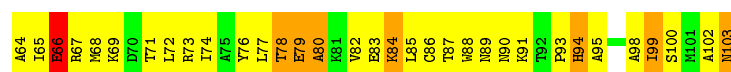




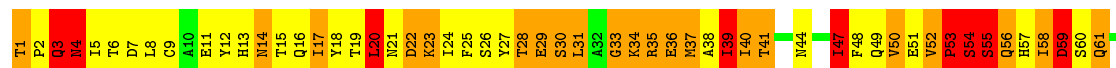
● Molecule 3: CHOLERA TOXIN



● Molecule 3: CHOLERA TOXIN



● Molecule 3: CHOLERA TOXIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.00 Å 92.20 Å 60.60 Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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	0.97	2/1581 (0.1%)	1.87	42/2153 (2.0%)
2	C	1.04	0/374	1.51	5/498 (1.0%)
3	D	0.95	0/833	1.71	9/1125 (0.8%)
3	E	0.99	0/833	1.75	12/1125 (1.1%)
3	F	0.96	0/833	1.72	11/1125 (1.0%)
3	G	1.15	2/833 (0.2%)	1.79	22/1125 (2.0%)
3	H	0.98	1/833 (0.1%)	1.91	17/1125 (1.5%)
All	All	1.00	5/6120 (0.1%)	1.79	118/8276 (1.4%)

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	A	0	15
2	C	0	2
3	D	0	8
3	E	0	2
3	F	0	4
3	G	0	9
3	H	0	10
All	All	0	50

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	THR	C-N	12.81	1.58	1.34
1	A	19	SER	C-N	10.39	1.51	1.33
3	H	53	PRO	C-N	-5.56	1.21	1.34
1	A	16	ILE	C-N	-5.27	1.22	1.34
3	G	45	GLY	N-CA	-5.01	1.38	1.46



All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	53	PRO	C-N-CA	19.24	169.80	121.70
3	H	54	SER	C-N-CA	18.47	167.88	121.70
1	A	15	GLU	O-C-N	-17.35	94.94	122.70
3	F	73	ARG	CD-NE-CZ	15.69	145.56	123.60
1	A	13	PRO	C-N-CA	14.48	157.89	121.70
3	D	67	ARG	NE-CZ-NH2	-11.91	114.34	120.30
1	A	67	ARG	NE-CZ-NH1	11.63	126.12	120.30
1	A	15	GLU	CA-C-N	11.39	142.26	117.20
3	E	79	GLU	C-N-CA	10.77	148.63	121.70
3	G	1	THR	O-C-N	-10.47	101.21	121.10
3	E	73	ARG	CD-NE-CZ	10.44	138.22	123.60
1	A	175	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	A	13	PRO	O-C-N	-10.40	106.05	122.70
3	H	53	PRO	O-C-N	-10.19	106.40	122.70
3	F	73	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	A	16	ILE	O-C-N	-9.38	107.69	122.70
1	A	14	ASP	O-C-N	-9.02	108.27	122.70
2	C	220	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	A	67	ARG	CD-NE-CZ	8.37	135.32	123.60
3	H	85	LEU	CA-CB-CG	8.23	134.22	115.30
3	E	73	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	99	ASP	CB-CG-OD1	8.03	125.52	118.30
3	E	73	ARG	NE-CZ-NH2	-7.97	116.32	120.30
3	E	53	PRO	C-N-CA	7.90	141.46	121.70
3	E	67	ARG	NE-CZ-NH1	-7.73	116.44	120.30
3	G	41	THR	CA-CB-CG2	7.57	122.99	112.40
3	H	4	ASN	CB-CA-C	-7.55	95.30	110.40
1	A	13	PRO	CA-C-N	7.49	133.68	117.20
3	G	45	GLY	N-CA-C	7.30	131.36	113.10
3	D	73	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	154	ASP	CB-CA-C	7.10	124.60	110.40
3	F	62	LYS	CA-CB-CG	6.94	128.66	113.40
3	G	44	ASN	C-N-CA	6.86	136.70	122.30
1	A	154	ASP	CB-CG-OD1	6.84	124.46	118.30
3	F	71	THR	CA-CB-CG2	6.82	121.95	112.40
3	H	79	GLU	N-CA-CB	6.82	122.88	110.60
1	A	32	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	129	ARG	NE-CZ-NH2	-6.71	116.95	120.30
3	D	84	LYS	N-CA-CB	6.68	122.63	110.60
1	A	192	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	11	ARG	NE-CZ-NH2	-6.63	116.98	120.30
3	H	91	LYS	N-CA-CB	6.59	122.46	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH1	6.58	123.59	120.30
3	G	1	THR	C-N-CD	-6.58	106.13	120.60
3	G	84	LYS	CG-CD-CE	6.54	131.51	111.90
3	D	22	ASP	CB-CG-OD1	-6.44	112.50	118.30
3	E	36	GLU	N-CA-CB	6.32	121.97	110.60
1	A	96	ASN	CB-CA-C	6.30	123.00	110.40
3	G	73	ARG	NE-CZ-NH2	6.28	123.44	120.30
3	D	70	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	A	15	GLU	C-N-CA	6.25	137.33	121.70
1	A	3	ASP	CB-CG-OD1	6.23	123.91	118.30
3	F	35	ARG	NE-CZ-NH1	-6.17	117.22	120.30
2	C	235	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	109	ASP	CB-CG-OD2	-6.11	112.81	118.30
3	G	6	THR	CA-CB-CG2	6.11	120.95	112.40
3	G	59	ASP	CB-CG-OD1	-6.05	112.85	118.30
3	H	30	SER	N-CA-CB	6.02	119.53	110.50
1	A	116	LEU	CB-CA-C	6.01	121.63	110.20
1	A	18	GLN	CA-C-N	-6.01	103.98	117.20
2	C	216	SER	O-C-N	-5.97	113.15	122.70
1	A	175	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	155	ILE	CA-C-N	5.96	130.32	117.20
3	G	73	ARG	NE-CZ-NH1	-5.93	117.34	120.30
3	E	67	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	99	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	155	ILE	N-CA-C	5.88	126.86	111.00
3	D	20	LEU	CA-CB-CG	5.87	128.80	115.30
3	G	54	SER	N-CA-CB	-5.85	101.72	110.50
3	H	55	SER	C-N-CA	5.82	136.24	121.70
3	H	83	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	3	ASP	CA-CB-CG	5.79	126.13	113.40
3	H	37	MET	CA-CB-CG	-5.72	103.58	113.30
3	H	3	GLN	C-N-CA	5.70	135.95	121.70
3	F	59	ASP	CB-CA-C	5.66	121.72	110.40
2	C	228	SER	O-C-N	-5.65	113.67	122.70
1	A	154	ASP	C-N-CA	5.63	135.79	121.70
3	D	14	ASN	CA-CB-CG	5.58	125.68	113.40
1	A	110	GLU	CB-CG-CD	5.58	129.26	114.20
1	A	153	LEU	N-CA-CB	-5.53	99.34	110.40
3	G	72	LEU	CB-CA-C	5.53	120.71	110.20
1	A	17	LYS	O-C-N	-5.51	113.89	122.70
3	G	2	PRO	CA-N-CD	-5.49	103.81	111.50
3	G	83	GLU	CG-CD-OE1	5.46	129.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	54	SER	CB-CA-C	5.43	120.41	110.10
3	G	49	GLN	CA-CB-CG	5.43	125.34	113.40
3	G	2	PRO	O-C-N	-5.42	114.02	122.70
1	A	152	ASN	CB-CG-OD1	-5.38	110.84	121.60
1	A	57	ASP	CB-CG-OD2	-5.38	113.46	118.30
3	G	73	ARG	CA-CB-CG	5.34	125.15	113.40
3	E	54	SER	N-CA-C	5.31	125.33	111.00
3	D	7	ASP	CB-CG-OD1	-5.27	113.56	118.30
3	E	53	PRO	N-CA-C	5.25	125.76	112.10
3	G	2	PRO	CB-CA-C	5.25	125.13	112.00
1	A	148	ARG	NE-CZ-NH2	-5.25	117.68	120.30
3	E	87	THR	CA-CB-CG2	5.24	119.74	112.40
1	A	116	LEU	CA-CB-CG	5.20	127.26	115.30
3	H	22	ASP	CB-CG-OD2	5.20	122.98	118.30
2	C	239	GLU	O-C-N	-5.18	114.41	122.70
1	A	67	ARG	NE-CZ-NH2	-5.17	117.71	120.30
3	F	73	ARG	CG-CD-NE	5.17	122.66	111.80
3	F	29	GLU	CG-CD-OE1	-5.17	107.96	118.30
1	A	112	GLU	CB-CA-C	-5.17	100.06	110.40
3	G	2	PRO	N-CD-CG	-5.16	95.46	103.20
3	E	63	LYS	N-CA-CB	5.13	119.83	110.60
1	A	28	SER	CB-CA-C	5.12	119.83	110.10
1	A	52	PHE	CA-CB-CG	5.09	126.11	113.90
3	F	11	GLU	CA-CB-CG	5.07	124.56	113.40
3	H	103	ASN	CA-CB-CG	5.07	124.56	113.40
3	G	29	GLU	OE1-CD-OE2	5.07	129.39	123.30
3	H	20	LEU	CA-CB-CG	5.07	126.97	115.30
3	H	85	LEU	O-C-N	5.04	130.77	122.70
1	A	16	ILE	CA-C-N	5.04	128.28	117.20
3	H	103	ASN	N-CA-CB	5.03	119.66	110.60
3	D	84	LYS	CA-CB-CG	5.02	124.45	113.40
3	F	62	LYS	N-CA-CB	5.02	119.63	110.60
3	G	7	ASP	CB-CG-OD1	5.00	122.80	118.30
3	G	35	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ASP	Mainchain
1	A	11	ARG	Sidechain
1	A	121	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	125	TYR	Sidechain
1	A	127	TRP	Mainchain
1	A	13	PRO	Peptide
1	A	14	ASP	Mainchain
1	A	148	ARG	Sidechain
1	A	152	ASN	Sidechain
1	A	16	ILE	Mainchain
1	A	17	LYS	Mainchain
1	A	18	GLN	Mainchain
1	A	35	THR	Mainchain
1	A	52	PHE	Mainchain
1	A	88	LEU	Mainchain
2	C	235	ARG	Sidechain
2	C	239	GLU	Mainchain
3	D	18	TYR	Mainchain
3	D	35	ARG	Mainchain
3	D	40	ILE	Mainchain
3	D	48	PHE	Mainchain
3	D	67	ARG	Sidechain
3	D	71	THR	Mainchain
3	D	81	LYS	Mainchain
3	D	85	LEU	Mainchain
3	E	65	ILE	Mainchain
3	E	81	LYS	Mainchain
3	F	13	HIS	Mainchain
3	F	61	GLN	Mainchain
3	F	70	ASP	Mainchain
3	F	76	TYR	Sidechain
3	G	1	THR	Mainchain
3	G	11	GLU	Sidechain
3	G	27	TYR	Mainchain
3	G	44	ASN	Mainchain
3	G	50	VAL	Mainchain
3	G	66	GLU	Mainchain
3	G	8	LEU	Mainchain
3	G	80	ALA	Mainchain
3	G	94	HIS	Mainchain
3	H	39	ILE	Mainchain
3	H	4	ASN	Mainchain
3	H	47	ILE	Mainchain
3	H	50	VAL	Mainchain
3	H	53	PRO	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
3	H	54	SER	Mainchain
3	H	70	ASP	Mainchain
3	H	73	ARG	Sidechain
3	H	81	LYS	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1532	0	1419	201	2
2	C	370	0	355	93	0
3	D	819	0	823	209	0
3	E	819	0	822	226	2
3	F	819	0	823	158	0
3	G	819	0	823	117	0
3	H	819	0	821	133	0
4	A	35	0	0	6	0
4	C	4	0	0	1	0
4	D	24	0	0	6	0
4	E	19	0	0	1	0
4	F	19	0	0	1	0
4	G	19	0	0	4	0
4	H	18	0	0	0	0
All	All	6135	0	5886	983	2

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 83.

All (983) 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:A:129:ARG:NH2	1:A:131:HIS:HB3	1.25	1.47
2:C:235:ARG:HH22	2:C:239:GLU:CB	1.35	1.37
3:F:70:ASP:O	3:F:74:ILE:HG23	1.20	1.32
2:C:235:ARG:NH2	2:C:239:GLU:CB	1.90	1.30
1:A:170:GLU:HB3	1:A:192:ARG:NH2	1.47	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1:THR:CG2	3:H:2:PRO:HD2	1.64	1.27
3:G:55:SER:O	3:G:56:GLN:HG2	1.30	1.26
2:C:235:ARG:NH2	2:C:239:GLU:HB2	0.94	1.24
1:A:143:ARG:NH1	1:A:146:ARG:HH21	1.36	1.22
3:E:22:ASP:O	3:E:81:LYS:HA	1.03	1.19
3:D:5:ILE:HG23	3:D:84:LYS:HZ2	1.02	1.19
1:A:76:ILE:O	1:A:78:SER:N	1.76	1.19
2:C:228:SER:OG	3:D:74:ILE:HG13	1.01	1.18
3:H:1:THR:HG22	3:H:2:PRO:CD	1.74	1.17
1:A:32:ASP:HB3	1:A:35:THR:HB	1.21	1.17
3:E:22:ASP:O	3:E:81:LYS:CA	1.93	1.16
1:A:175:ARG:HA	1:A:180:ILE:CD1	1.77	1.14
1:A:189:ASN:HB3	1:A:191:PRO:HD2	1.18	1.14
1:A:143:ARG:NH1	1:A:146:ARG:NH2	1.95	1.13
1:A:185:PRO:CD	2:C:202:LYS:HG2	1.78	1.13
3:F:56:GLN:HG2	3:F:57:HIS:CE1	1.82	1.13
3:E:42:PHE:HZ	3:E:82:VAL:CG1	1.63	1.12
2:C:224:SER:OG	3:E:77:LEU:HB3	1.51	1.11
1:A:129:ARG:NH2	1:A:131:HIS:CB	2.12	1.11
2:C:228:SER:OG	3:D:74:ILE:CG1	1.98	1.10
3:E:83:GLU:HG2	3:E:84:LYS:HG3	1.29	1.10
1:A:68:SER:O	1:A:72:VAL:HG13	1.52	1.09
2:C:227:GLN:HA	2:C:230:ILE:HG12	1.33	1.09
3:D:48:PHE:CE2	3:D:85:LEU:HD23	1.87	1.09
3:F:56:GLN:HG2	3:F:57:HIS:ND1	1.69	1.08
3:E:5:ILE:CG2	3:E:84:LYS:HZ3	1.66	1.08
3:F:25:PHE:HE1	3:G:103:ASN:OXT	1.37	1.07
1:A:185:PRO:HD2	2:C:202:LYS:CG	1.85	1.06
3:E:89:ASN:C	3:E:89:ASN:HD22	1.58	1.05
3:F:29:GLU:OE2	3:G:71:THR:HG21	1.54	1.05
3:G:55:SER:O	3:G:56:GLN:CG	2.04	1.05
3:E:5:ILE:CG2	3:E:84:LYS:NZ	2.20	1.04
3:F:25:PHE:CE1	3:G:103:ASN:OXT	2.10	1.04
2:C:234:ASN:O	2:C:238:ASP:HB2	1.56	1.04
3:G:85:LEU:HD23	3:G:99:ILE:HD13	1.35	1.03
1:A:131:HIS:CE1	1:A:136:ASP:HB2	1.93	1.02
3:D:20:LEU:HD23	3:D:42:PHE:CZ	1.94	1.02
1:A:155:ILE:O	1:A:156:ALA:HB3	1.58	1.02
1:A:40:ASN:ND2	1:A:43:ASP:H	1.56	1.02
3:E:42:PHE:CZ	3:E:82:VAL:CG1	2.43	1.01
3:E:77:LEU:CD1	3:F:78:THR:HG21	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:ILE:HG23	3:D:84:LYS:NZ	1.74	1.01
3:F:33:GLY:O	3:F:34:LYS:HG2	1.58	1.00
2:C:227:GLN:HA	2:C:230:ILE:CG1	1.91	1.00
3:E:25:PHE:HA	3:F:103:ASN:ND2	1.78	0.98
1:A:175:ARG:HA	1:A:180:ILE:HD13	1.45	0.98
3:E:5:ILE:HG22	3:E:84:LYS:NZ	1.79	0.97
3:F:70:ASP:O	3:F:74:ILE:CG2	2.11	0.97
3:H:39:ILE:HD13	3:H:39:ILE:C	1.84	0.97
3:F:24:ILE:HG21	3:F:40:ILE:HG13	1.44	0.96
3:G:74:ILE:O	3:G:78:THR:HB	1.66	0.96
3:D:65:ILE:HD12	3:H:31:LEU:HD11	1.47	0.96
2:C:235:ARG:HH21	2:C:239:GLU:HB2	1.21	0.95
3:D:31:LEU:HD22	3:E:97:ALA:HA	1.46	0.95
3:E:42:PHE:CZ	3:E:82:VAL:HG13	2.02	0.95
1:A:185:PRO:HD2	2:C:202:LYS:HG2	0.96	0.95
1:A:175:ARG:HA	1:A:180:ILE:HD12	1.46	0.94
3:G:24:ILE:HG22	3:G:76:TYR:HD1	1.31	0.94
3:H:8:LEU:HD23	3:H:8:LEU:C	1.88	0.94
1:A:170:GLU:CB	1:A:192:ARG:NH2	2.31	0.94
3:E:80:ALA:C	3:E:81:LYS:HG2	1.88	0.94
3:E:42:PHE:HZ	3:E:82:VAL:HG11	1.29	0.94
3:F:58:ILE:HD13	3:F:60:SER:OG	1.68	0.94
2:C:218:VAL:O	2:C:222:ILE:HG22	1.68	0.94
3:G:103:ASN:ND2	3:G:103:ASN:O	2.01	0.94
2:C:217:LYS:NZ	4:C:106:HOH:O	2.00	0.93
3:D:14:ASN:HB3	3:D:90:ASN:ND2	1.83	0.93
3:D:58:ILE:HG22	3:D:60:SER:OG	1.68	0.93
3:F:56:GLN:CG	3:F:57:HIS:CE1	2.52	0.93
3:G:86:CYS:HB3	3:G:98:ALA:HB3	1.49	0.93
3:D:2:PRO:HG2	3:D:8:LEU:HD12	1.51	0.92
3:E:49:GLN:O	3:E:96:ILE:HD12	1.68	0.92
3:E:14:ASN:HB3	3:E:90:ASN:HB3	1.47	0.92
1:A:15:GLU:HA	1:A:18:GLN:HG2	1.50	0.92
2:C:240:LEU:HD12	3:F:63:LYS:NZ	1.85	0.91
3:E:22:ASP:O	3:E:81:LYS:HE2	1.69	0.91
3:F:30:SER:OG	3:F:35:ARG:O	1.87	0.91
3:E:83:GLU:CG	3:E:84:LYS:HG3	1.99	0.91
3:D:20:LEU:CD2	3:D:42:PHE:CZ	2.53	0.91
1:A:129:ARG:HH22	1:A:131:HIS:HB3	1.25	0.91
3:D:74:ILE:O	3:D:78:THR:HG22	1.72	0.90
1:A:189:ASN:HB3	1:A:191:PRO:CD	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:ILE:HD12	3:H:31:LEU:CD1	1.99	0.90
1:A:40:ASN:HD22	1:A:43:ASP:H	1.19	0.90
3:D:67:ARG:O	3:D:70:ASP:HB2	1.71	0.90
1:A:32:ASP:CB	1:A:35:THR:HB	2.01	0.90
3:E:5:ILE:HG22	3:E:84:LYS:HZ3	1.33	0.90
1:A:131:HIS:HE1	1:A:136:ASP:HB2	1.36	0.89
3:D:74:ILE:O	3:D:78:THR:CG2	2.20	0.89
3:E:33:GLY:O	3:E:34:LYS:HB2	1.67	0.89
3:G:18:TYR:HE1	3:G:87:THR:HG1	1.21	0.89
3:E:34:LYS:C	3:E:35:ARG:HD2	1.93	0.88
2:C:229:ASP:OD2	3:D:73:ARG:NH1	2.06	0.88
1:A:13:PRO:HD3	1:A:84:TYR:CE2	2.07	0.88
3:D:50:VAL:HG11	3:D:69:LYS:HG3	1.54	0.88
1:A:143:ARG:HH12	1:A:146:ARG:HH21	1.21	0.88
3:D:13:HIS:O	3:D:14:ASN:HB2	1.72	0.88
3:F:51:GLU:OE2	3:F:91:LYS:HE2	1.72	0.88
3:D:18:TYR:OH	3:D:94:HIS:HD2	1.57	0.88
3:D:58:ILE:O	3:D:61:GLN:HB2	1.75	0.87
3:E:14:ASN:HD22	3:E:90:ASN:CB	1.86	0.87
3:G:102:ALA:O	3:G:103:ASN:HB3	1.72	0.87
1:A:76:ILE:C	1:A:78:SER:H	1.77	0.86
3:F:58:ILE:CD1	3:F:60:SER:OG	2.23	0.86
3:G:43:LYS:H	3:G:43:LYS:HE2	1.40	0.86
3:D:5:ILE:CG2	3:D:84:LYS:NZ	2.39	0.86
2:C:220:ARG:O	2:C:224:SER:HB2	1.74	0.86
3:E:25:PHE:HA	3:F:103:ASN:HD21	1.38	0.86
3:D:91:LYS:NZ	3:E:1:THR:OG1	2.07	0.86
3:E:87:THR:CG2	3:E:94:HIS:HB3	2.06	0.85
3:F:74:ILE:O	3:F:78:THR:HB	1.76	0.85
2:C:228:SER:HG	3:D:74:ILE:CG1	1.85	0.85
3:D:2:PRO:HG3	3:D:11:GLU:OE1	1.76	0.85
2:C:228:SER:HG	3:D:74:ILE:HG13	1.06	0.85
3:E:77:LEU:HD12	3:F:78:THR:HG21	1.56	0.84
1:A:187:CYS:O	1:A:189:ASN:N	2.10	0.84
1:A:175:ARG:HD3	1:A:189:ASN:O	1.77	0.84
3:G:24:ILE:HG22	3:G:76:TYR:CD1	2.11	0.84
3:H:51:GLU:OE2	3:H:91:LYS:HE2	1.78	0.83
3:G:1:THR:HA	4:G:104:HOH:O	1.79	0.83
3:D:18:TYR:OH	3:D:94:HIS:CD2	2.32	0.83
3:D:49:GLN:HG2	3:D:93:PRO:O	1.79	0.83
3:D:54:SER:O	3:D:57:HIS:CD2	2.32	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:42:PHE:CD2	3:G:46:ALA:HB3	2.14	0.83
3:G:82:VAL:CG1	3:G:99:ILE:HD11	2.10	0.82
3:F:36:GLU:O	3:F:52:VAL:HG22	1.79	0.82
1:A:33:ARG:HH12	3:F:23:LYS:NZ	1.77	0.82
3:E:59:ASP:HA	3:E:62:LYS:HE2	1.59	0.82
3:G:58:ILE:O	3:G:62:LYS:HG3	1.79	0.82
3:G:99:ILE:HD12	3:G:100:SER:H	1.42	0.82
3:G:31:LEU:HD23	3:G:31:LEU:C	2.00	0.82
1:A:170:GLU:HB3	1:A:192:ARG:HH21	1.40	0.82
3:H:48:PHE:CE1	3:H:87:THR:HG21	2.14	0.82
2:C:230:ILE:HG13	2:C:231:ASP:H	1.42	0.81
3:D:73:ARG:HG3	3:D:73:ARG:O	1.80	0.81
3:D:96:ILE:O	3:D:96:ILE:HG22	1.78	0.81
1:A:72:VAL:O	1:A:76:ILE:HD12	1.79	0.81
1:A:139:LEU:O	1:A:141:ARG:NH2	2.14	0.81
3:D:76:TYR:O	3:D:78:THR:N	2.14	0.81
3:G:85:LEU:CD2	3:G:99:ILE:HD13	2.11	0.81
3:G:18:TYR:OH	3:G:94:HIS:CD2	2.34	0.81
1:A:18:GLN:HG3	1:A:19:SER:N	1.96	0.80
1:A:91:ALA:HB1	1:A:92:PRO:HD2	1.64	0.80
1:A:15:GLU:CA	1:A:18:GLN:HG2	2.11	0.80
2:C:227:GLN:O	2:C:230:ILE:HG13	1.82	0.80
3:D:20:LEU:HD23	3:D:42:PHE:CE2	2.16	0.80
3:G:2:PRO:HB2	3:G:8:LEU:HD23	1.63	0.80
1:A:48:THR:O	1:A:49:GLN:HB2	1.80	0.80
3:D:28:THR:OG1	3:D:39:ILE:CG2	2.30	0.80
3:F:15:THR:HG21	3:F:86:CYS:SG	2.21	0.80
3:E:89:ASN:ND2	3:E:89:ASN:C	2.31	0.79
1:A:143:ARG:HH11	1:A:146:ARG:HH21	1.28	0.79
3:E:15:THR:OG1	3:E:86:CYS:SG	2.41	0.79
2:C:198:THR:O	2:C:202:LYS:HB2	1.82	0.79
3:E:83:GLU:HG2	3:E:84:LYS:N	1.96	0.79
3:D:56:GLN:HE21	3:D:57:HIS:CE1	2.00	0.79
3:H:24:ILE:HG22	3:H:26:SER:O	1.82	0.79
1:A:15:GLU:O	1:A:18:GLN:CG	2.31	0.79
1:A:88:LEU:HD23	1:A:119:ILE:HG21	1.63	0.79
1:A:129:ARG:HH22	1:A:131:HIS:CB	1.86	0.78
2:C:197:ASN:O	2:C:201:GLU:HB2	1.84	0.78
1:A:143:ARG:HH21	3:D:80:ALA:HA	1.46	0.78
1:A:27:GLN:OE1	1:A:35:THR:CG2	2.31	0.78
3:E:67:ARG:HH11	3:E:67:ARG:HG3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:28:THR:CB	3:D:39:ILE:CG2	2.63	0.77
3:F:27:TYR:HD1	3:F:40:ILE:HD11	1.47	0.77
3:E:28:THR:O	3:E:38:ALA:HA	1.84	0.77
3:E:47:ILE:HG21	3:F:3:GLN:HB3	1.65	0.77
3:D:41:THR:HG23	4:D:125:HOH:O	1.85	0.77
3:E:59:ASP:CG	3:E:62:LYS:HZ1	1.86	0.77
3:E:9:CYS:SG	3:E:15:THR:OG1	2.42	0.77
3:G:18:TYR:OH	3:G:94:HIS:NE2	2.18	0.77
3:E:59:ASP:OD1	3:E:62:LYS:NZ	2.17	0.77
3:E:65:ILE:O	3:E:69:LYS:HG3	1.85	0.76
1:A:129:ARG:HH21	1:A:131:HIS:HB3	0.96	0.76
3:G:33:GLY:N	3:H:61:GLN:NE2	2.34	0.76
3:D:8:LEU:O	3:D:11:GLU:HB2	1.86	0.76
3:F:50:VAL:HG12	3:F:65:ILE:CG2	2.15	0.76
3:D:26:SER:OG	3:D:41:THR:CG2	2.33	0.76
3:D:2:PRO:CG	3:D:8:LEU:HD12	2.15	0.76
1:A:175:ARG:CA	1:A:180:ILE:HD13	2.15	0.76
3:D:5:ILE:CG2	3:D:84:LYS:HZ2	1.89	0.76
1:A:70:HIS:CD2	1:A:74:GLN:OE1	2.39	0.76
3:F:27:TYR:HD1	3:F:40:ILE:CD1	1.99	0.75
2:C:235:ARG:HD2	3:F:67:ARG:HB2	1.67	0.75
2:C:227:GLN:NE2	3:F:74:ILE:HA	2.00	0.75
1:A:190:ALA:N	1:A:191:PRO:CD	2.48	0.75
3:D:35:ARG:NH2	3:E:2:PRO:HD3	2.02	0.75
3:D:28:THR:CB	3:D:39:ILE:HG22	2.16	0.75
3:D:47:ILE:HD13	3:E:3:GLN:HG2	1.69	0.75
3:D:32:ALA:O	3:D:35:ARG:O	2.04	0.75
1:A:98:ASN:OD1	1:A:111:GLN:HG2	1.87	0.75
2:C:235:ARG:HH22	2:C:239:GLU:HB3	1.50	0.74
3:F:84:LYS:HB2	3:F:100:SER:OG	1.85	0.74
3:E:5:ILE:HG21	3:E:84:LYS:NZ	2.01	0.74
3:F:93:PRO:HD2	3:G:1:THR:H3	1.51	0.74
3:H:36:GLU:H	3:H:36:GLU:CD	1.89	0.74
3:E:59:ASP:HA	3:E:62:LYS:CE	2.17	0.74
3:H:18:TYR:HB3	3:H:20:LEU:CD2	2.18	0.74
3:E:14:ASN:HD22	3:E:90:ASN:HB2	1.52	0.74
3:E:54:SER:HA	3:E:57:HIS:HB2	1.68	0.74
3:D:47:ILE:O	3:D:48:PHE:CD1	2.41	0.74
3:D:67:ARG:NH1	3:H:69:LYS:HB2	2.03	0.74
3:D:14:ASN:HB3	3:D:90:ASN:HD22	1.53	0.73
3:E:62:LYS:O	3:E:66:GLU:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:61:GLN:O	3:E:64:ALA:N	2.18	0.73
1:A:148:ARG:CZ	3:E:79:GLU:O	2.36	0.73
2:C:230:ILE:HG13	2:C:231:ASP:N	2.04	0.73
3:F:19:THR:HG23	3:F:84:LYS:NZ	2.02	0.73
1:A:76:ILE:HG22	1:A:77:LEU:N	2.03	0.73
3:F:56:GLN:CG	3:F:57:HIS:HE1	2.00	0.73
2:C:234:ASN:O	2:C:238:ASP:CB	2.33	0.72
3:D:67:ARG:NH2	3:H:70:ASP:OD1	2.22	0.72
3:F:69:LYS:CB	3:G:67:ARG:NH2	2.52	0.72
2:C:228:SER:HB2	3:D:77:LEU:HD23	1.71	0.72
3:G:46:ALA:HB1	3:G:48:PHE:CE1	2.25	0.72
1:A:129:ARG:NH2	1:A:131:HIS:CG	2.56	0.72
1:A:15:GLU:O	1:A:18:GLN:HG2	1.88	0.72
3:D:5:ILE:HG12	3:D:17:ILE:HD11	1.71	0.72
2:C:224:SER:OG	3:E:77:LEU:CB	2.35	0.72
2:C:230:ILE:CG2	3:H:74:ILE:HD13	2.18	0.72
2:C:227:GLN:HE22	3:F:74:ILE:HA	1.53	0.72
3:E:89:ASN:HA	3:E:94:HIS:ND1	2.04	0.72
2:C:219:LYS:O	2:C:223:PHE:HB2	1.90	0.72
3:H:18:TYR:HB3	3:H:20:LEU:HD21	1.71	0.72
1:A:86:TYR:O	1:A:88:LEU:HD12	1.89	0.72
3:H:18:TYR:O	3:H:84:LYS:HA	1.90	0.71
3:D:16:GLN:OE1	3:D:89:ASN:HB3	1.90	0.71
3:D:28:THR:HB	3:D:39:ILE:CG2	2.20	0.71
3:F:33:GLY:O	3:F:34:LYS:CG	2.37	0.71
1:A:4:LYS:HG2	1:A:87:VAL:CG1	2.20	0.71
3:E:14:ASN:CB	3:E:90:ASN:HB3	2.20	0.71
3:E:48:PHE:HE1	3:E:87:THR:HG21	1.55	0.71
3:H:8:LEU:HD23	3:H:8:LEU:O	1.89	0.71
1:A:33:ARG:HH12	3:F:23:LYS:HZ3	1.36	0.71
3:E:76:TYR:CZ	3:F:101:MET:O	2.43	0.71
3:D:47:ILE:HG21	3:E:3:GLN:HG3	1.72	0.71
3:D:47:ILE:CD1	3:E:3:GLN:HG2	2.21	0.71
1:A:96:ASN:O	1:A:100:VAL:HG23	1.91	0.71
3:D:58:ILE:CG2	3:D:60:SER:OG	2.38	0.71
1:A:14:ASP:OD2	4:A:197:HOH:O	2.09	0.71
3:D:28:THR:OG1	3:D:39:ILE:HG21	1.89	0.71
1:A:27:GLN:OE1	1:A:35:THR:HG22	1.91	0.71
1:A:9:ASP:HB3	1:A:86:TYR:HE2	1.55	0.71
2:C:227:GLN:HB2	2:C:231:ASP:OD1	1.91	0.70
3:G:4:ASN:O	3:G:8:LEU:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:HH12	1:A:55:HIS:HB3	1.55	0.70
1:A:129:ARG:HH22	1:A:131:HIS:CG	2.08	0.70
2:C:227:GLN:CA	2:C:230:ILE:HG12	2.17	0.70
3:D:47:ILE:HG21	3:E:3:GLN:CG	2.21	0.70
3:E:42:PHE:CE2	3:E:82:VAL:HG13	2.26	0.70
3:D:14:ASN:O	3:D:88:TRP:HD1	1.74	0.70
3:E:5:ILE:HG12	3:E:5:ILE:O	1.92	0.70
1:A:155:ILE:O	1:A:156:ALA:CB	2.27	0.70
3:E:58:ILE:HG22	3:E:60:SER:H	1.57	0.70
3:H:29:GLU:O	3:H:29:GLU:CG	2.40	0.70
1:A:190:ALA:H	1:A:191:PRO:HD3	1.56	0.70
3:F:53:PRO:HA	3:F:57:HIS:CD2	2.26	0.69
3:E:77:LEU:HD11	3:F:78:THR:HG21	1.74	0.69
3:F:69:LYS:HB2	3:G:67:ARG:NH2	2.07	0.69
1:A:129:ARG:HH21	1:A:131:HIS:CB	1.87	0.69
2:C:240:LEU:HD12	3:F:63:LYS:HZ2	1.54	0.69
3:G:74:ILE:HD12	3:G:77:LEU:HB2	1.74	0.69
3:H:37:MET:HG3	3:H:38:ALA:N	2.06	0.69
3:H:68:MET:O	3:H:68:MET:HG3	1.90	0.69
3:E:20:LEU:O	3:E:21:ASN:C	2.30	0.69
1:A:12:PRO:HA	1:A:84:TYR:CE2	2.27	0.69
3:E:33:GLY:O	3:E:34:LYS:CB	2.41	0.69
1:A:88:LEU:O	1:A:89:ALA:O	2.11	0.69
3:F:31:LEU:HG	3:F:31:LEU:O	1.93	0.69
2:C:227:GLN:O	2:C:228:SER:O	2.10	0.69
1:A:188:GLY:O	1:A:189:ASN:HB2	1.91	0.69
3:D:20:LEU:HD22	3:D:82:VAL:HG11	1.75	0.69
3:E:14:ASN:HD22	3:E:90:ASN:HB3	1.57	0.69
3:D:26:SER:OG	3:D:41:THR:HG21	1.92	0.69
3:G:54:SER:OG	3:G:57:HIS:HD2	1.74	0.68
3:H:65:ILE:HG22	3:H:66:GLU:OE1	1.93	0.68
1:A:107:HIS:O	1:A:110:GLU:HB2	1.93	0.68
3:D:23:LYS:HB3	3:D:81:LYS:HG3	1.73	0.68
3:H:29:GLU:O	3:H:29:GLU:HG3	1.91	0.68
1:A:76:ILE:HG22	1:A:77:LEU:H	1.58	0.68
3:F:87:THR:CG2	3:F:94:HIS:HB3	2.23	0.68
3:F:69:LYS:CB	3:G:67:ARG:HH21	2.07	0.68
3:D:36:GLU:O	3:D:52:VAL:HA	1.94	0.68
1:A:82:THR:HA	1:A:130:VAL:O	1.93	0.68
2:C:239:GLU:OE1	2:C:239:GLU:HA	1.94	0.68
3:F:67:ARG:HH11	3:F:67:ARG:HG3	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:PRO:CB	3:D:8:LEU:HD12	2.23	0.68
3:H:5:ILE:HD11	3:H:98:ALA:HB3	1.76	0.68
3:E:13:HIS:CD2	3:E:13:HIS:C	2.67	0.68
1:A:132:PHE:H	1:A:132:PHE:HD1	1.42	0.68
2:C:223:PHE:O	2:C:227:GLN:HG2	1.94	0.67
2:C:239:GLU:O	2:C:240:LEU:HB2	1.94	0.67
3:H:5:ILE:CD1	3:H:98:ALA:HB3	2.24	0.67
3:E:80:ALA:O	3:E:81:LYS:HG2	1.95	0.67
3:D:48:PHE:CD2	3:D:85:LEU:HD23	2.30	0.67
3:D:68:MET:C	3:D:70:ASP:H	1.98	0.67
3:G:23:LYS:O	3:G:43:LYS:NZ	2.27	0.67
3:F:83:GLU:HG3	3:F:84:LYS:N	2.09	0.67
3:E:74:ILE:HD13	3:E:74:ILE:C	2.15	0.67
3:D:19:THR:HG21	4:D:106:HOH:O	1.95	0.67
3:F:70:ASP:OD1	3:G:67:ARG:NH1	2.27	0.67
3:D:48:PHE:HE2	3:D:85:LEU:HD23	1.56	0.67
3:D:32:ALA:HB1	3:E:12:TYR:CE2	2.29	0.67
3:G:33:GLY:N	3:H:61:GLN:HE21	1.93	0.66
3:E:23:LYS:HA	3:E:80:ALA:HB3	1.78	0.66
3:E:5:ILE:HG21	3:E:84:LYS:HZ2	1.60	0.66
1:A:15:GLU:O	1:A:18:GLN:HG3	1.95	0.66
3:E:67:ARG:NH1	3:E:67:ARG:HG3	2.10	0.66
3:F:83:GLU:HG3	3:F:100:SER:OG	1.95	0.66
3:G:54:SER:OG	3:G:57:HIS:CD2	2.47	0.66
3:F:52:VAL:O	3:F:54:SER:N	2.22	0.66
3:E:58:ILE:O	3:E:61:GLN:HB2	1.94	0.66
3:H:88:TRP:CZ3	3:H:97:ALA:HB2	2.31	0.66
3:F:87:THR:HG23	3:F:94:HIS:HB3	1.76	0.66
3:D:70:ASP:OD1	3:E:67:ARG:NH1	2.28	0.66
3:H:36:GLU:N	3:H:36:GLU:CD	2.49	0.66
2:C:233:HIS:CE1	3:D:67:ARG:HG3	2.30	0.66
1:A:143:ARG:HH12	1:A:146:ARG:NH2	1.81	0.66
3:H:39:ILE:CD1	3:H:39:ILE:C	2.62	0.66
3:G:46:ALA:HB1	3:G:48:PHE:HE1	1.60	0.66
3:D:81:LYS:NZ	3:D:103:ASN:O	2.29	0.65
1:A:174:TRP:HA	1:A:174:TRP:CE3	2.31	0.65
1:A:106:PRO:O	1:A:107:HIS:CD2	2.49	0.65
3:E:76:TYR:OH	3:F:101:MET:O	2.14	0.65
3:E:48:PHE:CE1	3:E:87:THR:HG21	2.31	0.65
1:A:4:LYS:HG2	1:A:87:VAL:HG13	1.77	0.65
1:A:69:ALA:O	1:A:72:VAL:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:26:SER:HB2	3:E:41:THR:HB	1.78	0.65
1:A:190:ALA:HB3	1:A:191:PRO:HD3	1.77	0.65
3:F:29:GLU:OE2	3:G:71:THR:CG2	2.40	0.65
2:C:227:GLN:NE2	3:F:74:ILE:HB	2.11	0.65
3:D:2:PRO:HD3	3:H:35:ARG:HH21	1.62	0.65
3:F:54:SER:HB2	3:F:56:GLN:OE1	1.96	0.65
1:A:12:PRO:HA	1:A:84:TYR:HE2	1.62	0.65
3:G:2:PRO:HB2	3:G:8:LEU:CD2	2.27	0.65
3:H:1:THR:CG2	3:H:2:PRO:CD	2.53	0.65
3:E:83:GLU:CG	3:E:84:LYS:N	2.60	0.65
3:F:46:ALA:HB1	3:F:48:PHE:CZ	2.31	0.65
3:E:42:PHE:CZ	3:E:82:VAL:HG11	2.21	0.65
3:E:89:ASN:HD22	3:E:90:ASN:N	1.95	0.65
3:E:58:ILE:CG2	3:E:60:SER:OG	2.44	0.65
3:F:78:THR:HG22	3:F:80:ALA:H	1.61	0.64
3:D:28:THR:HB	3:D:39:ILE:HG22	1.78	0.64
3:E:44:ASN:O	3:E:44:ASN:OD1	2.14	0.64
3:D:47:ILE:HD12	3:E:3:GLN:OE1	1.96	0.64
3:E:35:ARG:HD2	3:E:35:ARG:N	2.11	0.64
3:E:20:LEU:HD22	3:E:42:PHE:CD2	2.32	0.64
3:D:52:VAL:O	3:D:54:SER:N	2.31	0.64
3:F:90:ASN:N	3:F:90:ASN:OD1	2.29	0.64
3:D:15:THR:CG2	3:D:88:TRP:NE1	2.61	0.64
3:F:15:THR:CG2	3:F:86:CYS:SG	2.86	0.64
3:F:21:ASN:HA	3:F:83:GLU:HA	1.80	0.64
3:E:67:ARG:CG	3:E:67:ARG:HH11	2.08	0.64
3:H:66:GLU:OE1	3:H:69:LYS:NZ	2.25	0.64
3:E:89:ASN:HA	3:E:94:HIS:CE1	2.33	0.64
3:G:48:PHE:CE2	3:G:87:THR:HG21	2.32	0.64
3:E:72:LEU:HA	3:E:75:ALA:HB3	1.78	0.64
3:G:99:ILE:HD12	3:G:100:SER:N	2.13	0.64
3:F:69:LYS:HB3	3:G:67:ARG:HH21	1.63	0.63
1:A:190:ALA:H	1:A:191:PRO:CD	2.08	0.63
3:E:54:SER:OG	3:E:62:LYS:NZ	2.30	0.63
3:G:42:PHE:HB2	3:G:46:ALA:HB3	1.80	0.63
1:A:31:PHE:CE1	2:C:219:LYS:HG3	2.32	0.63
3:D:28:THR:CB	3:D:39:ILE:HG21	2.28	0.63
3:H:51:GLU:OE2	3:H:91:LYS:CE	2.46	0.63
3:F:24:ILE:HD13	3:F:42:PHE:CZ	2.34	0.63
3:F:19:THR:HG23	3:F:84:LYS:HZ2	1.62	0.63
3:D:20:LEU:HD21	3:D:42:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2:PRO:HB2	3:D:8:LEU:HD12	1.81	0.63
3:F:93:PRO:CD	3:G:1:THR:H3	2.11	0.63
2:C:227:GLN:CA	2:C:230:ILE:CG1	2.72	0.63
1:A:33:ARG:NH1	3:F:23:LYS:NZ	2.47	0.63
1:A:143:ARG:HD3	1:A:144:GLY:N	2.13	0.63
3:G:61:GLN:O	3:G:65:ILE:HG13	1.98	0.63
3:H:1:THR:HG22	3:H:2:PRO:HD2	0.77	0.62
3:F:50:VAL:HG12	3:F:65:ILE:HG23	1.81	0.62
3:D:32:ALA:HB1	3:E:12:TYR:CZ	2.34	0.62
3:E:68:MET:O	3:E:70:ASP:N	2.32	0.62
2:C:233:HIS:CE1	3:H:73:ARG:HH22	2.17	0.62
3:F:92:THR:O	3:G:1:THR:N	2.32	0.62
3:E:77:LEU:HD12	3:F:78:THR:CG2	2.30	0.62
3:G:3:GLN:O	3:G:4:ASN:HB3	2.00	0.62
3:G:40:ILE:HG13	3:G:40:ILE:O	1.98	0.62
3:H:87:THR:HB	3:H:94:HIS:HB3	1.82	0.62
4:D:109:HOH:O	3:E:1:THR:HG21	2.00	0.62
3:E:24:ILE:HD13	3:E:40:ILE:HG13	1.81	0.62
1:A:59:TYR:CZ	1:A:116:LEU:HD22	2.34	0.62
3:D:1:THR:HG22	3:D:2:PRO:HD2	1.81	0.62
3:F:73:ARG:HA	3:F:76:TYR:HB3	1.80	0.62
3:G:58:ILE:O	3:G:62:LYS:CG	2.47	0.62
3:E:80:ALA:O	3:E:81:LYS:CG	2.47	0.61
1:A:143:ARG:NH2	3:D:80:ALA:HA	2.14	0.61
3:D:8:LEU:HD21	3:H:30:SER:HB2	1.83	0.61
1:A:143:ARG:HD3	1:A:144:GLY:H	1.65	0.61
1:A:106:PRO:O	1:A:107:HIS:CG	2.53	0.61
3:F:27:TYR:CD1	3:F:40:ILE:HD11	2.34	0.61
3:F:67:ARG:NH1	3:F:67:ARG:HG3	2.13	0.61
3:D:96:ILE:O	3:D:96:ILE:CG2	2.47	0.61
3:E:14:ASN:ND2	3:E:90:ASN:HB3	2.15	0.61
3:E:58:ILE:CG2	3:E:60:SER:H	2.13	0.61
3:E:58:ILE:HG22	3:E:60:SER:OG	2.01	0.61
3:E:82:VAL:HG23	3:E:99:ILE:HD13	1.83	0.61
3:D:15:THR:HG22	3:D:88:TRP:CD1	2.35	0.60
1:A:40:ASN:ND2	1:A:43:ASP:OD2	2.34	0.60
3:H:5:ILE:CD1	3:H:98:ALA:CB	2.79	0.60
1:A:175:ARG:HD2	1:A:180:ILE:HD11	1.83	0.60
3:D:48:PHE:CE2	3:D:85:LEU:CD2	2.75	0.60
3:H:68:MET:HE3	3:H:99:ILE:HG21	1.84	0.60
1:A:173:ALA:O	1:A:179:TRP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:58:ILE:O	3:H:60:SER:N	2.35	0.60
3:D:65:ILE:HD12	3:H:31:LEU:HD12	1.81	0.60
1:A:77:LEU:H	1:A:77:LEU:HD22	1.67	0.60
1:A:185:PRO:CG	2:C:202:LYS:HG2	2.32	0.60
3:E:58:ILE:HG22	3:E:60:SER:N	2.17	0.59
3:G:9:CYS:C	3:G:11:GLU:H	2.04	0.59
2:C:227:GLN:HA	2:C:230:ILE:CD1	2.32	0.59
3:E:54:SER:OG	3:E:62:LYS:HD2	2.03	0.59
1:A:13:PRO:HD3	1:A:84:TYR:CZ	2.36	0.59
3:H:14:ASN:OD1	3:H:14:ASN:N	2.36	0.59
3:E:24:ILE:CG2	3:E:26:SER:O	2.51	0.59
3:E:27:TYR:OH	3:E:29:GLU:HG3	2.02	0.59
1:A:190:ALA:N	1:A:191:PRO:HD3	2.16	0.59
3:H:41:THR:HG22	3:H:47:ILE:HG23	1.84	0.59
3:D:39:ILE:CG2	3:D:39:ILE:O	2.49	0.59
3:G:58:ILE:HD12	3:G:60:SER:OG	2.02	0.59
3:G:91:LYS:HD2	4:G:107:HOH:O	2.02	0.59
3:H:57:HIS:O	3:H:58:ILE:C	2.41	0.59
1:A:132:PHE:N	1:A:132:PHE:CD1	2.70	0.59
1:A:143:ARG:HH11	1:A:146:ARG:NH2	1.89	0.59
1:A:174:TRP:CE3	1:A:183:ALA:HB2	2.37	0.59
3:F:58:ILE:HD11	3:F:60:SER:OG	2.02	0.59
3:E:20:LEU:O	3:E:22:ASP:N	2.36	0.58
3:F:83:GLU:OE1	3:F:84:LYS:HD2	2.03	0.58
3:D:56:GLN:HE21	3:D:57:HIS:HE1	1.47	0.58
3:D:35:ARG:CZ	3:E:2:PRO:HD3	2.32	0.58
2:C:227:GLN:O	2:C:231:ASP:HB2	2.03	0.58
3:E:49:GLN:O	3:E:96:ILE:CD1	2.49	0.58
3:F:58:ILE:HG12	3:F:59:ASP:N	2.17	0.58
3:G:32:ALA:C	3:H:61:GLN:HE21	2.07	0.58
1:A:98:ASN:HD21	1:A:108:PRO:HA	1.67	0.58
2:C:229:ASP:OD1	3:D:73:ARG:HG2	2.04	0.58
3:F:9:CYS:SG	3:F:15:THR:CG2	2.92	0.58
3:D:78:THR:HG23	3:D:80:ALA:HB2	1.86	0.58
1:A:170:GLU:CB	1:A:192:ARG:HH21	2.05	0.58
3:D:14:ASN:HB3	3:D:90:ASN:HD21	1.65	0.58
3:D:27:TYR:HD1	3:D:40:ILE:HD11	1.66	0.58
1:A:88:LEU:CD2	1:A:119:ILE:HG21	2.34	0.58
2:C:227:GLN:HE21	3:F:74:ILE:HB	1.69	0.58
3:E:15:THR:HA	3:E:87:THR:O	2.04	0.58
1:A:35:THR:HG22	1:A:35:THR:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:C	1:A:18:GLN:HG2	2.23	0.57
2:C:229:ASP:HB2	3:D:74:ILE:HB	1.86	0.57
3:D:50:VAL:HG11	3:D:69:LYS:CG	2.29	0.57
3:G:42:PHE:HD2	3:G:46:ALA:HB3	1.67	0.57
1:A:148:ARG:NH1	3:E:79:GLU:O	2.38	0.57
3:H:74:ILE:O	3:H:78:THR:HB	2.04	0.57
2:C:203:THR:O	2:C:206:LEU:HB2	2.05	0.57
3:F:57:HIS:N	3:F:57:HIS:ND1	2.51	0.57
3:D:5:ILE:CG2	3:D:84:LYS:HZ1	2.15	0.57
3:H:37:MET:CG	3:H:38:ALA:N	2.62	0.57
3:H:68:MET:O	3:H:72:LEU:HG	2.03	0.57
3:H:75:ALA:O	3:H:80:ALA:N	2.38	0.57
3:D:54:SER:O	3:D:57:HIS:HD2	1.86	0.57
3:D:34:LYS:HE2	3:E:58:ILE:HG13	1.87	0.57
3:E:87:THR:HG23	3:E:94:HIS:HB3	1.85	0.57
3:E:65:ILE:O	3:E:65:ILE:HG22	2.05	0.57
3:D:5:ILE:HB	3:H:28:THR:HG21	1.87	0.57
3:E:89:ASN:ND2	3:E:90:ASN:N	2.53	0.56
3:F:27:TYR:CD1	3:F:40:ILE:CD1	2.86	0.56
3:G:31:LEU:HD23	3:G:32:ALA:N	2.20	0.56
2:C:231:ASP:OD2	3:F:74:ILE:CG2	2.54	0.56
3:E:73:ARG:O	3:E:77:LEU:HD23	2.05	0.56
3:E:83:GLU:HG2	3:E:84:LYS:CG	2.19	0.56
1:A:40:ASN:CG	1:A:43:ASP:OD2	2.43	0.56
3:D:67:ARG:NH1	3:H:70:ASP:OD1	2.38	0.56
3:F:20:LEU:HD23	3:F:85:LEU:HD23	1.87	0.56
3:D:82:VAL:HG22	3:D:99:ILE:HD11	1.88	0.56
3:G:2:PRO:CB	3:G:8:LEU:HD23	2.35	0.56
3:F:31:LEU:CG	3:F:31:LEU:O	2.52	0.56
2:C:232:THR:HG21	3:D:73:ARG:HH22	1.69	0.56
3:D:103:ASN:OD1	3:H:25:PHE:HE1	1.89	0.56
3:G:31:LEU:C	3:G:31:LEU:CD2	2.73	0.56
2:C:230:ILE:HG21	3:H:74:ILE:HD13	1.88	0.56
3:E:89:ASN:C	3:E:91:LYS:H	2.09	0.56
3:F:31:LEU:HB2	3:G:64:ALA:HB1	1.88	0.56
3:E:74:ILE:HD12	3:E:74:ILE:H	1.69	0.56
2:C:230:ILE:HG23	3:H:74:ILE:HD13	1.87	0.56
3:G:54:SER:HB2	3:G:55:SER:O	2.05	0.56
3:E:82:VAL:CG2	3:E:99:ILE:HD13	2.35	0.56
1:A:16:ILE:HD13	1:A:22:LEU:HD23	1.88	0.56
3:E:13:HIS:CD2	3:E:13:HIS:O	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASN:ND2	1:A:3:ASP:CG	2.59	0.56
1:A:109:ASP:HB2	1:A:110:GLU:OE1	2.06	0.55
1:A:110:GLU:HG3	4:A:217:HOH:O	2.05	0.55
1:A:63:SER:HB2	1:A:69:ALA:HB2	1.88	0.55
3:E:25:PHE:O	3:F:102:ALA:HA	2.06	0.55
3:H:90:ASN:HD22	3:H:91:LYS:HD3	1.72	0.55
3:G:31:LEU:HA	3:H:64:ALA:HB1	1.89	0.55
3:F:56:GLN:OE1	3:F:57:HIS:CE1	2.60	0.55
3:F:32:ALA:O	3:F:35:ARG:HB2	2.06	0.55
1:A:92:PRO:HD3	1:A:153:LEU:HG	1.88	0.55
1:A:81:SER:O	1:A:130:VAL:O	2.24	0.55
3:E:27:TYR:HD1	3:E:40:ILE:HD11	1.71	0.55
1:A:64:ILE:O	1:A:64:ILE:HG13	2.05	0.55
1:A:54:ARG:HG3	1:A:61:SER:HB3	1.89	0.55
3:E:76:TYR:O	3:E:77:LEU:C	2.45	0.55
3:G:82:VAL:HG11	3:G:99:ILE:HD11	1.87	0.55
3:D:73:ARG:O	3:D:73:ARG:CG	2.52	0.55
3:G:26:SER:HA	3:H:101:MET:O	2.07	0.55
3:D:99:ILE:O	3:H:28:THR:HA	2.06	0.55
3:D:68:MET:O	3:D:70:ASP:N	2.40	0.55
1:A:12:PRO:HB2	1:A:14:ASP:OD2	2.07	0.55
1:A:91:ALA:O	1:A:94:MET:HG2	2.07	0.55
3:G:35:ARG:HE	3:H:11:GLU:CD	2.10	0.55
1:A:176:GLU:O	1:A:180:ILE:HB	2.07	0.55
3:H:4:ASN:HB3	3:H:6:THR:H	1.72	0.55
1:A:175:ARG:C	1:A:180:ILE:HD13	2.28	0.54
1:A:119:ILE:HG23	1:A:123:GLN:HB3	1.88	0.54
3:D:73:ARG:HH11	3:D:73:ARG:HB3	1.72	0.54
3:D:14:ASN:O	3:D:88:TRP:CD1	2.59	0.54
3:F:46:ALA:HB1	3:F:48:PHE:CE2	2.41	0.54
3:G:2:PRO:CB	3:G:8:LEU:CD2	2.85	0.54
1:A:129:ARG:NH2	1:A:131:HIS:ND1	2.56	0.54
3:D:4:ASN:C	3:D:4:ASN:OD1	2.45	0.54
3:G:16:GLN:CD	3:G:89:ASN:HD22	2.11	0.54
3:E:82:VAL:CG2	3:E:99:ILE:CD1	2.85	0.54
3:D:11:GLU:HB3	3:D:12:TYR:CD1	2.43	0.54
3:F:84:LYS:CB	3:F:100:SER:OG	2.53	0.54
3:F:69:LYS:HB3	3:G:67:ARG:NH2	2.20	0.54
1:A:170:GLU:HB3	1:A:192:ARG:CZ	2.33	0.54
3:F:37:MET:HA	3:F:69:LYS:NZ	2.23	0.54
3:F:79:GLU:O	3:F:80:ALA:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:22:ASP:O	3:E:81:LYS:CE	2.52	0.54
3:D:48:PHE:CD2	3:D:85:LEU:CD2	2.91	0.54
3:G:20:LEU:HD11	3:G:85:LEU:HD12	1.89	0.54
3:H:8:LEU:CD2	3:H:8:LEU:C	2.67	0.54
3:H:88:TRP:CE3	3:H:97:ALA:HB2	2.42	0.54
1:A:16:ILE:CD1	1:A:22:LEU:CD2	2.86	0.54
3:D:26:SER:HG	3:D:41:THR:HG21	1.71	0.54
1:A:40:ASN:HD22	1:A:43:ASP:N	1.96	0.54
3:F:56:GLN:CD	3:F:57:HIS:CE1	2.81	0.54
3:G:25:PHE:CD2	3:G:41:THR:HG22	2.43	0.54
3:E:19:THR:HG22	3:E:21:ASN:OD1	2.07	0.53
3:E:30:SER:O	3:E:36:GLU:OE1	2.26	0.53
3:E:58:ILE:HG21	3:E:60:SER:OG	2.08	0.53
1:A:16:ILE:CD1	1:A:22:LEU:HD23	2.38	0.53
3:H:58:ILE:HG22	3:H:59:ASP:OD1	2.08	0.53
1:A:119:ILE:CG2	1:A:123:GLN:HB3	2.39	0.53
3:F:24:ILE:HG21	3:F:40:ILE:CG1	2.28	0.53
3:E:17:ILE:HG22	3:E:18:TYR:N	2.22	0.53
3:H:39:ILE:HD13	3:H:40:ILE:N	2.24	0.53
3:H:87:THR:HA	3:H:95:ALA:O	2.07	0.53
2:C:202:LYS:O	2:C:206:LEU:HG	2.08	0.53
1:A:13:PRO:HB3	1:A:127:TRP:CZ2	2.44	0.53
3:D:3:GLN:OE1	3:H:47:ILE:HD13	2.08	0.53
3:E:83:GLU:CD	3:E:84:LYS:HE3	2.29	0.53
3:D:73:ARG:HH11	3:D:73:ARG:CB	2.22	0.53
1:A:174:TRP:HA	1:A:174:TRP:HE3	1.70	0.53
3:D:31:LEU:CD2	3:E:97:ALA:HA	2.28	0.53
3:E:47:ILE:HD13	3:F:3:GLN:HB3	1.91	0.53
2:C:231:ASP:HB3	3:E:73:ARG:HH22	1.73	0.53
1:A:131:HIS:CE1	1:A:136:ASP:CB	2.80	0.52
3:H:5:ILE:HD13	3:H:98:ALA:HB1	1.91	0.52
1:A:9:ASP:OD1	1:A:10:SER:N	2.42	0.52
3:F:19:THR:HG23	3:F:84:LYS:HZ1	1.75	0.52
3:F:83:GLU:HG3	3:F:84:LYS:H	1.74	0.52
3:D:76:TYR:C	3:D:78:THR:H	2.12	0.52
2:C:234:ASN:HD22	2:C:234:ASN:N	2.06	0.52
1:A:131:HIS:HE1	1:A:136:ASP:CB	2.13	0.52
1:A:175:ARG:HD2	1:A:180:ILE:CD1	2.40	0.52
3:D:15:THR:HG22	3:D:88:TRP:NE1	2.23	0.52
3:G:24:ILE:HG21	3:G:76:TYR:HB2	1.90	0.52
3:D:39:ILE:HA	3:D:48:PHE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:8:LEU:O	3:F:11:GLU:HB3	2.10	0.52
3:F:2:PRO:HB3	3:F:7:ASP:HB2	1.92	0.52
3:E:14:ASN:HB3	3:E:90:ASN:CB	2.32	0.52
3:E:81:LYS:NZ	3:E:81:LYS:HB3	2.25	0.52
1:A:40:ASN:HD21	1:A:43:ASP:H	1.53	0.52
3:H:15:THR:HA	3:H:87:THR:O	2.09	0.52
3:H:9:CYS:SG	3:H:15:THR:HB	2.49	0.52
1:A:59:TYR:CZ	1:A:116:LEU:CD2	2.93	0.52
3:E:13:HIS:HB2	4:E:109:HOH:O	2.09	0.52
3:F:73:ARG:NH1	3:G:71:THR:OG1	2.43	0.52
3:H:18:TYR:O	3:H:84:LYS:HB3	2.10	0.52
3:G:32:ALA:O	3:G:36:GLU:HG3	2.09	0.52
3:F:24:ILE:HD11	3:F:82:VAL:HG21	1.92	0.51
3:E:47:ILE:HG21	3:F:3:GLN:CB	2.36	0.51
3:H:24:ILE:CG2	3:H:26:SER:O	2.54	0.51
3:F:82:VAL:HG22	3:F:99:ILE:HD11	1.93	0.51
3:D:65:ILE:CD1	3:H:31:LEU:HD11	2.29	0.51
3:E:2:PRO:HB2	3:E:8:LEU:HD23	1.92	0.51
3:D:15:THR:CG2	3:D:88:TRP:CD1	2.94	0.51
1:A:91:ALA:CB	1:A:92:PRO:HD2	2.37	0.51
3:F:8:LEU:C	3:F:8:LEU:HD23	2.31	0.51
3:H:50:VAL:HG21	3:H:72:LEU:HD12	1.91	0.51
2:C:235:ARG:HH22	2:C:239:GLU:HB2	0.68	0.51
1:A:188:GLY:O	1:A:189:ASN:CB	2.57	0.51
3:D:20:LEU:HD11	3:D:48:PHE:CE2	2.45	0.51
3:F:53:PRO:HB3	3:F:65:ILE:HD12	1.93	0.51
1:A:108:PRO:O	1:A:109:ASP:C	2.49	0.51
3:F:22:ASP:HA	3:F:81:LYS:HG3	1.92	0.51
3:E:31:LEU:HD23	3:E:32:ALA:N	2.25	0.51
3:H:27:TYR:C	3:H:27:TYR:CD1	2.82	0.51
2:C:227:GLN:NE2	3:F:74:ILE:CA	2.73	0.51
3:D:47:ILE:O	3:D:48:PHE:HD1	1.89	0.51
3:E:31:LEU:HD23	3:E:31:LEU:C	2.31	0.51
1:A:60:VAL:CG2	1:A:118:GLY:HA2	2.41	0.51
1:A:1:ASN:HD21	1:A:3:ASP:CG	2.14	0.51
2:C:240:LEU:HD12	3:F:63:LYS:HZ1	1.72	0.50
1:A:74:GLN:HB3	1:A:83:TYR:OH	2.11	0.50
1:A:66:LEU:O	1:A:67:ARG:C	2.49	0.50
3:D:65:ILE:HA	3:H:31:LEU:CD1	2.41	0.50
1:A:12:PRO:HG2	4:A:197:HOH:O	2.11	0.50
3:D:66:GLU:O	3:E:67:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:9:CYS:SG	3:F:15:THR:HG21	2.52	0.50
1:A:21:GLY:C	1:A:23:MET:HE2	2.31	0.50
3:E:77:LEU:CD1	3:F:78:THR:CG2	2.80	0.50
1:A:169:PRO:O	1:A:188:GLY:HA2	2.11	0.50
1:A:185:PRO:HG2	2:C:202:LYS:HE2	1.92	0.50
3:D:68:MET:C	3:D:70:ASP:N	2.61	0.50
3:G:26:SER:OG	3:G:41:THR:HB	2.11	0.50
1:A:70:HIS:NE2	1:A:74:GLN:OE1	2.44	0.50
3:G:41:THR:HA	3:G:46:ALA:O	2.11	0.50
3:E:57:HIS:HD2	3:E:61:GLN:OE1	1.94	0.50
1:A:42:TYR:O	1:A:46:ARG:HG2	2.11	0.50
2:C:228:SER:CB	3:D:77:LEU:HD23	2.41	0.50
3:F:53:PRO:HA	3:F:57:HIS:NE2	2.26	0.50
3:H:5:ILE:O	3:H:9:CYS:N	2.37	0.50
1:A:88:LEU:CD2	1:A:119:ILE:HG12	2.41	0.50
1:A:150:TYR:C	1:A:152:ASN:H	2.15	0.50
3:F:28:THR:HA	3:G:99:ILE:O	2.12	0.50
3:H:24:ILE:HG21	3:H:40:ILE:HB	1.93	0.50
2:C:233:HIS:CE1	3:D:67:ARG:HA	2.47	0.50
3:D:14:ASN:CB	3:D:90:ASN:HD22	2.23	0.50
3:E:2:PRO:HG2	3:E:8:LEU:HD22	1.94	0.50
1:A:174:TRP:CZ3	1:A:179:TRP:HB3	2.46	0.49
3:G:74:ILE:CD1	3:G:77:LEU:HB2	2.39	0.49
1:A:174:TRP:O	1:A:180:ILE:HD12	2.12	0.49
3:F:40:ILE:O	3:F:47:ILE:HA	2.11	0.49
3:H:73:ARG:O	3:H:76:TYR:HB3	2.12	0.49
1:A:59:TYR:CE2	1:A:116:LEU:HB2	2.47	0.49
3:H:27:TYR:O	3:H:27:TYR:HD1	1.95	0.49
3:E:83:GLU:HB2	3:E:102:ALA:CB	2.43	0.49
3:E:83:GLU:HB2	3:E:102:ALA:HB3	1.94	0.49
3:G:43:LYS:N	3:G:43:LYS:HE2	2.19	0.49
3:D:58:ILE:N	3:D:58:ILE:HD13	2.27	0.49
3:D:58:ILE:O	3:D:61:GLN:N	2.43	0.49
3:E:71:THR:O	3:E:74:ILE:HD13	2.13	0.49
1:A:184:PRO:HG2	1:A:187:CYS:SG	2.52	0.49
3:G:20:LEU:O	3:G:21:ASN:C	2.50	0.49
3:H:37:MET:HB2	3:H:50:VAL:O	2.13	0.49
3:G:18:TYR:HH	3:G:94:HIS:HE2	1.59	0.49
3:D:24:ILE:HG21	3:D:40:ILE:HG13	1.93	0.49
3:D:6:THR:O	3:D:7:ASP:O	2.31	0.49
3:D:2:PRO:HB3	3:D:8:LEU:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:58:ILE:HG12	3:F:59:ASP:H	1.77	0.49
3:H:91:LYS:O	3:H:94:HIS:HA	2.13	0.49
3:G:87:THR:OG1	3:G:94:HIS:HD2	1.96	0.49
1:A:88:LEU:O	1:A:89:ALA:C	2.50	0.49
3:E:53:PRO:HB3	3:E:62:LYS:HG3	1.94	0.49
3:D:19:THR:CG2	4:D:106:HOH:O	2.58	0.49
1:A:25:ARG:HD2	1:A:56:ASP:OD1	2.13	0.49
3:E:2:PRO:HB2	3:E:8:LEU:CD2	2.42	0.49
3:H:14:ASN:O	3:H:88:TRP:HD1	1.96	0.49
3:H:4:ASN:ND2	3:H:7:ASP:OD2	2.46	0.49
3:D:75:ALA:CA	3:D:78:THR:HG22	2.43	0.49
3:D:66:GLU:OE1	3:E:63:LYS:NZ	2.46	0.49
3:G:18:TYR:CD1	3:G:87:THR:HG23	2.48	0.49
3:G:42:PHE:CG	3:G:46:ALA:HB3	2.46	0.49
3:F:87:THR:HG21	3:F:94:HIS:HB3	1.94	0.49
3:H:83:GLU:HB3	3:H:100:SER:OG	2.13	0.49
2:C:219:LYS:O	2:C:223:PHE:CB	2.58	0.49
3:G:30:SER:HB3	3:G:35:ARG:O	2.12	0.49
3:F:24:ILE:HG22	3:F:41:THR:O	2.13	0.48
2:C:211:LEU:O	2:C:215:GLN:HG3	2.13	0.48
2:C:219:LYS:O	2:C:223:PHE:N	2.40	0.48
3:F:72:LEU:O	3:F:73:ARG:HB3	2.13	0.48
3:D:2:PRO:CG	3:D:11:GLU:OE1	2.56	0.48
1:A:108:PRO:O	1:A:110:GLU:N	2.46	0.48
3:E:24:ILE:HG22	3:E:26:SER:O	2.13	0.48
2:C:220:ARG:NE	3:E:77:LEU:O	2.46	0.48
3:E:25:PHE:CD1	3:F:103:ASN:ND2	2.81	0.48
3:E:57:HIS:CD2	3:E:61:GLN:OE1	2.66	0.48
2:C:239:GLU:OE1	2:C:239:GLU:CA	2.61	0.48
1:A:174:TRP:CE3	1:A:179:TRP:HB3	2.48	0.48
3:D:39:ILE:O	3:D:40:ILE:HD12	2.12	0.48
3:G:42:PHE:CD2	3:G:46:ALA:CB	2.91	0.48
3:F:93:PRO:CD	3:G:1:THR:N	2.75	0.48
3:F:15:THR:HG22	3:F:16:GLN:H	1.78	0.48
1:A:98:ASN:HB2	1:A:111:GLN:NE2	2.28	0.48
2:C:204:GLN:O	2:C:205:SER:C	2.52	0.48
3:D:66:GLU:HG3	3:E:67:ARG:NH2	2.28	0.48
3:D:67:ARG:NH1	3:H:69:LYS:CB	2.74	0.48
3:D:91:LYS:CG	4:D:117:HOH:O	2.60	0.48
3:G:78:THR:O	3:G:79:GLU:HB2	2.14	0.48
1:A:76:ILE:CG2	1:A:77:LEU:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:36:GLU:HG2	3:F:64:ALA:HB2	1.96	0.48
3:G:41:THR:O	3:G:42:PHE:CD2	2.67	0.48
1:A:10:SER:O	1:A:11:ARG:C	2.51	0.48
1:A:120:PRO:O	1:A:122:SER:N	2.47	0.48
2:C:230:ILE:CG1	2:C:231:ASP:N	2.75	0.48
3:E:20:LEU:O	3:E:22:ASP:HB2	2.14	0.48
1:A:170:GLU:CB	1:A:192:ARG:CZ	2.92	0.48
3:D:2:PRO:HD3	3:H:35:ARG:NH2	2.27	0.48
3:D:43:LYS:HE2	3:D:43:LYS:HB3	1.51	0.48
3:E:48:PHE:HD1	3:E:94:HIS:O	1.97	0.47
3:F:19:THR:HA	3:F:83:GLU:O	2.14	0.47
1:A:143:ARG:NH2	3:D:78:THR:O	2.26	0.47
3:D:93:PRO:CD	3:E:1:THR:HB	2.44	0.47
3:D:75:ALA:HA	3:D:78:THR:HG22	1.95	0.47
3:F:76:TYR:C	3:F:76:TYR:CD1	2.87	0.47
3:F:40:ILE:HG22	3:F:48:PHE:HB2	1.97	0.47
3:F:93:PRO:HD2	3:G:1:THR:N	2.25	0.47
3:D:73:ARG:HE	3:E:71:THR:HA	1.79	0.47
3:E:76:TYR:O	3:E:78:THR:N	2.48	0.47
2:C:231:ASP:OD2	3:F:74:ILE:HG22	2.13	0.47
3:E:92:THR:N	3:E:93:PRO:O	2.48	0.47
3:G:1:THR:HB	3:G:2:PRO:HD2	1.97	0.47
3:E:62:LYS:H	3:E:62:LYS:HD3	1.79	0.47
3:G:66:GLU:HA	3:G:66:GLU:OE1	2.15	0.47
3:E:68:MET:O	3:E:69:LYS:C	2.53	0.47
3:D:92:THR:O	3:E:1:THR:OG1	2.19	0.47
3:G:9:CYS:C	3:G:11:GLU:N	2.67	0.47
1:A:191:PRO:O	1:A:192:ARG:HB2	2.14	0.47
3:E:82:VAL:HG21	3:E:99:ILE:CD1	2.45	0.47
3:G:18:TYR:O	3:G:84:LYS:HA	2.14	0.47
3:E:91:LYS:O	3:E:92:THR:OG1	2.27	0.47
3:D:49:GLN:OE1	3:D:91:LYS:HE3	2.15	0.47
1:A:154:ASP:CB	4:A:222:HOH:O	2.62	0.47
3:D:28:THR:HB	3:D:39:ILE:HG21	1.91	0.47
3:H:51:GLU:OE1	3:H:57:HIS:HE1	1.97	0.47
3:D:12:TYR:O	3:D:13:HIS:ND1	2.49	0.46
3:F:72:LEU:O	3:F:73:ARG:CB	2.63	0.46
3:D:53:PRO:HG3	3:E:63:LYS:NZ	2.30	0.46
3:D:49:GLN:O	3:D:95:ALA:HA	2.15	0.46
1:A:8:ALA:HB2	1:A:85:LEU:HD11	1.96	0.46
3:D:102:ALA:HB1	3:D:103:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:72:LEU:O	3:E:75:ALA:HB3	2.15	0.46
1:A:183:ALA:O	1:A:184:PRO:O	2.34	0.46
3:E:82:VAL:HG21	3:E:99:ILE:HD11	1.97	0.46
3:D:15:THR:HG23	3:D:88:TRP:NE1	2.29	0.46
1:A:21:GLY:C	1:A:23:MET:CE	2.84	0.46
2:C:233:HIS:HE1	3:H:73:ARG:HH22	1.59	0.46
3:E:72:LEU:HA	3:E:75:ALA:CB	2.46	0.46
1:A:75:THR:HG21	4:A:216:HOH:O	2.15	0.46
3:E:71:THR:O	3:E:75:ALA:HB2	2.16	0.46
3:H:75:ALA:O	3:H:80:ALA:HB2	2.15	0.46
3:E:103:ASN:HA	3:E:103:ASN:HD22	1.50	0.46
3:H:52:VAL:HA	3:H:53:PRO:HD3	1.84	0.46
2:C:227:GLN:CB	2:C:230:ILE:HD11	2.45	0.46
3:D:5:ILE:HB	3:H:28:THR:CG2	2.45	0.46
3:G:41:THR:HG23	3:G:42:PHE:H	1.81	0.46
3:E:54:SER:OG	3:E:62:LYS:CE	2.64	0.46
2:C:227:GLN:C	2:C:230:ILE:HG13	2.36	0.46
3:E:65:ILE:HG22	3:E:69:LYS:HE2	1.98	0.46
3:F:61:GLN:O	3:F:65:ILE:HG13	2.16	0.46
1:A:91:ALA:HB3	1:A:123:GLN:NE2	2.31	0.46
3:D:92:THR:HG22	3:D:92:THR:O	2.16	0.46
3:F:90:ASN:ND2	4:F:111:HOH:O	2.14	0.46
3:D:34:LYS:NZ	3:E:60:SER:OG	2.36	0.46
3:E:17:ILE:CG2	3:E:84:LYS:HB3	2.46	0.45
3:D:39:ILE:HG23	3:D:39:ILE:O	2.15	0.45
3:F:2:PRO:HG2	3:F:8:LEU:HA	1.98	0.45
3:G:51:GLU:HG3	3:G:95:ALA:CB	2.45	0.45
3:E:88:TRP:HB3	3:E:90:ASN:OD1	2.16	0.45
3:D:101:MET:O	3:H:26:SER:HA	2.16	0.45
3:G:36:GLU:OE2	3:H:61:GLN:HG2	2.16	0.45
3:G:66:GLU:OE1	3:G:69:LYS:NZ	2.35	0.45
2:C:239:GLU:OE2	3:G:63:LYS:HD2	2.16	0.45
1:A:98:ASN:ND2	1:A:105:SER:OG	2.50	0.45
3:H:27:TYR:O	3:H:27:TYR:CD1	2.69	0.45
2:C:231:ASP:OD2	3:F:74:ILE:HG21	2.15	0.45
3:H:33:GLY:O	3:H:34:LYS:HB3	2.16	0.45
3:D:16:GLN:CD	3:D:89:ASN:HB3	2.37	0.45
3:F:9:CYS:SG	3:F:15:THR:HG22	2.56	0.45
1:A:154:ASP:HB2	4:A:222:HOH:O	2.15	0.45
3:D:59:ASP:O	3:D:62:LYS:HB2	2.17	0.45
3:E:19:THR:O	3:E:20:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:26:SER:OG	3:D:41:THR:HG22	2.13	0.45
3:D:47:ILE:HG21	3:E:3:GLN:HG2	1.97	0.45
1:A:107:HIS:O	1:A:108:PRO:C	2.55	0.45
1:A:45:ALA:HB1	1:A:106:PRO:HD2	1.98	0.45
3:H:54:SER:O	3:H:56:GLN:NE2	2.50	0.45
1:A:184:PRO:O	1:A:187:CYS:HB2	2.16	0.45
3:D:7:ASP:O	3:D:8:LEU:C	2.54	0.45
3:D:8:LEU:CD2	3:H:30:SER:HB2	2.47	0.45
3:D:67:ARG:CZ	3:H:70:ASP:OD1	2.64	0.45
1:A:85:LEU:HD13	1:A:130:VAL:HG21	1.98	0.45
1:A:125:TYR:C	1:A:125:TYR:CD1	2.89	0.45
3:E:65:ILE:CG2	3:E:65:ILE:O	2.65	0.45
3:E:86:CYS:SG	3:E:87:THR:N	2.90	0.45
2:C:229:ASP:OD2	3:D:73:ARG:CZ	2.65	0.45
1:A:9:ASP:HB3	1:A:86:TYR:CE2	2.45	0.45
3:H:85:LEU:CD1	3:H:96:ILE:HG12	2.47	0.45
3:E:48:PHE:HB3	3:E:96:ILE:HD11	1.99	0.45
3:G:42:PHE:CB	3:G:46:ALA:HB3	2.46	0.45
3:F:18:TYR:HB2	3:F:85:LEU:HB2	1.99	0.45
3:H:39:ILE:HA	3:H:48:PHE:O	2.17	0.45
3:E:54:SER:HG	3:E:62:LYS:HD2	1.80	0.45
2:C:228:SER:OG	2:C:229:ASP:N	2.50	0.44
3:E:76:TYR:HD1	3:E:77:LEU:HD22	1.83	0.44
3:E:91:LYS:HG3	3:E:95:ALA:CB	2.48	0.44
3:E:54:SER:HG	3:E:62:LYS:NZ	2.13	0.44
3:H:83:GLU:HG3	3:H:102:ALA:CB	2.47	0.44
3:D:65:ILE:HG23	3:D:69:LYS:HE2	1.99	0.44
3:E:30:SER:OG	3:E:31:LEU:N	2.51	0.44
1:A:88:LEU:HD23	1:A:119:ILE:HG12	1.98	0.44
3:H:85:LEU:HD12	3:H:96:ILE:HG12	1.97	0.44
3:E:14:ASN:ND2	3:E:90:ASN:CB	2.66	0.44
3:H:20:LEU:O	3:H:21:ASN:HB2	2.16	0.44
2:C:217:LYS:HG2	2:C:217:LYS:H	1.69	0.44
3:H:61:GLN:O	3:H:65:ILE:HD12	2.18	0.44
3:D:93:PRO:HD3	3:E:1:THR:HB	1.99	0.44
3:D:2:PRO:HB2	3:D:8:LEU:CD1	2.47	0.44
1:A:120:PRO:O	1:A:123:GLN:N	2.42	0.44
3:D:23:LYS:HD2	3:D:79:GLU:HB3	2.00	0.44
3:D:80:ALA:O	3:D:81:LYS:HB2	2.17	0.44
3:D:53:PRO:HG3	3:E:63:LYS:HZ3	1.83	0.44
2:C:225:GLY:O	2:C:228:SER:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:20:LEU:HD21	3:D:42:PHE:CE1	2.53	0.44
3:D:67:ARG:O	3:D:70:ASP:CB	2.54	0.44
1:A:119:ILE:HG23	1:A:123:GLN:CB	2.47	0.44
1:A:86:TYR:O	1:A:88:LEU:CD1	2.61	0.44
3:F:19:THR:CG2	3:F:84:LYS:HZ1	2.31	0.44
3:E:85:LEU:CD1	3:E:99:ILE:HG12	2.48	0.44
3:D:12:TYR:CD1	3:D:12:TYR:N	2.86	0.44
3:D:16:GLN:HG3	3:D:18:TYR:CE1	2.53	0.44
3:D:91:LYS:HD2	4:D:119:HOH:O	2.18	0.44
1:A:33:ARG:NH1	3:F:23:LYS:HZ3	2.10	0.44
3:F:69:LYS:C	3:G:67:ARG:HH22	2.20	0.44
3:F:13:HIS:O	3:F:14:ASN:HB2	2.17	0.44
3:H:16:GLN:N	3:H:87:THR:O	2.46	0.43
3:H:93:PRO:O	3:H:94:HIS:C	2.55	0.43
1:A:49:GLN:HE21	1:A:49:GLN:HB2	1.35	0.43
3:F:14:ASN:ND2	3:F:90:ASN:HB3	2.33	0.43
3:G:15:THR:HG23	3:G:88:TRP:CD1	2.53	0.43
2:C:227:GLN:O	2:C:228:SER:C	2.56	0.43
3:D:64:ALA:HB1	3:H:31:LEU:HA	2.00	0.43
3:E:32:ALA:O	3:E:35:ARG:HB2	2.17	0.43
3:G:93:PRO:HD3	3:H:1:THR:HB	2.00	0.43
1:A:76:ILE:CG2	1:A:77:LEU:H	2.23	0.43
1:A:106:PRO:C	1:A:107:HIS:CG	2.92	0.43
1:A:175:ARG:CD	1:A:180:ILE:HD11	2.49	0.43
3:F:50:VAL:CG1	3:F:65:ILE:CG2	2.92	0.43
3:E:13:HIS:HD2	3:E:13:HIS:C	2.17	0.43
3:E:5:ILE:CG1	3:E:5:ILE:O	2.65	0.43
3:E:92:THR:HA	3:E:93:PRO:C	2.38	0.43
3:E:52:VAL:HG23	3:E:52:VAL:H	1.45	0.43
3:E:88:TRP:O	3:E:91:LYS:HB2	2.19	0.43
3:E:58:ILE:O	3:E:61:GLN:N	2.45	0.43
3:E:17:ILE:HG22	3:E:18:TYR:H	1.82	0.43
3:E:14:ASN:O	3:E:88:TRP:HA	2.19	0.43
3:D:6:THR:HA	3:D:17:ILE:HD12	2.00	0.43
3:H:20:LEU:HD12	3:H:44:ASN:HD21	1.82	0.43
2:C:233:HIS:CD2	3:D:67:ARG:HH21	2.37	0.43
3:D:66:GLU:CD	3:E:63:LYS:HZ2	2.21	0.43
2:C:229:ASP:CG	3:D:73:ARG:HG2	2.39	0.43
2:C:233:HIS:HE1	3:D:67:ARG:HG3	1.78	0.43
3:G:18:TYR:HE1	3:G:87:THR:OG1	1.90	0.43
3:H:81:LYS:HG2	3:H:103:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:TYR:N	3:H:12:TYR:CD1	2.87	0.43
3:D:74:ILE:O	3:D:78:THR:HB	2.19	0.43
2:C:221:GLN:NE2	3:E:78:THR:O	2.52	0.43
3:E:48:PHE:CE1	3:E:94:HIS:HB2	2.54	0.43
3:H:18:TYR:HE2	3:H:94:HIS:HD2	1.67	0.42
3:E:76:TYR:CD1	3:E:77:LEU:HD22	2.54	0.42
3:E:78:THR:O	3:E:79:GLU:HB2	2.19	0.42
3:E:17:ILE:CG2	3:E:18:TYR:N	2.82	0.42
3:E:18:TYR:O	3:E:84:LYS:HA	2.20	0.42
3:D:61:GLN:HE21	3:H:33:GLY:H	1.66	0.42
3:G:42:PHE:HD2	3:G:46:ALA:CB	2.30	0.42
2:C:225:GLY:O	2:C:228:SER:HB3	2.19	0.42
1:A:176:GLU:O	1:A:180:ILE:HG22	2.19	0.42
3:D:15:THR:HG23	3:D:88:TRP:HE1	1.84	0.42
3:D:20:LEU:HD22	3:D:82:VAL:CG1	2.47	0.42
2:C:235:ARG:HB2	3:E:70:ASP:OD2	2.20	0.42
3:F:73:ARG:C	3:F:76:TYR:H	2.23	0.42
3:H:81:LYS:O	3:H:101:MET:HG3	2.19	0.42
3:F:84:LYS:N	3:F:100:SER:OG	2.52	0.42
3:D:74:ILE:O	3:D:78:THR:CB	2.68	0.42
3:E:20:LEU:C	3:E:22:ASP:N	2.71	0.42
3:D:7:ASP:O	3:D:9:CYS:N	2.53	0.42
3:F:33:GLY:O	3:F:34:LYS:CB	2.65	0.42
3:G:28:THR:HG23	3:H:99:ILE:O	2.20	0.42
3:F:22:ASP:N	3:F:82:VAL:O	2.53	0.42
3:H:13:HIS:CD2	3:H:14:ASN:ND2	2.87	0.42
3:E:17:ILE:CG2	3:E:18:TYR:H	2.33	0.42
3:H:58:ILE:C	3:H:60:SER:N	2.73	0.42
3:D:65:ILE:O	3:D:69:LYS:HE2	2.20	0.42
3:G:41:THR:O	3:G:42:PHE:CG	2.73	0.42
3:H:83:GLU:HG3	3:H:102:ALA:HB3	2.01	0.42
3:H:2:PRO:O	3:H:2:PRO:HG2	2.20	0.42
3:E:88:TRP:HB2	3:E:95:ALA:HB3	2.01	0.42
2:C:234:ASN:ND2	2:C:234:ASN:N	2.66	0.42
3:G:3:GLN:O	3:G:4:ASN:CB	2.66	0.42
1:A:139:LEU:HD23	1:A:140:HIS:N	2.35	0.42
3:G:77:LEU:HD22	3:H:78:THR:HG21	2.03	0.41
3:F:57:HIS:HB2	3:F:62:LYS:HZ1	1.85	0.41
1:A:156:ALA:HA	1:A:157:PRO:HD2	1.72	0.41
3:E:1:THR:HA	3:E:2:PRO:HD3	1.90	0.41
1:A:105:SER:O	1:A:108:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:18:TYR:HE1	3:E:87:THR:HB	1.84	0.41
3:E:91:LYS:HG3	3:E:95:ALA:HB2	2.01	0.41
3:F:58:ILE:HG23	3:F:61:GLN:HG3	2.01	0.41
3:H:40:ILE:HD13	3:H:72:LEU:HD13	2.02	0.41
3:D:56:GLN:HG3	3:D:57:HIS:CE1	2.54	0.41
1:A:11:ARG:HA	1:A:12:PRO:HD3	1.82	0.41
3:G:89:ASN:C	3:G:91:LYS:H	2.22	0.41
1:A:134:VAL:O	1:A:134:VAL:CG1	2.67	0.41
3:F:37:MET:HB3	3:F:37:MET:HE2	1.62	0.41
3:E:83:GLU:HG2	3:E:84:LYS:H	1.80	0.41
3:D:8:LEU:HD21	3:H:30:SER:CB	2.48	0.41
3:E:25:PHE:CA	3:F:103:ASN:ND2	2.67	0.41
3:D:57:HIS:HB3	3:D:61:GLN:OE1	2.20	0.41
3:H:75:ALA:O	3:H:80:ALA:CA	2.69	0.41
3:F:20:LEU:HD12	3:F:44:ASN:HD21	1.85	0.41
1:A:95:PHE:CE2	1:A:164:LEU:HD12	2.55	0.41
3:F:57:HIS:CD2	3:F:65:ILE:HD11	2.54	0.41
1:A:94:MET:SD	1:A:115:ALA:HB2	2.61	0.41
3:D:14:ASN:CB	3:D:90:ASN:ND2	2.70	0.41
3:F:53:PRO:O	3:F:54:SER:O	2.38	0.41
3:H:49:GLN:NE2	3:H:91:LYS:HG3	2.36	0.41
1:A:119:ILE:HA	1:A:120:PRO:HD2	1.80	0.41
4:G:112:HOH:O	3:H:67:ARG:HD2	2.20	0.41
3:G:47:ILE:HG21	3:H:3:GLN:HB3	2.02	0.41
3:G:56:GLN:HG3	3:G:57:HIS:CD2	2.56	0.41
3:D:24:ILE:HG22	3:D:26:SER:O	2.19	0.41
3:D:47:ILE:HD12	3:E:3:GLN:HG2	1.97	0.41
1:A:91:ALA:HB1	1:A:92:PRO:CD	2.43	0.41
3:F:15:THR:CG2	3:F:87:THR:O	2.68	0.41
3:F:18:TYR:HB2	3:F:85:LEU:CB	2.50	0.41
3:G:53:PRO:HG2	4:G:115:HOH:O	2.19	0.41
3:E:42:PHE:CE2	3:E:82:VAL:CG1	2.93	0.41
2:C:227:GLN:HA	2:C:230:ILE:HD11	2.01	0.41
3:F:67:ARG:O	3:F:70:ASP:HB2	2.20	0.41
3:E:86:CYS:HB3	3:E:98:ALA:HB3	2.02	0.41
1:A:6:TYR:CD1	1:A:66:LEU:HD23	2.55	0.41
3:G:68:MET:O	3:G:68:MET:HG3	2.21	0.41
3:E:68:MET:C	3:E:70:ASP:N	2.72	0.41
3:E:74:ILE:N	3:E:74:ILE:CD1	2.84	0.41
3:D:39:ILE:C	3:D:40:ILE:HD12	2.41	0.41
3:D:40:ILE:HD13	3:D:72:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:36:GLU:H	3:F:36:GLU:HG3	1.55	0.41
3:H:58:ILE:C	3:H:60:SER:H	2.24	0.41
3:H:5:ILE:HD11	3:H:98:ALA:CB	2.44	0.41
3:E:54:SER:HG	3:E:62:LYS:HZ2	1.61	0.41
3:F:2:PRO:HG2	3:F:8:LEU:CA	2.50	0.41
3:F:52:VAL:C	3:F:54:SER:N	2.75	0.41
3:E:20:LEU:N	3:E:83:GLU:O	2.53	0.40
3:E:5:ILE:HD11	3:E:86:CYS:H	1.86	0.40
3:D:99:ILE:HG22	3:H:29:GLU:HG2	2.03	0.40
3:F:30:SER:CB	3:F:35:ARG:O	2.68	0.40
3:G:48:PHE:CD2	3:G:87:THR:HG21	2.56	0.40
3:H:17:ILE:HD13	3:H:17:ILE:HA	1.76	0.40
1:A:155:ILE:O	1:A:156:ALA:O	2.39	0.40
3:H:24:ILE:CG2	3:H:40:ILE:HB	2.52	0.40
1:A:83:TYR:HE2	1:A:85:LEU:CD1	2.34	0.40
2:C:219:LYS:HG2	2:C:223:PHE:CE2	2.56	0.40
3:D:73:ARG:O	3:D:77:LEU:HB2	2.22	0.40
3:F:78:THR:O	3:F:79:GLU:HB2	2.20	0.40
3:D:20:LEU:HD11	3:D:48:PHE:HE2	1.85	0.40
3:F:50:VAL:CG1	3:F:65:ILE:HG23	2.49	0.40
3:G:1:THR:O	3:G:3:GLN:N	2.53	0.40
3:D:34:LYS:HZ1	3:E:58:ILE:HG21	1.87	0.40
3:E:62:LYS:O	3:E:66:GLU:CG	2.66	0.40
3:E:94:HIS:CD2	3:E:94:HIS:N	2.89	0.40
3:F:36:GLU:CD	3:G:60:SER:HB2	2.42	0.40
3:D:58:ILE:HD12	3:D:58:ILE:HA	1.72	0.40
3:G:25:PHE:CD2	3:G:41:THR:CG2	3.04	0.40
3:G:9:CYS:SG	3:G:17:ILE:HG12	2.61	0.40
3:H:22:ASP:CG	3:H:23:LYS:H	2.25	0.40
3:D:23:LYS:HA	3:D:81:LYS:HA	2.03	0.40
3:E:80:ALA:O	3:E:81:LYS:CB	2.69	0.40
3:E:54:SER:OG	3:E:62:LYS:CD	2.68	0.40
1:A:83:TYR:CZ	1:A:130:VAL:HG11	2.57	0.40
3:H:4:ASN:HB2	3:H:7:ASP:H	1.86	0.40
1:A:124:ILE:O	1:A:142:ASN:ND2	2.55	0.40

All (2) 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:A:192:ARG:O	3:E:14:ASN:ND2[1_655]	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:CD	3:E:13:HIS:NE2[1_655]	2.11	0.09

## 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	190/194 (98%)	149 (78%)	22 (12%)	19 (10%)	1	0
2	C	43/46 (94%)	40 (93%)	2 (5%)	1 (2%)	8	8
3	D	101/103 (98%)	81 (80%)	11 (11%)	9 (9%)	1	0
3	E	101/103 (98%)	73 (72%)	18 (18%)	10 (10%)	1	0
3	F	101/103 (98%)	87 (86%)	8 (8%)	6 (6%)	2	0
3	G	101/103 (98%)	80 (79%)	15 (15%)	6 (6%)	2	0
3	H	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	3	1
All	All	738/755 (98%)	593 (80%)	89 (12%)	56 (8%)	1	0

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	49	GLN
1	A	77	LEU
1	A	111	GLN
1	A	155	ILE
1	A	188	GLY
1	A	189	ASN
2	C	228	SER
3	D	7	ASP
3	D	8	LEU
3	E	54	SER
3	E	62	LYS

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Mol	Chain	Res	Type
3	E	80	ALA
3	F	33	GLY
3	F	54	SER
3	G	2	PRO
3	H	54	SER
3	H	59	ASP
3	H	81	LYS
1	A	66	LEU
1	A	89	ALA
1	A	109	ASP
1	A	121	TYR
3	D	34	LYS
3	D	55	SER
3	D	59	ASP
3	D	77	LEU
3	E	21	ASN
3	E	69	LYS
3	E	79	GLU
3	E	81	LYS
3	E	83	GLU
3	F	80	ALA
3	G	4	ASN
3	G	45	GLY
3	G	80	ALA
3	H	55	SER
1	A	14	ASP
1	A	65	SER
1	A	76	ILE
3	D	53	PRO
3	D	69	LYS
3	D	94	HIS
3	F	14	ASN
3	F	73	ARG
3	G	10	ALA
1	A	108	PRO
1	A	151	SER
1	A	156	ALA
3	H	33	GLY
1	A	184	PRO
3	F	53	PRO
3	G	58	ILE
3	E	77	LEU

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Mol	Chain	Res	Type
1	A	133	GLY
3	E	53	PRO

### 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	158/160 (99%)	123 (78%)	35 (22%)	1	1
2	C	43/44 (98%)	27 (63%)	16 (37%)	0	0
3	D	90/90 (100%)	67 (74%)	23 (26%)	0	0
3	E	90/90 (100%)	70 (78%)	20 (22%)	1	1
3	F	90/90 (100%)	65 (72%)	25 (28%)	0	0
3	G	90/90 (100%)	73 (81%)	17 (19%)	2	2
3	H	90/90 (100%)	54 (60%)	36 (40%)	0	0
All	All	651/654 (100%)	479 (74%)	172 (26%)	0	0

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LEU
1	A	15	GLU
1	A	16	ILE
1	A	17	LYS
1	A	18	GLN
1	A	29	GLU
1	A	35	THR
1	A	36	GLN
1	A	37	MET
1	A	41	LEU
1	A	49	GLN
1	A	53	VAL
1	A	55	HIS
1	A	56	ASP

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Mol	Chain	Res	Type
1	A	61	SER
1	A	64	ILE
1	A	66	LEU
1	A	70	HIS
1	A	71	LEU
1	A	77	LEU
1	A	81	SER
1	A	111	GLN
1	A	116	LEU
1	A	125	TYR
1	A	134	VAL
1	A	137	GLU
1	A	139	LEU
1	A	141	ARG
1	A	143	ARG
1	A	146	ARG
1	A	174	TRP
1	A	180	ILE
1	A	189	ASN
1	A	192	ARG
2	C	196	SER
2	C	197	ASN
2	C	200	ASP
2	C	202	LYS
2	C	203	THR
2	C	217	LYS
2	C	224	SER
2	C	229	ASP
2	C	231	ASP
2	C	233	HIS
2	C	235	ARG
2	C	236	ILE
2	C	237	LYS
2	C	238	ASP
2	C	239	GLU
2	C	240	LEU
3	D	1	THR
3	D	3	GLN
3	D	6	THR
3	D	8	LEU
3	D	11	GLU
3	D	17	ILE

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Mol	Chain	Res	Type
3	D	19	THR
3	D	21	ASN
3	D	26	SER
3	D	28	THR
3	D	31	LEU
3	D	34	LYS
3	D	37	MET
3	D	39	ILE
3	D	51	GLU
3	D	58	ILE
3	D	59	ASP
3	D	73	ARG
3	D	81	LYS
3	D	84	LYS
3	D	92	THR
3	D	94	HIS
3	D	96	ILE
3	E	1	THR
3	E	8	LEU
3	E	13	HIS
3	E	16	GLN
3	E	21	ASN
3	E	31	LEU
3	E	35	ARG
3	E	40	ILE
3	E	51	GLU
3	E	52	VAL
3	E	58	ILE
3	E	63	LYS
3	E	74	ILE
3	E	81	LYS
3	E	82	VAL
3	E	89	ASN
3	E	99	ILE
3	E	100	SER
3	E	101	MET
3	E	103	ASN
3	F	6	THR
3	F	14	ASN
3	F	15	THR
3	F	19	THR
3	F	20	LEU

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Mol	Chain	Res	Type
3	F	22	ASP
3	F	24	ILE
3	F	31	LEU
3	F	37	MET
3	F	40	ILE
3	F	41	THR
3	F	43	LYS
3	F	56	GLN
3	F	57	HIS
3	F	58	ILE
3	F	59	ASP
3	F	60	SER
3	F	72	LEU
3	F	73	ARG
3	F	74	ILE
3	F	77	LEU
3	F	78	THR
3	F	81	LYS
3	F	83	GLU
3	F	85	LEU
3	G	8	LEU
3	G	11	GLU
3	G	30	SER
3	G	31	LEU
3	G	34	LYS
3	G	37	MET
3	G	43	LYS
3	G	49	GLN
3	G	54	SER
3	G	58	ILE
3	G	62	LYS
3	G	66	GLU
3	G	78	THR
3	G	79	GLU
3	G	90	ASN
3	G	99	ILE
3	G	103	ASN
3	H	1	THR
3	H	3	GLN
3	H	14	ASN
3	H	17	ILE
3	H	19	THR

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Mol	Chain	Res	Type
3	H	20	LEU
3	H	23	LYS
3	H	28	THR
3	H	29	GLU
3	H	31	LEU
3	H	34	LYS
3	H	35	ARG
3	H	36	GLU
3	H	39	ILE
3	H	40	ILE
3	H	41	THR
3	H	47	ILE
3	H	52	VAL
3	H	54	SER
3	H	55	SER
3	H	56	GLN
3	H	58	ILE
3	H	59	ASP
3	H	61	GLN
3	H	66	GLU
3	H	68	MET
3	H	77	LEU
3	H	78	THR
3	H	82	VAL
3	H	83	GLU
3	H	84	LYS
3	H	90	ASN
3	H	91	LYS
3	H	94	HIS
3	H	99	ILE
3	H	101	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	18	GLN
1	A	40	ASN
1	A	49	GLN
1	A	70	HIS
1	A	80	HIS
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	111	GLN
1	A	123	GLN
1	A	131	HIS
2	C	227	GLN
2	C	233	HIS
2	C	234	ASN
3	D	57	HIS
3	D	89	ASN
3	D	94	HIS
3	D	103	ASN
3	E	13	HIS
3	E	14	ASN
3	E	16	GLN
3	E	44	ASN
3	E	89	ASN
3	E	103	ASN
3	F	14	ASN
3	F	44	ASN
3	F	57	HIS
3	F	61	GLN
3	F	103	ASN
3	G	3	GLN
3	G	57	HIS
3	G	89	ASN
3	H	4	ASN
3	H	13	HIS
3	H	56	GLN
3	H	57	HIS
3	H	61	GLN
3	H	94	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.