



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:46 PM UTC

PDB ID : 1A2V / pdb_00001a2v
Title : COPPER AMINE OXIDASE FROM HANSENULA POLYMORPHA
Authors : Li, R.; Mathews, F.S.
Deposited on : 1998-01-12
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

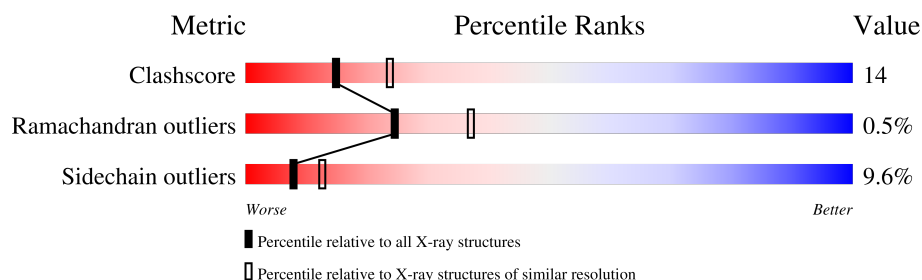
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	655	70% 24% 5%
1	B	655	68% 26% 5%
1	C	655	69% 25% 5%
1	D	655	65% 30% .
1	E	655	67% 27% 6%
1	F	655	69% 25% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33726 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 METHYLAMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5194	3305	892	974	23			
1	B	655	Total	C	N	O	S	0	0	0
			5194	3305	892	974	23			
1	C	655	Total	C	N	O	S	0	0	0
			5194	3305	892	974	23			
1	D	655	Total	C	N	O	S	0	0	0
			5194	3305	892	974	23			
1	E	655	Total	C	N	O	S	0	0	0
			5194	3305	892	974	23			
1	F	655	Total	C	N	O	S	0	0	0
			5194	3305	892	974	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	TPQ	TYR	modified residue	UNP P12807
B	405	TPQ	TYR	modified residue	UNP P12807
C	405	TPQ	TYR	modified residue	UNP P12807
D	405	TPQ	TYR	modified residue	UNP P12807
E	405	TPQ	TYR	modified residue	UNP P12807
F	405	TPQ	TYR	modified residue	UNP P12807

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Cu 1	0	0
2	E	1	Total 1	Cu 1	0	0
2	F	1	Total 1	Cu 1	0	0

- Molecule 3 is water.

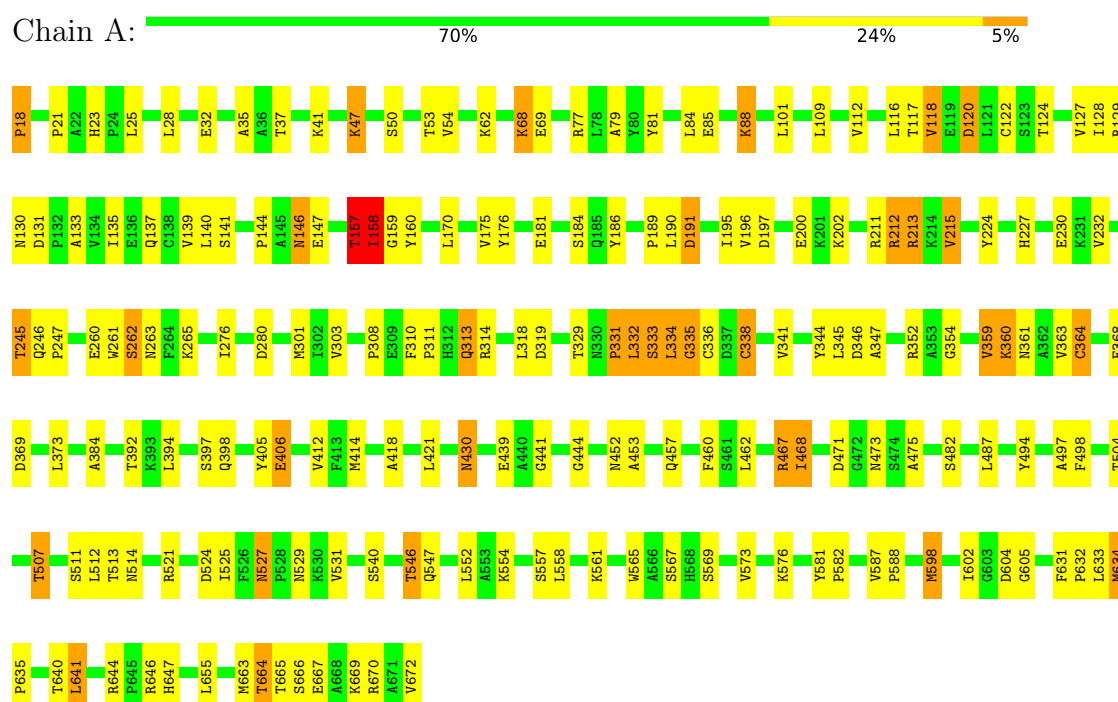
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	499	Total 499	O 499	0	0
3	B	453	Total 453	O 453	0	0
3	C	474	Total 474	O 474	0	0
3	D	415	Total 415	O 415	0	0
3	E	335	Total 335	O 335	0	0
3	F	380	Total 380	O 380	0	0

3 Residue-property plots

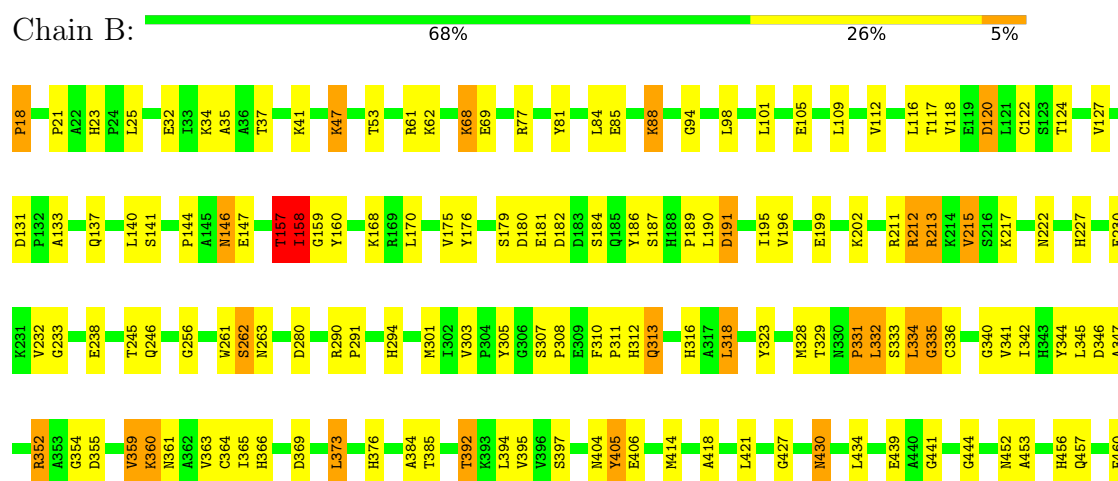
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

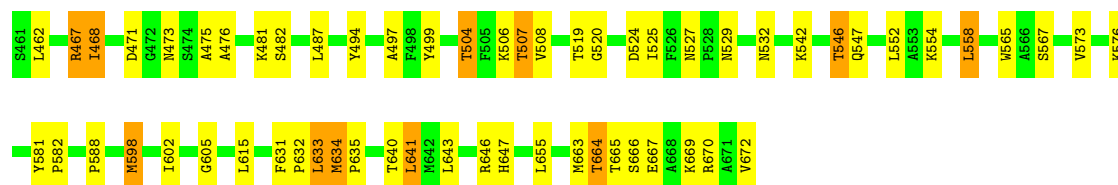
Note EDS was not executed.

• Molecule 1: METHYLAMINE OXIDASE



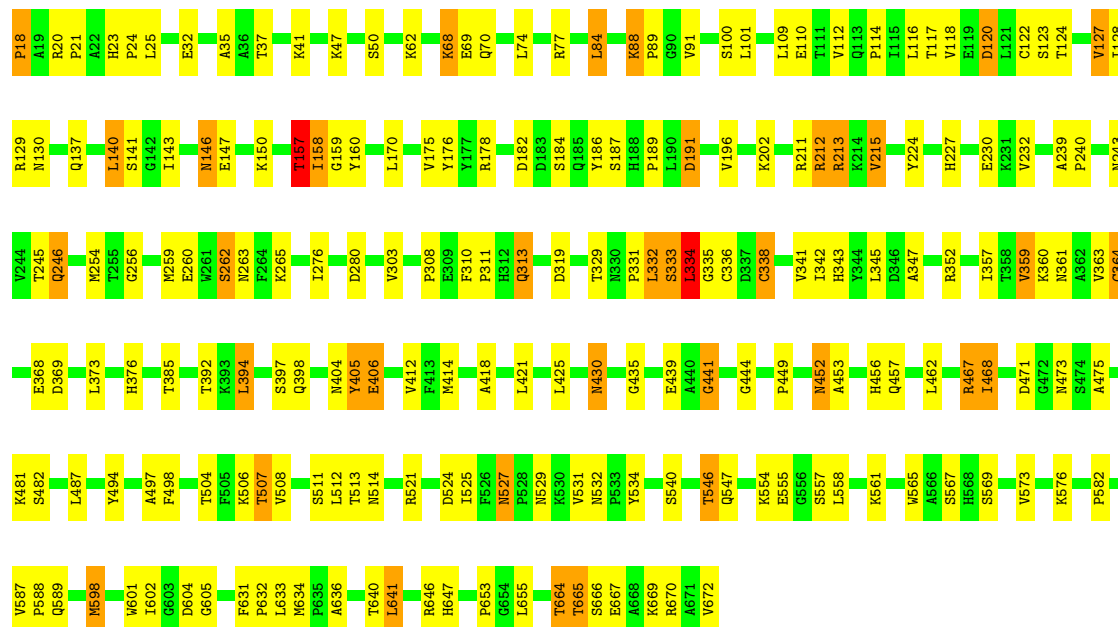
• Molecule 1: METHYLAMINE OXIDASE





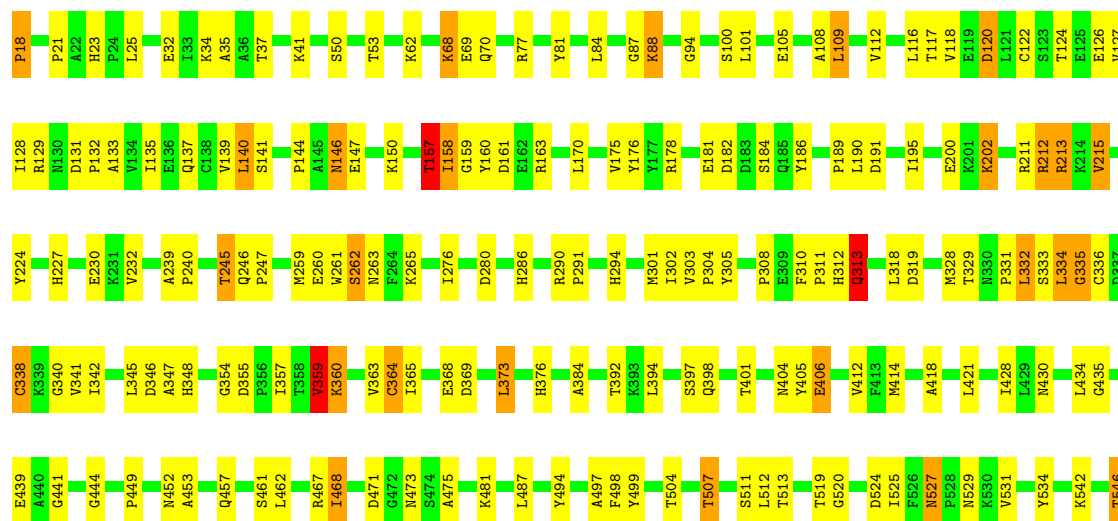
• Molecule 1: METHYLAMINE OXIDASE

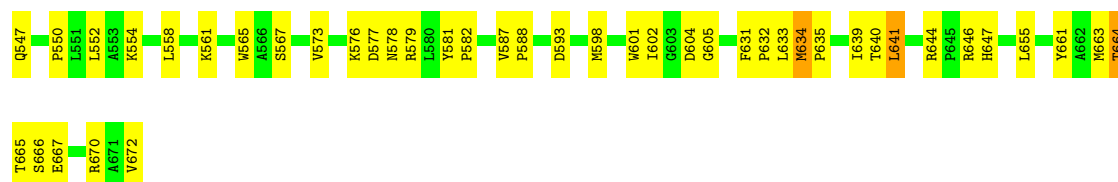
Chain C: 69% 25% 5%



• Molecule 1: METHYLAMINE OXIDASE

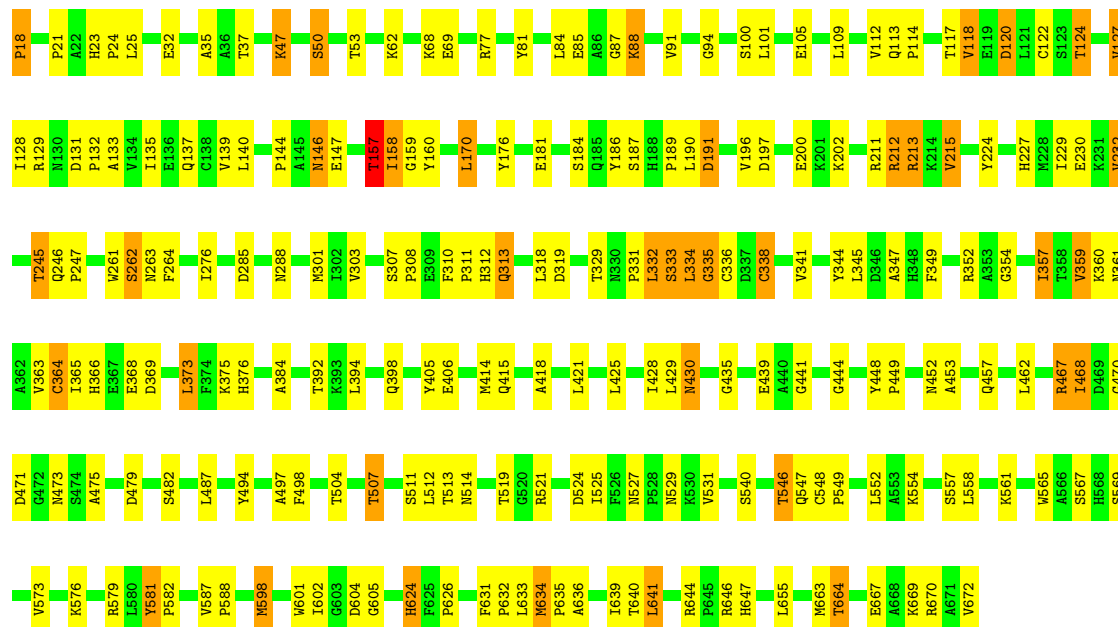
Chain D: 65% 30% 5%





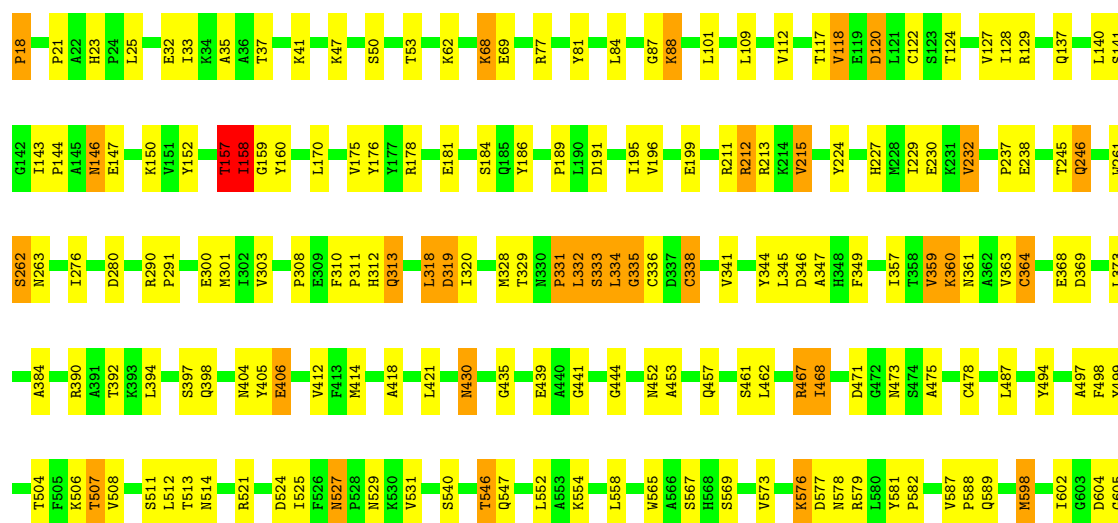
• Molecule 1: METHYLAMINE OXIDASE

Chain E: 67% 27% 6%



• Molecule 1: METHYLAMINE OXIDASE

Chain F: 69% 25% 5%



F631	P632	L633	M634	P635
T640	L641	R644	P645	R646
L655	S660	T664	T665	S666
E667	A668	K669	R670	A671
V672				

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.77Å 148.22Å 234.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40	Depositor
% Data completeness (in resolution range)	83.6 (100.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.184 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33726	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.61	1/5329 (0.0%)	1.06	29/7251 (0.4%)
1	B	0.66	2/5329 (0.0%)	1.10	32/7251 (0.4%)
1	C	0.67	3/5329 (0.1%)	1.10	32/7251 (0.4%)
1	D	0.64	1/5329 (0.0%)	1.09	29/7251 (0.4%)
1	E	0.63	2/5329 (0.0%)	1.08	32/7251 (0.4%)
1	F	0.64	2/5329 (0.0%)	1.10	28/7251 (0.4%)
All	All	0.64	11/31974 (0.0%)	1.09	182/43506 (0.4%)

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	D	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	598	MET	SD-CE	-8.45	1.58	1.79
1	C	598	MET	SD-CE	-7.04	1.61	1.79
1	E	634	MET	SD-CE	7.04	1.97	1.79
1	A	598	MET	SD-CE	-6.46	1.63	1.79
1	F	598	MET	SD-CE	-6.18	1.64	1.79
1	B	598	MET	SD-CE	-5.98	1.64	1.79
1	C	456	HIS	CD2-NE2	5.98	1.44	1.37
1	B	404	ASN	CG-OD1	5.40	1.33	1.23
1	F	404	ASN	CG-OD1	5.23	1.33	1.23
1	C	404	ASN	CG-ND2	-5.07	1.22	1.33
1	D	404	ASN	CG-OD1	5.05	1.33	1.23

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	332	LEU	N-CA-C	10.20	123.65	111.82
1	A	332	LEU	N-CA-C	9.73	123.10	111.82
1	B	332	LEU	N-CA-C	9.63	122.99	111.82
1	D	332	LEU	N-CA-C	9.58	122.93	111.82
1	E	332	LEU	N-CA-C	9.30	122.61	111.82
1	B	157	THR	N-CA-C	-8.84	98.87	110.53
1	D	157	THR	N-CA-C	-8.63	99.14	110.53
1	A	157	THR	N-CA-C	-8.51	99.29	110.53
1	E	157	THR	N-CA-C	-8.30	99.58	110.53
1	C	332	LEU	N-CA-C	8.20	123.06	112.89
1	F	157	THR	N-CA-C	-8.19	99.72	110.53
1	B	384	ALA	N-CA-C	-8.14	102.35	111.14
1	C	157	THR	N-CA-C	-8.11	99.83	110.53
1	F	184	SER	N-CA-C	-7.99	95.71	108.73
1	E	525	ILE	N-CA-C	-7.75	96.43	107.75
1	D	158	ILE	N-CA-C	-7.58	103.15	113.00
1	A	158	ILE	N-CA-C	-7.54	103.20	113.00
1	C	525	ILE	N-CA-C	-7.50	96.80	107.75
1	B	184	SER	N-CA-C	-7.37	95.60	108.20
1	E	634	MET	N-CA-C	7.30	119.27	110.07
1	D	184	SER	N-CA-C	-7.30	95.72	108.20
1	F	525	ILE	N-CA-C	-7.06	97.45	107.75
1	A	184	SER	N-CA-C	-7.01	96.21	108.20
1	A	525	ILE	N-CA-C	-7.00	97.53	107.75
1	D	124	THR	N-CA-C	6.98	119.77	111.33
1	B	158	ILE	N-CA-C	-6.95	103.96	113.00
1	F	331	PRO	N-CA-C	-6.94	100.31	110.80
1	F	158	ILE	N-CA-C	-6.90	104.03	113.00
1	B	233	GLY	N-CA-C	6.88	121.22	112.83
1	C	175	VAL	N-CA-C	6.86	117.94	108.89
1	A	634	MET	N-CA-C	6.86	118.71	110.07
1	B	482	SER	N-CA-C	-6.85	101.49	110.53
1	B	581	TYR	CA-C-N	6.80	126.50	119.56
1	B	581	TYR	C-N-CA	6.80	126.50	119.56
1	C	184	SER	N-CA-C	-6.80	96.57	108.20
1	B	232	VAL	N-CA-C	-6.78	98.47	108.97
1	D	525	ILE	N-CA-C	-6.77	97.86	107.75
1	F	122	CYS	N-CA-C	6.75	119.47	111.71
1	E	186	TYR	N-CA-C	6.66	120.86	112.87
1	E	184	SER	N-CA-C	-6.54	97.02	108.20
1	F	373	LEU	N-CA-C	-6.48	105.02	113.12
1	C	191	ASP	N-CA-C	6.42	121.11	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	VAL	N-CA-C	-6.37	99.33	109.20
1	E	158	ILE	N-CA-C	-6.37	104.72	113.00
1	A	186	TYR	N-CA-C	6.35	120.49	112.87
1	E	581	TYR	CA-C-N	6.34	126.03	119.56
1	E	581	TYR	C-N-CA	6.34	126.03	119.56
1	C	373	LEU	N-CA-C	-6.33	103.66	112.45
1	E	384	ALA	N-CA-C	-6.27	104.44	111.28
1	B	124	THR	N-CA-C	6.21	118.57	111.11
1	E	334	LEU	N-CA-C	6.21	121.55	111.37
1	A	319	ASP	N-CA-C	6.15	118.49	111.11
1	E	373	LEU	N-CA-C	-6.13	105.46	113.12
1	F	319	ASP	N-CA-C	6.13	118.74	111.33
1	D	186	TYR	N-CA-C	6.12	120.22	112.87
1	E	319	ASP	N-CA-C	6.12	118.45	111.11
1	A	175	VAL	N-CA-C	6.09	116.94	108.89
1	D	634	MET	N-CA-C	6.08	117.73	110.07
1	F	587	VAL	N-CA-C	6.07	122.00	108.88
1	C	186	TYR	N-CA-C	6.07	120.16	112.87
1	C	430	ASN	N-CA-C	-6.05	100.14	109.76
1	F	318	LEU	N-CA-C	-6.04	100.53	109.11
1	E	430	ASN	N-CA-C	-6.03	100.18	109.76
1	F	175	VAL	N-CA-C	6.02	117.40	109.21
1	C	334	LEU	N-CA-C	6.00	121.27	111.37
1	D	428	ILE	N-CA-C	6.00	117.12	108.48
1	A	122	CYS	N-CA-C	6.00	119.86	112.54
1	B	191	ASP	N-CA-C	5.99	120.59	113.16
1	A	482	SER	N-CA-C	-5.99	102.62	110.53
1	C	232	VAL	N-CA-C	-5.99	99.69	108.97
1	D	232	VAL	N-CA-C	-5.99	99.95	109.17
1	D	319	ASP	N-CA-C	5.97	118.27	111.11
1	C	122	CYS	N-CA-C	5.96	119.81	112.54
1	B	318	LEU	N-CA-C	-5.95	100.67	109.11
1	E	124	THR	N-CA-C	5.94	118.52	111.33
1	F	634	MET	N-CA-C	5.94	118.50	110.31
1	A	334	LEU	N-CA-C	5.93	121.15	111.37
1	A	124	THR	N-CA-C	5.92	118.50	111.33
1	D	334	LEU	N-CA-C	5.89	121.09	111.37
1	B	335	GLY	N-CA-C	5.88	120.93	114.40
1	B	307	SER	N-CA-C	-5.87	102.38	109.72
1	A	191	ASP	N-CA-C	5.86	120.43	113.28
1	A	331	PRO	N-CA-C	-5.83	101.36	110.50
1	C	521	ARG	N-CA-C	5.80	118.41	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	186	TYR	N-CA-C	5.79	119.82	112.87
1	B	331	PRO	N-CA-C	-5.78	101.43	110.50
1	F	232	VAL	N-CA-C	-5.77	100.28	109.17
1	C	587	VAL	N-CA-C	5.77	121.35	108.88
1	B	334	LEU	N-CA-C	5.76	120.88	111.37
1	D	397	SER	N-CA-C	5.76	118.95	109.85
1	A	232	VAL	N-CA-C	-5.76	100.31	109.17
1	C	634	MET	N-CA-C	5.73	118.22	110.31
1	D	122	CYS	N-CA-C	5.72	118.46	111.82
1	C	331	PRO	N-CA-C	-5.69	101.57	110.50
1	A	196	VAL	N-CA-C	5.68	116.06	108.11
1	E	335	GLY	N-CA-C	5.67	121.25	113.99
1	F	397	SER	N-CA-C	5.67	118.49	109.81
1	B	430	ASN	N-CA-C	-5.65	101.48	109.96
1	A	384	ALA	N-CA-C	-5.65	105.03	111.07
1	D	359	VAL	N-CA-C	-5.64	99.42	107.77
1	A	587	VAL	N-CA-C	5.58	120.94	108.88
1	C	482	SER	N-CA-C	-5.57	103.18	110.53
1	E	191	ASP	N-CA-C	5.56	119.90	113.18
1	D	313	GLN	N-CA-C	-5.55	106.01	112.89
1	C	397	SER	N-CA-C	5.54	118.60	109.85
1	C	412	VAL	N-CA-C	5.54	115.86	108.11
1	E	122	CYS	N-CA-C	5.53	119.28	112.54
1	B	186	TYR	N-CA-C	5.51	119.49	112.87
1	D	412	VAL	N-CA-C	5.51	115.89	108.17
1	E	415	GLN	N-CA-C	5.51	119.75	113.19
1	A	430	ASN	N-CA-C	-5.49	101.73	109.96
1	B	525	ILE	N-CA-C	-5.48	98.56	107.28
1	B	634	MET	N-CA-C	5.48	117.87	110.31
1	C	256	GLY	N-CA-C	-5.46	101.67	110.95
1	A	373	LEU	N-CA-C	-5.46	104.87	112.45
1	E	482	SER	N-CA-C	-5.43	103.36	110.53
1	F	334	LEU	N-CA-C	5.43	120.33	111.37
1	B	175	VAL	N-CA-C	5.43	116.59	109.21
1	C	532	ASN	N-CA-C	-5.42	102.83	109.65
1	E	587	VAL	N-CA-C	5.41	120.56	108.88
1	B	196	VAL	N-CA-C	5.38	115.64	108.11
1	C	158	ILE	N-CA-C	-5.37	104.52	112.04
1	B	122	CYS	N-CA-C	5.37	119.09	112.54
1	D	550	PRO	N-CA-C	-5.36	102.72	111.68
1	A	581	TYR	CA-C-N	5.36	125.03	119.56
1	A	581	TYR	C-N-CA	5.36	125.03	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	ASN	N-CA-C	-5.36	102.90	109.65
1	C	187	SER	N-CA-C	-5.36	106.75	113.28
1	F	335	GLY	N-CA-C	5.34	120.54	114.67
1	B	395	VAL	N-CA-C	5.34	115.54	107.75
1	D	587	VAL	N-CA-C	5.33	120.40	108.88
1	F	384	ALA	N-CA-C	-5.31	105.39	111.07
1	D	384	ALA	N-CA-C	-5.30	105.40	111.07
1	C	124	THR	N-CA-C	5.28	117.71	111.33
1	B	187	SER	N-CA-C	-5.27	106.85	113.28
1	D	373	LEU	N-CA-C	-5.27	105.12	112.45
1	E	187	SER	N-CA-C	-5.26	106.86	113.28
1	F	430	ASN	N-CA-C	-5.25	102.08	109.96
1	C	540	SER	N-CA-C	5.24	116.81	108.79
1	F	521	ARG	N-CA-C	5.23	117.82	110.23
1	C	18	PRO	N-CA-CB	5.23	108.75	103.00
1	C	653	PRO	N-CA-C	5.23	120.46	114.03
1	E	307	SER	N-CA-C	-5.23	103.19	109.72
1	D	175	VAL	N-CA-C	5.21	116.08	108.58
1	C	319	ASP	N-CA-C	5.20	117.34	111.11
1	B	373	LEU	N-CA-C	-5.19	105.24	112.45
1	F	196	VAL	N-CA-C	5.18	115.94	108.48
1	C	196	VAL	N-CA-C	5.18	115.94	108.48
1	B	98	LEU	N-CA-C	5.17	117.65	111.71
1	D	18	PRO	N-CA-CB	5.16	108.68	103.00
1	F	124	THR	N-CA-C	5.16	117.57	111.33
1	E	331	PRO	N-CA-C	-5.16	102.41	110.50
1	D	331	PRO	N-CA-C	-5.15	102.41	110.50
1	E	540	SER	N-CA-C	5.15	116.12	108.60
1	F	589	GLN	N-CA-C	5.15	119.41	113.38
1	B	18	PRO	N-CA-CB	5.15	108.66	103.00
1	F	18	PRO	N-CA-CB	5.14	108.66	103.00
1	A	521	ARG	N-CA-C	5.14	117.68	110.23
1	F	246	GLN	CA-C-N	5.13	125.17	119.32
1	F	246	GLN	C-N-CA	5.13	125.17	119.32
1	E	521	ARG	N-CA-C	5.13	117.88	110.28
1	A	335	GLY	N-CA-C	5.13	120.55	113.99
1	E	170	LEU	N-CA-C	5.13	118.08	110.14
1	E	428	ILE	N-CA-C	5.12	115.86	108.48
1	E	624	HIS	N-CA-C	5.09	116.91	108.20
1	E	18	PRO	N-CA-CB	5.08	108.59	103.00
1	D	587	VAL	CA-C-N	-5.07	114.73	119.90
1	D	587	VAL	C-N-CA	-5.07	114.73	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	335	GLY	N-CA-C	5.06	120.47	113.99
1	B	256	GLY	N-CA-C	-5.06	102.35	110.95
1	A	18	PRO	N-CA-CB	5.06	108.56	103.00
1	A	397	SER	N-CA-C	5.06	117.84	109.85
1	E	196	VAL	N-CA-C	5.06	115.76	108.48
1	B	397	SER	N-CA-C	5.05	117.83	109.85
1	A	412	VAL	N-CA-C	5.04	115.17	108.11
1	D	581	TYR	CA-C-N	5.03	124.69	119.56
1	D	581	TYR	C-N-CA	5.03	124.69	119.56
1	A	540	SER	N-CA-C	5.03	115.94	108.60
1	F	412	VAL	N-CA-C	5.01	115.19	108.17
1	C	589	GLN	N-CA-C	5.01	118.97	112.86
1	C	246	GLN	CA-C-N	5.01	125.03	119.32
1	C	246	GLN	C-N-CA	5.01	125.03	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	305	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5194	0	5033	136	0
1	B	5194	0	5034	148	0
1	C	5194	0	5034	139	0
1	D	5194	0	5033	165	0
1	E	5194	0	5033	155	0
1	F	5194	0	5033	144	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	499	0	0	7	0
3	B	453	0	0	6	0
3	C	474	0	0	5	0
3	D	415	0	0	9	0
3	E	335	0	0	5	0
3	F	380	0	0	7	0
All	All	33726	0	30200	838	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 14.

All (838) 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:C:546:THR:CG2	1:D:546:THR:HG21	1.57	1.32
1:A:546:THR:HG21	1:B:546:THR:CG2	1.64	1.27
1:E:546:THR:CG2	1:F:546:THR:HG21	1.64	1.26
1:A:546:THR:CG2	1:B:546:THR:HG21	1.67	1.24
1:C:546:THR:HG21	1:D:546:THR:CG2	1.69	1.22
1:E:546:THR:HG21	1:F:546:THR:CG2	1.81	1.09
1:D:664:THR:HG22	1:D:667:GLU:H	1.15	1.09
1:C:664:THR:HG22	1:C:667:GLU:H	1.17	1.07
1:A:664:THR:HG22	1:A:667:GLU:H	1.20	1.06
1:E:664:THR:HG22	1:E:667:GLU:H	1.20	1.05
1:E:439:GLU:HG3	1:E:441:GLY:H	1.22	1.00
1:F:664:THR:HG22	1:F:667:GLU:H	1.24	0.98
1:C:23:HIS:HD2	1:C:25:LEU:H	1.13	0.97
1:B:664:THR:HG22	1:B:667:GLU:H	1.30	0.96
1:A:494:TYR:CD1	1:B:313:GLN:HG2	2.02	0.95
1:C:130:ASN:HB3	3:C:716:HOH:O	1.68	0.93
1:D:23:HIS:HD2	1:D:25:LEU:H	1.14	0.93
1:E:311:PRO:HA	1:E:313:GLN:NE2	1.84	0.93
1:D:311:PRO:HA	1:D:313:GLN:NE2	1.83	0.93
1:A:23:HIS:HD2	1:A:25:LEU:H	1.16	0.92
1:E:311:PRO:HA	1:E:313:GLN:HE22	1.32	0.92
1:C:439:GLU:HG3	1:C:441:GLY:H	1.33	0.92
1:A:311:PRO:HA	1:A:313:GLN:NE2	1.85	0.91
1:A:130:ASN:HB3	3:A:1134:HOH:O	1.71	0.90
1:B:347:ALA:HB3	1:B:359:VAL:HG13	1.53	0.90
1:E:546:THR:HG21	1:F:546:THR:HG21	0.92	0.89
1:A:439:GLU:HG3	1:A:441:GLY:H	1.33	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:PRO:HA	1:C:313:GLN:NE2	1.89	0.88
1:B:311:PRO:HA	1:B:313:GLN:NE2	1.89	0.87
1:E:23:HIS:HD2	1:E:25:LEU:H	1.13	0.87
1:B:23:HIS:HD2	1:B:25:LEU:H	1.16	0.86
1:B:439:GLU:HG3	1:B:441:GLY:H	1.41	0.85
1:E:439:GLU:HG3	1:E:441:GLY:N	1.92	0.85
1:A:311:PRO:HA	1:A:313:GLN:HE22	1.42	0.84
1:F:439:GLU:HG3	1:F:441:GLY:H	1.41	0.84
1:F:598:MET:HE2	1:F:602:ILE:HG13	1.57	0.84
1:F:23:HIS:HD2	1:F:25:LEU:H	1.26	0.83
1:D:439:GLU:HG3	1:D:441:GLY:H	1.44	0.83
1:D:573:VAL:HG11	1:D:598:MET:HE1	1.60	0.83
1:F:311:PRO:HA	1:F:313:GLN:NE2	1.95	0.82
1:E:313:GLN:HG2	1:F:494:TYR:CD1	2.14	0.81
1:C:311:PRO:HA	1:C:313:GLN:HE22	1.46	0.81
1:C:598:MET:HE2	1:C:602:ILE:HG13	1.61	0.80
1:D:468:ILE:H	1:D:473:ASN:HD21	1.24	0.80
1:C:146:ASN:C	1:C:146:ASN:HD22	1.88	0.80
1:D:527:ASN:HD22	1:D:529:ASN:H	1.29	0.80
1:A:313:GLN:HG2	1:B:494:TYR:CD1	2.17	0.79
1:C:347:ALA:HB3	1:C:359:VAL:HG13	1.65	0.78
1:C:494:TYR:CD1	1:D:313:GLN:HG2	2.18	0.78
1:F:21:PRO:HG3	1:F:77:ARG:CZ	2.12	0.78
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.13	0.78
1:E:347:ALA:HB3	1:E:359:VAL:HG13	1.65	0.78
1:F:527:ASN:HD22	1:F:529:ASN:H	1.33	0.76
1:C:468:ILE:H	1:C:473:ASN:HD21	1.32	0.76
1:C:313:GLN:HG2	1:D:494:TYR:CD1	2.20	0.76
1:D:311:PRO:HA	1:D:313:GLN:HE22	1.51	0.76
1:D:527:ASN:HD21	1:D:529:ASN:HB2	1.51	0.75
1:F:467:ARG:HD2	1:F:471:ASP:OD1	1.85	0.75
1:A:468:ILE:H	1:A:473:ASN:HD21	1.33	0.75
1:D:439:GLU:C	1:D:441:GLY:H	1.92	0.74
1:C:70:GLN:HG2	3:C:825:HOH:O	1.86	0.74
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.17	0.74
1:A:79:ALA:HB1	3:A:944:HOH:O	1.86	0.74
1:A:347:ALA:HB3	1:A:359:VAL:HG13	1.68	0.74
1:F:468:ILE:H	1:F:473:ASN:HD21	1.35	0.74
1:B:157:THR:HG21	1:B:588:PRO:HB3	1.69	0.74
1:C:573:VAL:HG11	1:C:598:MET:HE1	1.68	0.74
1:A:146:ASN:C	1:A:146:ASN:HD22	1.95	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:TYR:CD1	1:F:313:GLN:HG2	2.23	0.73
1:F:347:ALA:HB3	1:F:359:VAL:HG13	1.70	0.73
1:E:468:ILE:H	1:E:473:ASN:HD21	1.35	0.73
1:D:146:ASN:C	1:D:146:ASN:HD22	1.94	0.73
1:B:146:ASN:HD22	1:B:146:ASN:C	1.96	0.73
1:A:439:GLU:HG3	1:A:441:GLY:N	2.03	0.73
1:E:527:ASN:HD22	1:E:529:ASN:H	1.37	0.73
1:D:598:MET:HE2	1:D:602:ILE:HG13	1.70	0.73
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.18	0.72
1:F:18:PRO:HG3	1:F:32:GLU:HA	1.70	0.72
1:B:527:ASN:HD22	1:B:529:ASN:H	1.37	0.72
1:E:439:GLU:C	1:E:441:GLY:H	1.96	0.72
1:B:137:GLN:OE1	1:B:212:ARG:NH2	2.22	0.72
1:E:18:PRO:HG3	1:E:32:GLU:HA	1.71	0.72
1:F:146:ASN:C	1:F:146:ASN:HD22	1.96	0.72
1:C:527:ASN:HD22	1:C:529:ASN:H	1.36	0.72
1:A:527:ASN:HD22	1:A:529:ASN:H	1.37	0.72
1:E:23:HIS:CD2	1:E:25:LEU:H	2.04	0.72
1:B:468:ILE:H	1:B:473:ASN:HD21	1.38	0.71
1:D:335:GLY:O	1:D:336:CYS:HB2	1.91	0.71
1:D:338:CYS:HG	1:D:364:CYS:CB	2.03	0.71
1:A:439:GLU:C	1:A:441:GLY:H	1.97	0.71
1:C:137:GLN:OE1	1:C:212:ARG:NH2	2.23	0.71
1:A:598:MET:HE2	1:A:602:ILE:HG13	1.73	0.71
1:B:439:GLU:C	1:B:441:GLY:H	1.98	0.71
1:B:467:ARG:HD2	1:B:471:ASP:OD1	1.92	0.70
1:E:573:VAL:HG11	1:E:598:MET:HE1	1.74	0.70
1:C:439:GLU:C	1:C:441:GLY:H	2.00	0.69
1:C:37:THR:O	1:C:41:LYS:HG3	1.92	0.69
1:C:527:ASN:HD22	1:C:527:ASN:C	2.00	0.69
1:D:467:ARG:HD2	1:D:471:ASP:OD1	1.92	0.69
1:C:565:TRP:CD1	1:C:582:PRO:HB2	2.28	0.69
1:C:439:GLU:HG3	1:C:441:GLY:N	2.05	0.69
1:A:573:VAL:HG11	1:A:598:MET:HE1	1.75	0.69
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.22	0.69
1:C:406:GLU:OE2	1:D:376:HIS:ND1	2.20	0.69
1:D:21:PRO:HG3	1:D:77:ARG:CZ	2.23	0.69
1:D:507:THR:HG23	1:D:605:GLY:O	1.93	0.69
1:E:335:GLY:O	1:E:336:CYS:HB2	1.93	0.69
1:B:507:THR:HG23	1:B:605:GLY:O	1.93	0.69
1:D:68:LYS:HE2	1:D:280:ASP:OD2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:507:THR:HG23	1:E:605:GLY:O	1.94	0.68
1:D:157:THR:HB	1:D:159:GLY:H	1.57	0.68
1:C:546:THR:HG21	1:D:546:THR:HG21	0.76	0.68
1:E:565:TRP:CD1	1:E:582:PRO:HB2	2.29	0.68
1:B:311:PRO:HA	1:B:313:GLN:HE22	1.56	0.68
1:B:168:LYS:HE2	3:B:944:HOH:O	1.93	0.68
1:C:335:GLY:O	1:C:336:CYS:HB2	1.92	0.68
1:F:338:CYS:HG	1:F:364:CYS:HG	0.76	0.68
1:B:507:THR:HG21	3:B:965:HOH:O	1.94	0.67
1:C:141:SER:O	1:C:215:VAL:HG23	1.93	0.67
1:E:137:GLN:OE1	1:E:212:ARG:NH2	2.27	0.67
1:E:527:ASN:HD21	1:E:529:ASN:HD22	1.42	0.67
1:C:546:THR:CG2	1:D:546:THR:CG2	2.48	0.67
1:E:546:THR:CG2	1:F:546:THR:CG2	2.55	0.67
1:A:467:ARG:HD2	1:A:471:ASP:OD1	1.93	0.67
1:C:146:ASN:HD22	1:C:147:GLU:N	1.92	0.67
1:B:439:GLU:HG3	1:B:441:GLY:N	2.10	0.67
1:A:18:PRO:HG3	1:A:32:GLU:HA	1.76	0.67
1:E:467:ARG:HD2	1:E:471:ASP:OD1	1.95	0.67
1:A:335:GLY:O	1:A:336:CYS:HB2	1.94	0.67
1:F:573:VAL:HG11	1:F:598:MET:HE1	1.77	0.67
1:A:137:GLN:OE1	1:A:212:ARG:NH2	2.28	0.67
1:B:345:LEU:HB2	1:B:363:VAL:HB	1.77	0.67
1:E:211:ARG:HD3	1:E:213:ARG:HD2	1.77	0.66
1:E:669:LYS:HE3	1:F:181:GLU:OE1	1.96	0.66
1:B:262:SER:O	1:B:263:ASN:HB2	1.96	0.66
1:C:157:THR:HB	1:C:159:GLY:H	1.60	0.66
1:F:598:MET:HE3	1:F:598:MET:HA	1.77	0.66
1:E:573:VAL:CG1	1:E:598:MET:HE1	2.26	0.66
1:F:439:GLU:C	1:F:441:GLY:H	2.02	0.66
1:F:137:GLN:OE1	1:F:212:ARG:NH2	2.29	0.65
1:F:452:ASN:C	1:F:452:ASN:HD22	2.04	0.65
1:C:507:THR:HG23	1:C:605:GLY:O	1.97	0.65
1:D:37:THR:O	1:D:41:LYS:HG3	1.96	0.65
1:E:308:PRO:HB3	1:F:497:ALA:HB2	1.79	0.65
1:F:338:CYS:CB	1:F:364:CYS:HG	2.06	0.65
1:F:439:GLU:HG3	1:F:441:GLY:N	2.10	0.65
1:F:507:THR:HG23	1:F:605:GLY:O	1.97	0.65
1:C:23:HIS:CD2	1:C:25:LEU:H	2.05	0.65
1:F:146:ASN:HD22	1:F:147:GLU:N	1.94	0.65
1:D:18:PRO:HG3	1:D:32:GLU:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:THR:HG23	1:A:605:GLY:O	1.97	0.65
1:B:573:VAL:HG11	1:B:598:MET:HE1	1.78	0.65
1:D:439:GLU:HG3	1:D:441:GLY:N	2.11	0.65
1:E:452:ASN:HD22	1:E:453:ALA:N	1.95	0.65
1:F:37:THR:O	1:F:41:LYS:HG3	1.97	0.65
1:E:18:PRO:HG2	1:E:32:GLU:HG2	1.79	0.64
1:C:146:ASN:C	1:C:146:ASN:ND2	2.55	0.64
1:D:573:VAL:CG1	1:D:598:MET:HE1	2.27	0.64
1:E:211:ARG:CD	1:E:213:ARG:HD2	2.27	0.64
1:A:452:ASN:C	1:A:452:ASN:HD22	2.03	0.64
1:B:23:HIS:CD2	1:B:25:LEU:H	2.07	0.64
1:D:137:GLN:OE1	1:D:212:ARG:NH2	2.29	0.64
1:D:414:MET:HE3	1:D:418:ALA:HB3	1.80	0.64
1:A:157:THR:HG21	1:A:588:PRO:HB3	1.79	0.64
1:E:144:PRO:HB2	1:E:146:ASN:ND2	2.13	0.64
1:A:146:ASN:HD22	1:A:147:GLU:N	1.96	0.64
1:A:497:ALA:HB2	1:B:308:PRO:HB3	1.78	0.64
1:E:457:GLN:HE22	1:E:552:LEU:H	1.46	0.64
1:C:527:ASN:ND2	1:C:529:ASN:H	1.95	0.64
1:A:546:THR:HG21	1:B:546:THR:HG21	0.76	0.63
1:A:669:LYS:HE3	1:B:181:GLU:OE1	1.98	0.63
1:F:160:TYR:CD2	1:F:558:LEU:HD21	2.33	0.63
1:A:262:SER:O	1:A:263:ASN:HB2	1.97	0.63
1:C:452:ASN:C	1:C:452:ASN:HD22	2.06	0.63
1:B:573:VAL:CG1	1:B:598:MET:HE1	2.28	0.63
1:E:146:ASN:C	1:E:146:ASN:HD22	2.07	0.63
1:B:157:THR:CG2	1:B:588:PRO:HB3	2.29	0.63
1:F:18:PRO:HG2	1:F:32:GLU:HG2	1.81	0.63
1:D:468:ILE:N	1:D:473:ASN:HD21	1.96	0.62
1:F:414:MET:HE3	1:F:418:ALA:HB3	1.81	0.62
1:C:669:LYS:HE3	1:D:181:GLU:OE1	1.99	0.62
1:F:527:ASN:ND2	1:F:529:ASN:H	1.97	0.62
1:B:598:MET:HE2	1:B:602:ILE:HG13	1.82	0.62
1:D:157:THR:HG21	1:D:588:PRO:HB3	1.81	0.62
1:D:573:VAL:HG11	1:D:598:MET:CE	2.28	0.62
1:D:262:SER:O	1:D:263:ASN:HB2	2.00	0.62
1:E:191:ASP:OD2	1:E:212:ARG:NH1	2.31	0.62
1:B:157:THR:HB	1:B:159:GLY:H	1.63	0.62
1:A:308:PRO:HB3	1:B:497:ALA:HB2	1.80	0.62
1:E:527:ASN:ND2	1:E:529:ASN:H	1.98	0.62
1:E:439:GLU:C	1:E:441:GLY:N	2.57	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:HD11	1:D:157:THR:HG23	1.82	0.61
1:D:527:ASN:ND2	1:D:529:ASN:H	1.97	0.61
1:E:338:CYS:CB	1:E:364:CYS:HG	2.13	0.61
1:B:527:ASN:HD21	1:B:529:ASN:HD22	1.47	0.61
1:D:664:THR:HG22	1:D:667:GLU:N	2.00	0.61
1:C:18:PRO:HG3	1:C:32:GLU:HA	1.82	0.61
1:B:414:MET:HE3	1:B:418:ALA:HB3	1.82	0.61
1:D:439:GLU:C	1:D:441:GLY:N	2.55	0.61
1:B:452:ASN:C	1:B:452:ASN:HD22	2.09	0.61
1:A:160:TYR:CD2	1:A:558:LEU:HD21	2.35	0.61
1:A:573:VAL:CG1	1:A:598:MET:HE1	2.30	0.61
1:F:452:ASN:HD22	1:F:453:ALA:N	1.98	0.61
1:F:141:SER:O	1:F:215:VAL:HG23	2.00	0.61
1:C:160:TYR:CD2	1:C:558:LEU:HD21	2.36	0.60
1:C:527:ASN:HD21	1:C:529:ASN:HB2	1.66	0.60
1:E:452:ASN:HD22	1:E:452:ASN:C	2.08	0.60
1:A:527:ASN:HD22	1:A:527:ASN:C	2.10	0.60
1:A:565:TRP:CD1	1:A:582:PRO:HB2	2.36	0.60
1:A:157:THR:HB	1:A:159:GLY:H	1.67	0.60
1:F:335:GLY:O	1:F:336:CYS:HB2	2.01	0.60
1:D:23:HIS:CD2	1:D:25:LEU:H	2.07	0.60
1:E:310:PHE:HA	1:E:313:GLN:HE21	1.66	0.60
1:E:547:GLN:NE2	1:E:640:THR:H	2.00	0.60
1:F:146:ASN:C	1:F:146:ASN:ND2	2.59	0.60
1:B:146:ASN:HD22	1:B:147:GLU:N	1.98	0.60
1:F:345:LEU:HB2	1:F:363:VAL:HB	1.84	0.60
1:A:452:ASN:HD22	1:A:453:ALA:N	2.00	0.60
1:C:276:ILE:HD11	1:C:398:GLN:HB3	1.82	0.60
1:C:467:ARG:HD2	1:C:471:ASP:OD1	2.01	0.60
1:E:527:ASN:HD22	1:E:527:ASN:C	2.10	0.60
1:B:18:PRO:HG3	1:B:32:GLU:HA	1.83	0.59
1:F:527:ASN:HD22	1:F:527:ASN:C	2.09	0.59
1:A:18:PRO:HG2	1:A:32:GLU:HG2	1.85	0.59
1:D:565:TRP:CD1	1:D:582:PRO:HB2	2.37	0.59
1:A:439:GLU:C	1:A:441:GLY:N	2.57	0.59
1:D:146:ASN:C	1:D:146:ASN:ND2	2.57	0.59
1:E:146:ASN:HD22	1:E:147:GLU:N	2.01	0.59
1:B:35:ALA:HB1	1:B:101:LEU:HD21	1.83	0.59
1:E:157:THR:HB	1:E:159:GLY:H	1.68	0.59
1:E:527:ASN:ND2	1:E:529:ASN:HD22	1.99	0.59
1:A:527:ASN:ND2	1:A:529:ASN:H	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:TYR:CE1	1:B:189:PRO:HB3	2.38	0.59
1:E:262:SER:O	1:E:263:ASN:HB2	2.02	0.59
1:B:565:TRP:CD1	1:B:582:PRO:HB2	2.38	0.58
1:D:146:ASN:HD22	1:D:147:GLU:N	1.99	0.58
1:F:301:MET:HG3	1:F:320:ILE:HD12	1.84	0.58
1:E:176:TYR:CE1	1:E:189:PRO:HB3	2.39	0.58
1:F:68:LYS:HD2	3:F:873:HOH:O	2.02	0.58
1:C:157:THR:HG21	1:C:588:PRO:HB3	1.86	0.58
1:B:310:PHE:HA	1:B:313:GLN:HE21	1.69	0.58
1:F:439:GLU:C	1:F:441:GLY:N	2.60	0.58
1:C:439:GLU:C	1:C:441:GLY:N	2.58	0.58
1:C:468:ILE:N	1:C:473:ASN:HD21	2.02	0.57
1:A:468:ILE:N	1:A:473:ASN:HD21	2.01	0.57
1:E:47:LYS:HD2	1:E:85:GLU:OE2	2.04	0.57
1:E:276:ILE:HD11	1:E:398:GLN:HB3	1.87	0.57
1:A:68:LYS:HE2	1:A:280:ASP:OD2	2.04	0.57
1:C:414:MET:HE3	1:C:418:ALA:HB3	1.86	0.57
1:A:23:HIS:CD2	1:A:25:LEU:H	2.09	0.57
1:E:547:GLN:HE22	1:E:639:ILE:HA	1.70	0.57
1:F:68:LYS:HE2	1:F:280:ASP:OD2	2.05	0.57
1:D:452:ASN:HD22	1:D:453:ALA:N	2.02	0.57
1:D:457:GLN:HE22	1:D:552:LEU:H	1.52	0.57
1:D:641:LEU:C	1:D:641:LEU:HD23	2.30	0.57
1:E:414:MET:HE3	1:E:418:ALA:HB3	1.85	0.57
1:F:176:TYR:CE1	1:F:189:PRO:HB3	2.40	0.57
1:D:116:LEU:CD1	1:D:157:THR:HG23	2.35	0.57
1:F:641:LEU:C	1:F:641:LEU:HD23	2.29	0.57
1:C:117:THR:N	1:C:120:ASP:OD1	2.38	0.57
1:C:308:PRO:HB3	1:D:497:ALA:HB2	1.87	0.57
1:D:527:ASN:HD22	1:D:527:ASN:C	2.13	0.57
1:E:546:THR:HG23	1:F:546:THR:HG21	1.76	0.57
1:F:262:SER:O	1:F:263:ASN:HB2	2.04	0.57
1:A:414:MET:HE3	1:A:418:ALA:HB3	1.86	0.56
1:F:468:ILE:N	1:F:473:ASN:HD21	2.03	0.56
1:B:146:ASN:C	1:B:146:ASN:ND2	2.61	0.56
1:D:444:GLY:HA3	1:D:452:ASN:HD21	1.70	0.56
1:A:176:TYR:CE1	1:A:189:PRO:HB3	2.39	0.56
1:B:160:TYR:CD2	1:B:558:LEU:HD21	2.40	0.56
1:D:452:ASN:HD22	1:D:452:ASN:C	2.12	0.56
1:A:631:PHE:CG	1:A:632:PRO:HA	2.40	0.56
1:C:116:LEU:HD11	1:C:157:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLN:HB2	1:C:341:VAL:HG21	1.87	0.56
1:D:160:TYR:CD2	1:D:558:LEU:HD21	2.41	0.56
1:C:573:VAL:CG1	1:C:598:MET:HE1	2.35	0.56
1:E:211:ARG:NE	1:E:213:ARG:HD2	2.20	0.56
1:E:439:GLU:HG3	1:E:441:GLY:CA	2.36	0.56
1:A:246:GLN:HB2	1:A:341:VAL:HG21	1.88	0.56
1:C:444:GLY:HA3	1:C:452:ASN:HD21	1.71	0.56
1:E:160:TYR:CD2	1:E:558:LEU:HD21	2.41	0.55
1:B:439:GLU:C	1:B:441:GLY:N	2.58	0.55
1:E:573:VAL:HG11	1:E:598:MET:CE	2.36	0.55
1:F:311:PRO:HA	1:F:313:GLN:HE22	1.70	0.55
1:F:573:VAL:CG1	1:F:598:MET:HE1	2.37	0.55
1:A:546:THR:CG2	1:B:546:THR:CG2	2.50	0.55
1:B:344:TYR:CD1	1:B:361:ASN:HB3	2.41	0.55
1:D:70:GLN:HG2	3:D:980:HOH:O	2.06	0.55
1:F:261:TRP:CE3	1:F:262:SER:HB2	2.42	0.55
1:D:527:ASN:ND2	1:D:529:ASN:HB2	2.20	0.55
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.42	0.55
1:B:68:LYS:HE2	1:B:280:ASP:OD2	2.07	0.55
1:B:664:THR:CG2	1:B:667:GLU:H	2.09	0.55
1:D:261:TRP:CE3	1:D:262:SER:HB2	2.42	0.55
1:F:631:PHE:CG	1:F:632:PRO:HA	2.41	0.55
1:C:598:MET:HE3	1:C:598:MET:HA	1.89	0.55
1:D:547:GLN:NE2	1:D:640:THR:H	2.05	0.55
1:E:37:THR:HG21	1:E:354:GLY:HA2	1.88	0.55
1:F:157:THR:HB	1:F:159:GLY:H	1.72	0.55
1:A:345:LEU:HB2	1:A:363:VAL:HB	1.87	0.54
1:A:117:THR:N	1:A:120:ASP:OD1	2.40	0.54
1:C:69:GLU:CD	1:C:467:ARG:HH22	2.15	0.54
1:E:514:ASN:HA	1:E:569:SER:HB2	1.90	0.54
1:F:344:TYR:CD1	1:F:361:ASN:HB3	2.43	0.54
1:A:35:ALA:HB1	1:A:101:LEU:HD21	1.89	0.54
1:C:35:ALA:HB1	1:C:101:LEU:HD21	1.88	0.54
1:A:157:THR:CG2	1:A:588:PRO:HB3	2.37	0.54
1:B:527:ASN:ND2	1:B:529:ASN:HD22	2.05	0.54
1:F:310:PHE:HA	1:F:313:GLN:HE21	1.72	0.54
1:F:670:ARG:C	1:F:672:VAL:H	2.14	0.54
1:B:47:LYS:HD2	1:B:85:GLU:OE2	2.07	0.54
1:B:631:PHE:CG	1:B:632:PRO:HA	2.43	0.54
1:D:294:HIS:HD2	3:D:847:HOH:O	1.89	0.54
1:C:655:LEU:HD11	1:D:632:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLN:NE2	1:A:640:THR:H	2.06	0.54
1:B:527:ASN:ND2	1:B:529:ASN:H	2.02	0.54
1:D:631:PHE:CG	1:D:632:PRO:HA	2.43	0.54
1:F:157:THR:HG21	1:F:588:PRO:HB3	1.90	0.54
1:F:506:LYS:HG2	3:F:975:HOH:O	2.08	0.54
1:B:346:ASP:OD1	1:B:360:LYS:HA	2.08	0.54
1:C:89:PRO:HG2	1:C:110:GLU:HB3	1.89	0.54
1:E:670:ARG:C	1:E:672:VAL:H	2.16	0.54
1:A:181:GLU:OE1	1:B:669:LYS:HE3	2.09	0.53
1:B:261:TRP:CE3	1:B:262:SER:HB2	2.43	0.53
1:C:557:SER:O	1:C:561:LYS:HG3	2.09	0.53
1:E:468:ILE:N	1:E:473:ASN:HD21	2.04	0.53
1:A:670:ARG:C	1:A:672:VAL:H	2.15	0.53
1:C:262:SER:O	1:C:263:ASN:HB2	2.08	0.53
1:F:641:LEU:C	1:F:641:LEU:CD2	2.81	0.53
1:B:452:ASN:HD22	1:B:453:ALA:N	2.06	0.53
1:D:135:ILE:O	1:D:139:VAL:HG23	2.08	0.53
1:A:527:ASN:HD21	1:A:529:ASN:HB2	1.73	0.53
1:D:670:ARG:C	1:D:672:VAL:H	2.17	0.53
1:B:468:ILE:N	1:B:473:ASN:HD21	2.04	0.53
1:A:37:THR:O	1:A:41:LYS:HG3	2.09	0.53
1:B:392:THR:HG22	3:B:774:HOH:O	2.08	0.53
1:B:546:THR:HG23	1:B:546:THR:O	2.08	0.53
1:C:128:ILE:HG13	1:C:129:ARG:N	2.23	0.53
1:E:69:GLU:CD	1:E:467:ARG:HH22	2.17	0.53
1:E:181:GLU:OE1	1:F:669:LYS:HE3	2.09	0.53
1:F:527:ASN:HD21	1:F:529:ASN:HB2	1.73	0.53
1:C:338:CYS:HG	1:C:364:CYS:CB	2.20	0.53
1:C:573:VAL:HG11	1:C:598:MET:CE	2.38	0.53
1:B:117:THR:N	1:B:120:ASP:OD1	2.41	0.53
1:B:641:LEU:C	1:B:641:LEU:HD23	2.34	0.53
1:C:641:LEU:HD23	1:C:641:LEU:C	2.34	0.53
1:C:664:THR:CG2	1:C:667:GLU:H	2.07	0.53
1:D:157:THR:CG2	1:D:588:PRO:HB3	2.38	0.53
1:E:144:PRO:HB2	1:E:146:ASN:HD21	1.74	0.53
1:E:303:VAL:HA	1:E:457:GLN:O	2.09	0.53
1:A:141:SER:O	1:A:215:VAL:HG23	2.09	0.52
1:A:452:ASN:C	1:A:452:ASN:ND2	2.67	0.52
1:E:157:THR:HG21	1:E:588:PRO:HB3	1.91	0.52
1:B:180:ASP:OD2	1:B:182:ASP:HB2	2.09	0.52
1:C:452:ASN:HD22	1:C:453:ALA:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:565:TRP:CD1	1:F:582:PRO:HB2	2.43	0.52
1:A:276:ILE:HD11	1:A:398:GLN:HB3	1.91	0.52
1:B:211:ARG:HD3	1:B:213:ARG:HD2	1.92	0.52
1:B:527:ASN:HD22	1:B:527:ASN:C	2.17	0.52
1:C:68:LYS:HE2	1:C:280:ASP:OD2	2.09	0.52
1:F:191:ASP:OD2	1:F:212:ARG:NH1	2.42	0.52
1:C:497:ALA:HB2	1:D:308:PRO:HB3	1.90	0.52
1:E:641:LEU:C	1:E:641:LEU:HD23	2.34	0.52
1:C:670:ARG:C	1:C:672:VAL:H	2.16	0.52
1:A:146:ASN:C	1:A:146:ASN:ND2	2.60	0.52
1:B:547:GLN:NE2	1:B:640:THR:H	2.08	0.52
1:F:346:ASP:OD1	1:F:360:LYS:HA	2.09	0.52
1:A:310:PHE:HA	1:A:313:GLN:HE21	1.75	0.51
1:B:670:ARG:C	1:B:672:VAL:H	2.18	0.51
1:A:444:GLY:HA3	1:A:452:ASN:HD21	1.76	0.51
1:F:211:ARG:NH2	1:F:435:GLY:HA3	2.25	0.51
1:C:18:PRO:HG2	1:C:32:GLU:HG2	1.93	0.51
1:F:246:GLN:HB2	1:F:341:VAL:HG21	1.92	0.51
1:C:116:LEU:CD1	1:C:157:THR:HG23	2.41	0.51
1:D:176:TYR:CE1	1:D:189:PRO:HB3	2.46	0.51
1:E:452:ASN:C	1:E:452:ASN:ND2	2.67	0.51
1:B:444:GLY:HA3	1:B:452:ASN:HD21	1.76	0.51
1:F:670:ARG:C	1:F:672:VAL:N	2.68	0.51
1:E:345:LEU:HB2	1:E:363:VAL:HB	1.92	0.51
1:F:664:THR:HG22	1:F:667:GLU:HG3	1.91	0.51
1:A:261:TRP:CE3	1:A:262:SER:HB2	2.45	0.51
1:B:527:ASN:HD21	1:B:529:ASN:HB2	1.76	0.51
1:A:69:GLU:CD	1:A:467:ARG:HH22	2.18	0.51
1:B:335:GLY:O	1:B:336:CYS:HB2	2.10	0.51
1:F:35:ALA:HB1	1:F:101:LEU:HD21	1.93	0.51
1:B:21:PRO:HG3	1:B:77:ARG:NE	2.26	0.50
1:E:497:ALA:HB2	1:F:308:PRO:HB3	1.93	0.50
1:F:23:HIS:CD2	1:F:25:LEU:H	2.18	0.50
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.47	0.50
1:C:452:ASN:C	1:C:452:ASN:ND2	2.68	0.50
1:D:117:THR:N	1:D:120:ASP:OD1	2.43	0.50
1:F:468:ILE:H	1:F:473:ASN:ND2	2.08	0.50
1:A:573:VAL:HG11	1:A:598:MET:CE	2.40	0.50
1:D:246:GLN:HB2	1:D:341:VAL:HG21	1.92	0.50
1:E:146:ASN:ND2	1:E:146:ASN:C	2.69	0.50
1:A:69:GLU:OE2	1:A:467:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:THR:N	1:E:120:ASP:OD1	2.45	0.50
1:E:261:TRP:CE3	1:E:262:SER:HB2	2.47	0.50
1:F:444:GLY:HA3	1:F:452:ASN:HD21	1.75	0.50
1:A:457:GLN:HE22	1:A:552:LEU:H	1.57	0.50
1:A:670:ARG:C	1:A:672:VAL:N	2.70	0.50
1:B:246:GLN:HB2	1:B:341:VAL:HG21	1.92	0.50
1:C:259:MET:HE3	1:C:394:LEU:HD11	1.94	0.50
1:A:191:ASP:OD2	1:A:212:ARG:NH1	2.43	0.50
1:A:527:ASN:HD21	1:A:529:ASN:HD22	1.59	0.50
1:B:190:LEU:HD21	1:B:215:VAL:HG13	1.94	0.50
1:C:157:THR:CG2	1:C:588:PRO:HB3	2.41	0.50
1:E:246:GLN:HB2	1:E:341:VAL:HG21	1.94	0.50
1:F:452:ASN:C	1:F:452:ASN:ND2	2.66	0.50
1:C:632:PRO:HD2	1:D:655:LEU:HD11	1.93	0.50
1:D:191:ASP:OD2	1:D:212:ARG:NH1	2.44	0.50
1:D:311:PRO:HA	1:D:313:GLN:HE21	1.69	0.50
1:E:670:ARG:C	1:E:672:VAL:N	2.69	0.50
1:B:641:LEU:C	1:B:641:LEU:CD2	2.85	0.50
1:D:347:ALA:HB3	1:D:359:VAL:HG13	1.93	0.50
1:E:301:MET:O	1:E:318:LEU:HA	2.12	0.50
1:A:641:LEU:C	1:A:641:LEU:HD23	2.37	0.49
1:D:18:PRO:HG2	1:D:32:GLU:HG2	1.94	0.49
1:D:35:ALA:HB1	1:D:101:LEU:HD21	1.95	0.49
1:D:189:PRO:HD2	3:D:782:HOH:O	2.11	0.49
1:D:211:ARG:NH2	1:D:435:GLY:HA3	2.27	0.49
1:E:157:THR:CG2	1:E:588:PRO:HB3	2.42	0.49
1:E:444:GLY:HA3	1:E:452:ASN:HD21	1.77	0.49
1:F:664:THR:CG2	1:F:667:GLU:H	2.11	0.49
1:D:641:LEU:C	1:D:641:LEU:CD2	2.84	0.49
1:E:118:VAL:HG13	3:E:928:HOH:O	2.11	0.49
1:C:345:LEU:HB2	1:C:363:VAL:HB	1.94	0.49
1:C:631:PHE:CG	1:C:632:PRO:HA	2.47	0.49
1:F:69:GLU:OE2	1:F:467:ARG:NH2	2.44	0.49
1:F:144:PRO:HB2	1:F:146:ASN:ND2	2.27	0.49
1:A:439:GLU:HG3	1:A:441:GLY:CA	2.42	0.49
1:B:352:ARG:NH1	1:B:352:ARG:HG3	2.27	0.49
1:D:126:GLU:HB2	3:D:1060:HOH:O	2.11	0.49
1:D:200:GLU:HB3	1:D:202:LYS:HE3	1.94	0.49
1:E:310:PHE:HA	1:E:313:GLN:NE2	2.26	0.49
1:B:439:GLU:HG3	1:B:441:GLY:CA	2.43	0.49
1:C:141:SER:O	1:C:215:VAL:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ILE:O	1:E:139:VAL:HG23	2.12	0.49
1:F:664:THR:CG2	1:F:667:GLU:HG3	2.42	0.49
1:D:211:ARG:HD3	1:D:213:ARG:HD2	1.95	0.49
1:B:573:VAL:HG11	1:B:598:MET:CE	2.42	0.49
1:D:468:ILE:H	1:D:473:ASN:ND2	2.01	0.49
1:D:670:ARG:C	1:D:672:VAL:N	2.71	0.49
1:A:646:ARG:O	1:A:647:HIS:HB2	2.13	0.49
1:E:131:ASP:OD2	1:E:133:ALA:HB3	2.13	0.49
1:B:303:VAL:HA	1:B:457:GLN:O	2.13	0.48
1:A:546:THR:O	1:A:546:THR:HG23	2.13	0.48
1:C:176:TYR:CE1	1:C:189:PRO:HB3	2.48	0.48
1:D:348:HIS:HD2	3:D:936:HOH:O	1.95	0.48
1:E:211:ARG:HE	1:E:213:ARG:HD2	1.78	0.48
1:A:118:VAL:HG13	3:A:828:HOH:O	2.12	0.48
1:C:641:LEU:C	1:C:641:LEU:CD2	2.86	0.48
1:D:311:PRO:CA	1:D:313:GLN:NE2	2.66	0.48
1:C:333:SER:HB2	1:C:361:ASN:OD1	2.12	0.48
1:E:632:PRO:HD2	1:F:655:LEU:HD11	1.95	0.48
1:B:34:LYS:NZ	1:B:355:ASP:OD1	2.45	0.48
1:C:385:THR:OG1	1:C:665:THR:HA	2.14	0.48
1:C:468:ILE:H	1:C:473:ASN:ND2	2.07	0.48
1:C:546:THR:O	1:C:546:THR:HG23	2.13	0.48
1:D:260:GLU:HG2	1:D:265:LYS:HG3	1.95	0.48
1:E:479:ASP:HB3	1:E:519:THR:HB	1.95	0.48
1:A:632:PRO:HD2	1:B:655:LEU:HD11	1.95	0.48
1:E:128:ILE:HG13	1:E:129:ARG:N	2.29	0.48
1:B:476:ALA:CB	1:B:504:THR:HA	2.44	0.48
1:D:646:ARG:O	1:D:647:HIS:HB2	2.14	0.48
1:E:598:MET:HE2	1:E:602:ILE:HG13	1.96	0.48
1:A:311:PRO:CA	1:A:313:GLN:NE2	2.67	0.48
1:B:37:THR:HG21	1:B:354:GLY:HA2	1.94	0.48
1:C:303:VAL:HA	1:C:457:GLN:O	2.14	0.48
1:C:547:GLN:NE2	1:C:640:THR:H	2.11	0.48
1:D:577:ASP:O	1:D:578:ASN:HB2	2.13	0.48
1:D:190:LEU:HD21	1:D:215:VAL:HG13	1.96	0.47
1:D:301:MET:O	1:D:318:LEU:HA	2.14	0.47
1:A:211:ARG:HD3	1:A:213:ARG:HD2	1.95	0.47
1:C:182:ASP:OD1	1:D:664:THR:HG23	2.14	0.47
1:C:334:LEU:HD13	1:D:661:TYR:CZ	2.48	0.47
1:C:631:PHE:CD1	1:C:632:PRO:HA	2.49	0.47
1:E:579:ARG:HG2	1:E:601:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ARG:HG3	1:B:294:HIS:CE1	2.49	0.47
1:B:141:SER:O	1:B:215:VAL:HG23	2.14	0.47
1:C:143:ILE:HG13	1:C:215:VAL:HG21	1.97	0.47
1:E:224:TYR:HB2	1:E:227:HIS:ND1	2.29	0.47
1:E:261:TRP:O	1:E:264:PHE:HB2	2.13	0.47
1:F:546:THR:O	1:F:546:THR:HG23	2.14	0.47
1:C:646:ARG:O	1:C:647:HIS:HB2	2.15	0.47
1:D:211:ARG:CD	1:D:213:ARG:HD2	2.45	0.47
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.49	0.47
1:E:69:GLU:OE2	1:E:467:ARG:NH2	2.45	0.47
1:E:311:PRO:CA	1:E:313:GLN:NE2	2.67	0.47
1:F:514:ASN:HA	1:F:569:SER:HB2	1.97	0.47
1:A:303:VAL:HA	1:A:457:GLN:O	2.15	0.47
1:A:641:LEU:C	1:A:641:LEU:CD2	2.88	0.47
1:C:69:GLU:OE2	1:C:467:ARG:NH2	2.47	0.47
1:C:475:ALA:HA	1:C:524:ASP:O	2.15	0.47
1:E:549:PRO:HB3	3:E:758:HOH:O	2.14	0.47
1:A:116:LEU:HD11	1:A:157:THR:HG23	1.95	0.47
1:B:191:ASP:OD1	1:B:212:ARG:NH1	2.48	0.47
1:B:331:PRO:HB3	1:B:360:LYS:O	2.15	0.47
1:D:69:GLU:OE2	1:D:467:ARG:NH2	2.44	0.47
1:E:87:GLY:C	1:E:88:LYS:HZ2	2.22	0.47
1:E:190:LEU:HD21	1:E:215:VAL:HG13	1.97	0.47
1:E:467:ARG:HG3	1:E:470:GLY:O	2.14	0.47
1:E:631:PHE:CG	1:E:632:PRO:HA	2.50	0.47
1:F:69:GLU:CD	1:F:467:ARG:HH22	2.22	0.47
1:F:604:ASP:OD1	1:F:604:ASP:C	2.58	0.47
1:A:664:THR:HG23	1:A:665:THR:N	2.30	0.47
1:B:598:MET:CE	1:B:602:ILE:HG13	2.44	0.47
1:D:224:TYR:HB2	1:D:227:HIS:ND1	2.29	0.47
1:B:452:ASN:C	1:B:452:ASN:ND2	2.71	0.47
1:D:634:MET:HA	1:D:635:PRO:HD3	1.74	0.47
1:A:468:ILE:H	1:A:473:ASN:ND2	2.06	0.47
1:B:468:ILE:H	1:B:473:ASN:ND2	2.09	0.47
1:E:604:ASP:OD1	1:E:604:ASP:C	2.58	0.47
1:F:631:PHE:CD1	1:F:632:PRO:HA	2.49	0.47
1:B:664:THR:HG23	1:B:665:THR:N	2.30	0.46
1:C:507:THR:O	1:C:508:VAL:C	2.58	0.46
1:F:150:LYS:HB3	1:F:178:ARG:O	2.15	0.46
1:F:478:CYS:SG	3:F:902:HOH:O	2.60	0.46
1:A:144:PRO:HB2	1:A:146:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:MET:O	1:B:318:LEU:HA	2.15	0.46
1:E:245:THR:OG1	1:E:247:PRO:HD3	2.15	0.46
1:F:87:GLY:C	1:F:88:LYS:HZ2	2.23	0.46
1:C:664:THR:HG23	1:D:182:ASP:OD1	2.14	0.46
1:E:475:ALA:HA	1:E:524:ASP:O	2.16	0.46
1:F:439:GLU:HG3	1:F:441:GLY:CA	2.46	0.46
1:B:439:GLU:HG3	1:B:441:GLY:HA2	1.97	0.46
1:B:664:THR:HG23	1:B:666:SER:H	1.81	0.46
1:D:87:GLY:C	1:D:88:LYS:HZ2	2.24	0.46
1:A:224:TYR:HB2	1:A:227:HIS:ND1	2.30	0.46
1:A:655:LEU:HD11	1:B:632:PRO:HD2	1.98	0.46
1:B:340:GLY:O	1:B:342:ILE:HG12	2.16	0.46
1:B:457:GLN:HE22	1:B:552:LEU:H	1.64	0.46
1:E:53:THR:O	1:E:81:TYR:HA	2.15	0.46
1:E:349:PHE:HB2	1:E:357:ILE:HG13	1.96	0.46
1:F:158:ILE:HD12	1:F:195:ILE:HD12	1.98	0.46
1:B:53:THR:O	1:B:81:TYR:HA	2.16	0.46
1:C:664:THR:HG23	1:C:666:SER:H	1.80	0.46
1:C:664:THR:HG23	1:C:665:THR:N	2.30	0.46
1:D:53:THR:O	1:D:81:TYR:HA	2.15	0.46
1:D:140:LEU:HD13	3:D:977:HOH:O	2.15	0.46
1:E:23:HIS:CD2	1:E:24:PRO:HD2	2.51	0.46
1:E:191:ASP:OD1	1:E:212:ARG:NH1	2.49	0.46
1:E:581:TYR:HA	1:E:582:PRO:HD2	1.77	0.46
1:F:303:VAL:HA	1:F:457:GLN:O	2.15	0.46
1:A:664:THR:HG23	1:A:666:SER:H	1.81	0.46
1:E:333:SER:HB2	1:E:361:ASN:OD1	2.15	0.46
1:F:141:SER:O	1:F:215:VAL:CG2	2.64	0.46
1:F:576:LYS:HB2	1:F:579:ARG:HD2	1.97	0.46
1:A:135:ILE:O	1:A:139:VAL:HG23	2.16	0.46
1:A:557:SER:O	1:A:561:LYS:HG3	2.16	0.46
1:B:352:ARG:CG	1:B:352:ARG:HH11	2.29	0.46
1:C:160:TYR:HD2	1:C:558:LEU:HD21	1.80	0.46
1:C:335:GLY:O	1:C:336:CYS:CB	2.61	0.46
1:C:338:CYS:CB	1:C:364:CYS:HG	2.23	0.46
1:C:376:HIS:ND1	1:D:406:GLU:OE2	2.43	0.46
1:D:303:VAL:HA	1:D:457:GLN:O	2.16	0.46
1:D:598:MET:HE2	1:D:602:ILE:CG1	2.41	0.46
1:B:69:GLU:CD	1:B:467:ARG:HH22	2.24	0.46
1:D:69:GLU:CD	1:D:467:ARG:HH22	2.23	0.46
1:D:598:MET:HA	1:D:598:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:ILE:HG21	1:F:540:SER:HA	1.97	0.46
1:C:352:ARG:NH1	1:C:352:ARG:HG3	2.31	0.45
1:D:345:LEU:HB2	1:D:363:VAL:HB	1.99	0.45
1:D:542:LYS:HB2	1:D:542:LYS:HE2	1.83	0.45
1:D:598:MET:HE3	1:D:601:TRP:HB2	1.98	0.45
1:C:150:LYS:HB3	1:C:178:ARG:O	2.16	0.45
1:C:405:TPQ:C6	1:C:405:TPQ:H	2.28	0.45
1:E:557:SER:O	1:E:561:LYS:HG3	2.16	0.45
1:F:33:ILE:O	1:F:37:THR:HG23	2.17	0.45
1:D:439:GLU:HG3	1:D:441:GLY:CA	2.46	0.45
1:E:197:ASP:CG	1:E:200:GLU:HB2	2.42	0.45
1:F:21:PRO:HG3	1:F:77:ARG:NE	2.30	0.45
1:A:141:SER:O	1:A:215:VAL:CG2	2.64	0.45
1:B:37:THR:O	1:B:41:LYS:HG3	2.17	0.45
1:C:50:SER:HB3	3:C:770:HOH:O	2.16	0.45
1:C:211:ARG:HD3	1:C:213:ARG:HD2	1.98	0.45
1:D:37:THR:HG21	1:D:354:GLY:HA2	1.98	0.45
1:D:338:CYS:CB	1:D:364:CYS:SG	3.05	0.45
1:D:511:SER:O	1:D:513:THR:N	2.49	0.45
1:E:511:SER:O	1:E:513:THR:N	2.49	0.45
1:B:365:ILE:O	1:B:366:HIS:HB3	2.16	0.45
1:B:131:ASP:OD1	1:B:133:ALA:HB3	2.16	0.45
1:C:507:THR:HG21	3:C:759:HOH:O	2.15	0.45
1:F:499:TYR:CD1	1:F:499:TYR:N	2.84	0.45
1:A:598:MET:HE2	1:A:602:ILE:CG1	2.45	0.45
1:B:598:MET:HE2	1:B:602:ILE:CG1	2.46	0.45
1:C:670:ARG:C	1:C:672:VAL:N	2.71	0.45
1:F:117:THR:N	1:F:120:ASP:OD1	2.50	0.45
1:A:344:TYR:CD1	1:A:361:ASN:HB3	2.52	0.45
1:A:511:SER:O	1:A:513:THR:N	2.50	0.45
1:D:579:ARG:HG2	1:D:601:TRP:CE2	2.51	0.45
1:E:191:ASP:CG	1:E:212:ARG:NH1	2.74	0.45
1:A:514:ASN:HA	1:A:569:SER:HB2	1.99	0.45
1:B:476:ALA:HB2	1:B:504:THR:HA	1.99	0.45
1:E:124:THR:HA	1:E:127:VAL:HG13	1.99	0.45
1:F:157:THR:CG2	1:F:588:PRO:HB3	2.46	0.45
1:A:21:PRO:HG3	1:A:77:ARG:NE	2.32	0.45
1:B:499:TYR:N	1:B:499:TYR:CD1	2.85	0.45
1:C:20:ARG:HG3	1:C:20:ARG:HH11	1.82	0.45
1:C:406:GLU:CD	1:D:376:HIS:HA	2.41	0.45
1:D:302:ILE:HG12	1:D:304:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:MET:O	1:F:318:LEU:HA	2.17	0.45
1:F:573:VAL:HG11	1:F:598:MET:CE	2.46	0.45
1:C:534:TYR:CE1	1:D:449:PRO:HD3	2.52	0.44
1:D:144:PRO:HB2	1:D:146:ASN:ND2	2.32	0.44
1:D:161:ASP:OD1	1:D:163:ARG:HB2	2.17	0.44
1:E:634:MET:HA	1:E:635:PRO:HD3	1.78	0.44
1:B:144:PRO:HB2	1:B:146:ASN:ND2	2.32	0.44
1:F:224:TYR:HB2	1:F:227:HIS:ND1	2.32	0.44
1:A:128:ILE:HG13	1:A:129:ARG:N	2.33	0.44
1:C:514:ASN:HA	1:C:569:SER:HB2	1.98	0.44
1:D:519:THR:O	1:D:520:GLY:C	2.60	0.44
1:E:313:GLN:HG2	1:F:494:TYR:CE1	2.52	0.44
1:E:547:GLN:NE2	1:E:639:ILE:HA	2.33	0.44
1:A:604:ASP:OD1	1:A:604:ASP:C	2.60	0.44
1:B:385:THR:OG1	1:B:665:THR:HA	2.17	0.44
1:F:21:PRO:CD	1:F:77:ARG:HD3	2.47	0.44
1:F:290:ARG:HA	1:F:291:PRO:HD3	1.84	0.44
1:F:581:TYR:HB3	3:F:824:HOH:O	2.18	0.44
1:A:189:PRO:HD2	3:A:761:HOH:O	2.17	0.44
1:A:262:SER:O	1:A:263:ASN:CB	2.66	0.44
1:C:224:TYR:HB2	1:C:227:HIS:ND1	2.33	0.44
1:C:123:SER:O	1:C:127:VAL:HG13	2.17	0.44
1:A:439:GLU:O	1:A:441:GLY:N	2.51	0.44
1:B:634:MET:HA	1:B:635:PRO:HD3	1.75	0.44
1:B:664:THR:HG21	3:B:1053:HOH:O	2.17	0.44
1:C:498:PHE:CD1	1:C:498:PHE:C	2.96	0.44
1:C:604:ASP:OD1	1:C:604:ASP:C	2.60	0.44
1:D:157:THR:HG22	3:D:787:HOH:O	2.17	0.44
1:D:276:ILE:HD11	1:D:398:GLN:HB3	1.99	0.44
1:E:439:GLU:HG3	1:E:441:GLY:HA2	1.98	0.44
1:F:300:GLU:HG3	1:F:301:MET:N	2.33	0.44
1:D:601:TRP:N	1:D:601:TRP:CD1	2.85	0.44
1:C:254:MET:HE2	1:C:254:MET:HB3	1.91	0.44
1:A:53:THR:O	1:A:81:TYR:HA	2.18	0.43
1:D:259:MET:CE	1:D:365:ILE:HG21	2.48	0.43
1:D:312:HIS:HD2	3:D:755:HOH:O	2.01	0.43
1:E:598:MET:HE2	1:E:602:ILE:CG1	2.48	0.43
1:A:439:GLU:HG3	1:A:441:GLY:HA2	2.01	0.43
1:B:158:ILE:CD1	1:B:195:ILE:HD12	2.48	0.43
1:C:439:GLU:O	1:C:441:GLY:N	2.51	0.43
1:A:475:ALA:HA	1:A:524:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:SER:O	1:B:263:ASN:CB	2.65	0.43
1:B:405:TPQ:H	1:B:405:TPQ:C6	2.30	0.43
1:B:646:ARG:O	1:B:647:HIS:HB2	2.17	0.43
1:D:310:PHE:HA	1:D:313:GLN:HE21	1.84	0.43
1:E:641:LEU:C	1:E:641:LEU:CD2	2.91	0.43
1:B:141:SER:O	1:B:215:VAL:CG2	2.67	0.43
1:D:94:GLY:HA3	1:D:105:GLU:O	2.18	0.43
1:E:23:HIS:HD2	1:E:25:LEU:N	1.97	0.43
1:F:229:ILE:O	1:F:232:VAL:O	2.36	0.43
1:F:333:SER:HB2	1:F:361:ASN:OD1	2.18	0.43
1:F:527:ASN:HD21	1:F:529:ASN:HD22	1.66	0.43
1:A:598:MET:CE	1:A:602:ILE:HG13	2.47	0.43
1:A:664:THR:HG21	3:A:1103:HOH:O	2.19	0.43
1:B:21:PRO:CD	1:B:77:ARG:HD3	2.48	0.43
1:B:519:THR:O	1:B:520:GLY:C	2.61	0.43
1:B:670:ARG:C	1:B:672:VAL:N	2.72	0.43
1:D:340:GLY:O	1:D:342:ILE:HG12	2.19	0.43
1:D:439:GLU:O	1:D:441:GLY:N	2.51	0.43
1:D:452:ASN:C	1:D:452:ASN:ND2	2.76	0.43
1:E:373:LEU:HD12	1:E:373:LEU:HA	1.86	0.43
1:E:664:THR:CG2	1:E:667:GLU:HG3	2.48	0.43
1:F:189:PRO:HD2	3:F:772:HOH:O	2.18	0.43
1:F:457:GLN:HE22	1:F:552:LEU:H	1.64	0.43
1:D:604:ASP:C	1:D:604:ASP:OD1	2.62	0.43
1:E:113:GLN:OE1	1:E:113:GLN:HA	2.18	0.43
1:E:646:ARG:O	1:E:647:HIS:HB2	2.19	0.43
1:A:498:PHE:CD1	1:A:498:PHE:C	2.97	0.43
1:B:116:LEU:HD11	1:B:157:THR:HG23	2.01	0.43
1:D:239:ALA:O	1:D:240:PRO:C	2.59	0.43
1:E:94:GLY:HA3	1:E:105:GLU:O	2.17	0.43
1:E:211:ARG:HD3	1:E:213:ARG:CD	2.47	0.43
1:C:91:VAL:HG11	1:C:114:PRO:HG3	2.00	0.43
1:C:439:GLU:HG3	1:C:441:GLY:CA	2.48	0.43
1:F:312:HIS:HE1	3:F:742:HOH:O	2.01	0.43
1:A:211:ARG:CD	1:A:213:ARG:HD2	2.48	0.43
1:A:494:TYR:CE1	1:B:313:GLN:HG2	2.53	0.43
1:E:18:PRO:CG	1:E:32:GLU:HG2	2.47	0.43
1:E:100:SER:O	1:E:101:LEU:C	2.61	0.43
1:A:197:ASP:CG	1:A:200:GLU:HB2	2.44	0.43
1:A:352:ARG:NH1	1:A:352:ARG:HG3	2.33	0.43
1:B:434:LEU:HB2	1:B:452:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ASP:OD1	1:C:212:ARG:NH1	2.52	0.43
1:C:511:SER:O	1:C:513:THR:N	2.51	0.43
1:D:100:SER:O	1:D:101:LEU:C	2.62	0.43
1:D:461:SER:HB2	1:D:565:TRP:CE3	2.53	0.43
1:E:344:TYR:CD1	1:E:361:ASN:HB3	2.54	0.43
1:E:624:HIS:O	1:E:626:PRO:HD3	2.19	0.43
1:F:311:PRO:HA	1:F:313:GLN:HE21	1.79	0.43
1:F:511:SER:O	1:F:513:THR:N	2.51	0.43
1:A:190:LEU:HD21	1:A:215:VAL:HG13	2.00	0.42
1:F:143:ILE:HG13	1:F:215:VAL:HG21	2.01	0.42
1:A:88:LYS:HZ3	1:A:88:LYS:HG2	1.65	0.42
1:A:333:SER:HB2	1:A:361:ASN:OD1	2.19	0.42
1:B:158:ILE:HD12	1:B:195:ILE:HD12	2.00	0.42
1:D:34:LYS:NZ	1:D:355:ASP:OD1	2.52	0.42
1:D:546:THR:HG23	1:D:546:THR:O	2.19	0.42
1:E:50:SER:HB3	3:E:961:HOH:O	2.18	0.42
1:E:548:CYS:HB3	3:E:774:HOH:O	2.20	0.42
1:A:28:LEU:CD1	3:A:944:HOH:O	2.66	0.42
1:B:373:LEU:HD12	1:B:373:LEU:HA	1.86	0.42
1:D:150:LYS:HB3	1:D:178:ARG:O	2.20	0.42
1:F:439:GLU:HG3	1:F:441:GLY:HA2	2.01	0.42
1:F:507:THR:O	1:F:508:VAL:C	2.62	0.42
1:C:342:ILE:HG22	1:C:343:HIS:N	2.34	0.42
1:E:335:GLY:O	1:E:336:CYS:CB	2.63	0.42
1:E:425:LEU:O	1:E:636:ALA:HA	2.20	0.42
1:F:498:PHE:CD1	1:F:498:PHE:C	2.98	0.42
1:F:634:MET:HA	1:F:635:PRO:HD3	1.79	0.42
1:B:460:PHE:CD1	1:B:460:PHE:N	2.87	0.42
1:C:555:GLU:HG3	3:C:920:HOH:O	2.20	0.42
1:D:131:ASP:OD2	1:D:133:ALA:HB3	2.19	0.42
1:D:439:GLU:HG3	1:D:441:GLY:HA2	2.00	0.42
1:E:655:LEU:HD11	1:F:632:PRO:HD2	2.01	0.42
1:F:577:ASP:O	1:F:578:ASN:HB2	2.20	0.42
1:B:238:GLU:HG2	3:B:1092:HOH:O	2.19	0.42
1:B:323:TYR:HB2	1:B:328:MET:HE2	2.01	0.42
1:B:573:VAL:HG13	1:B:598:MET:HE1	2.00	0.42
1:D:475:ALA:HA	1:D:524:ASP:O	2.19	0.42
1:F:349:PHE:HB2	1:F:357:ILE:HG13	2.02	0.42
1:A:54:VAL:HG12	3:A:944:HOH:O	2.18	0.42
1:B:94:GLY:HA3	1:B:105:GLU:O	2.19	0.42
1:B:316:HIS:CE1	1:B:558:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LYS:O	1:B:643:LEU:HA	2.20	0.42
1:D:346:ASP:OD1	1:D:360:LYS:HA	2.19	0.42
1:E:35:ALA:HB1	1:E:101:LEU:HD21	2.01	0.42
1:F:390:ARG:HG3	1:F:660:SER:OG	2.19	0.42
1:C:24:PRO:HG3	1:C:74:LEU:HD11	2.02	0.42
1:D:664:THR:HG23	1:D:665:THR:N	2.33	0.42
1:F:475:ALA:HA	1:F:524:ASP:O	2.20	0.42
1:F:671:ALA:O	1:F:672:VAL:HB	2.19	0.42
1:E:262:SER:O	1:E:263:ASN:CB	2.67	0.42
1:E:429:LEU:HD13	1:E:453:ALA:CB	2.50	0.42
1:E:598:MET:CE	1:E:602:ILE:HG13	2.49	0.42
1:F:331:PRO:HB3	1:F:360:LYS:O	2.19	0.42
1:B:222:ASN:HB3	1:B:227:HIS:ND1	2.34	0.42
1:D:131:ASP:HA	1:D:132:PRO:HD3	1.95	0.42
1:D:498:PHE:CD1	1:D:498:PHE:C	2.98	0.42
1:E:229:ILE:O	1:E:232:VAL:O	2.37	0.42
1:F:237:PRO:O	1:F:238:GLU:C	2.62	0.42
1:B:88:LYS:HZ3	1:B:88:LYS:HG2	1.63	0.41
1:C:84:LEU:N	1:C:84:LEU:CD2	2.83	0.41
1:C:243:ASN:ND2	1:D:247:PRO:HG3	2.35	0.41
1:D:290:ARG:HA	1:D:291:PRO:HD3	1.87	0.41
1:E:285:ASP:N	1:E:288:ASN:O	2.51	0.41
1:E:312:HIS:HD2	3:E:779:HOH:O	2.03	0.41
1:E:376:HIS:ND1	1:F:406:GLU:OE2	2.37	0.41
1:B:212:ARG:HA	1:B:212:ARG:HD2	1.89	0.41
1:B:347:ALA:HB3	1:B:359:VAL:CG1	2.38	0.41
1:B:507:THR:O	1:B:508:VAL:C	2.61	0.41
1:D:158:ILE:HD12	1:D:195:ILE:HG23	2.02	0.41
1:E:37:THR:HG21	1:E:354:GLY:CA	2.48	0.41
1:E:211:ARG:NH2	1:E:435:GLY:HA3	2.35	0.41
1:A:47:LYS:HD2	1:A:85:GLU:OE2	2.21	0.41
1:A:158:ILE:HD12	1:A:195:ILE:HD12	2.01	0.41
1:A:634:MET:HA	1:A:635:PRO:HD3	1.76	0.41
1:B:211:ARG:CD	1:B:213:ARG:HD2	2.50	0.41
1:D:598:MET:CE	1:D:602:ILE:HG13	2.45	0.41
1:E:448:TYR:O	1:E:449:PRO:C	2.63	0.41
1:B:439:GLU:O	1:B:441:GLY:N	2.54	0.41
1:B:475:ALA:HA	1:B:524:ASP:O	2.21	0.41
1:D:128:ILE:HG13	1:D:129:ARG:N	2.32	0.41
1:D:328:MET:HB3	1:D:401:THR:O	2.21	0.41
1:F:160:TYR:HD2	1:F:558:LEU:HD21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG13	1:A:314:ARG:HD2	2.02	0.41
1:A:338:CYS:CB	1:A:364:CYS:SG	3.09	0.41
1:C:449:PRO:HD3	1:D:534:TYR:CE1	2.55	0.41
1:C:598:MET:HE3	1:C:601:TRP:HB2	2.02	0.41
1:D:245:THR:OG1	1:D:247:PRO:HD3	2.20	0.41
1:D:499:TYR:CD1	1:D:499:TYR:N	2.89	0.41
1:E:365:ILE:O	1:E:366:HIS:HB3	2.20	0.41
1:E:457:GLN:NE2	1:E:552:LEU:H	2.15	0.41
1:A:18:PRO:HD3	1:A:35:ALA:CB	2.51	0.41
1:A:245:THR:OG1	1:A:247:PRO:HD3	2.21	0.41
1:C:425:LEU:O	1:C:636:ALA:HA	2.20	0.41
1:D:191:ASP:OD1	1:D:212:ARG:NH1	2.54	0.41
1:D:664:THR:HG23	1:D:666:SER:H	1.85	0.41
1:F:53:THR:O	1:F:81:TYR:HA	2.21	0.41
1:A:565:TRP:CD1	1:A:565:TRP:H	2.38	0.41
1:B:305:TYR:CD2	1:B:456:HIS:HB3	2.56	0.41
1:B:427:GLY:O	1:B:633:LEU:HD23	2.21	0.41
1:C:35:ALA:HB1	1:C:101:LEU:CD2	2.50	0.41
1:C:100:SER:O	1:C:101:LEU:C	2.64	0.41
1:D:561:LYS:NZ	1:D:593:ASP:OD1	2.53	0.41
1:E:498:PHE:C	1:E:498:PHE:CD1	2.99	0.41
1:F:118:VAL:HG13	3:F:821:HOH:O	2.21	0.41
1:A:460:PHE:CD1	1:A:460:PHE:N	2.88	0.41
1:D:286:HIS:CE1	3:D:908:HOH:O	2.74	0.41
1:E:276:ILE:CD1	1:E:398:GLN:HB3	2.49	0.41
1:F:461:SER:HB2	1:F:565:TRP:CE3	2.55	0.41
1:F:664:THR:HG23	1:F:666:SER:H	1.84	0.41
1:A:301:MET:O	1:A:318:LEU:HA	2.20	0.41
1:B:190:LEU:CD2	1:B:215:VAL:HG13	2.50	0.41
1:B:352:ARG:HG3	1:B:352:ARG:HH11	1.84	0.41
1:C:88:LYS:HZ3	1:C:88:LYS:HG2	1.72	0.41
1:C:310:PHE:HA	1:C:313:GLN:HE21	1.86	0.41
1:D:108:ALA:C	1:D:109:LEU:HD13	2.46	0.41
1:D:141:SER:O	1:D:215:VAL:CG2	2.69	0.41
1:D:547:GLN:HE22	1:D:639:ILE:HA	1.86	0.41
1:E:347:ALA:HB3	1:E:359:VAL:CG1	2.42	0.41
1:E:565:TRP:CD1	1:E:565:TRP:H	2.38	0.41
1:F:212:ARG:HA	1:F:212:ARG:HD2	1.88	0.41
1:F:666:SER:O	1:F:669:LYS:HB2	2.21	0.41
1:A:37:THR:HG21	1:A:354:GLY:HA2	2.03	0.41
1:A:131:ASP:OD2	1:A:133:ALA:HB3	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:HG21	1:B:354:GLY:CA	2.51	0.41
1:C:239:ALA:O	1:C:240:PRO:C	2.64	0.41
1:C:260:GLU:HG2	1:C:265:LYS:HG3	2.03	0.41
1:D:211:ARG:NE	1:D:213:ARG:HD2	2.35	0.41
1:D:373:LEU:HD12	1:D:373:LEU:HA	1.90	0.41
1:E:114:PRO:O	1:E:588:PRO:HG2	2.20	0.41
1:F:276:ILE:HD11	1:F:398:GLN:HB3	2.03	0.41
1:B:615:LEU:HD23	1:B:615:LEU:HA	1.87	0.40
1:C:23:HIS:HD2	1:C:25:LEU:N	1.97	0.40
1:D:565:TRP:CD1	1:D:565:TRP:H	2.37	0.40
1:F:152:TYR:CD1	1:F:178:ARG:HG3	2.56	0.40
1:F:547:GLN:NE2	1:F:640:THR:H	2.19	0.40
1:A:346:ASP:OD1	1:A:360:LYS:HA	2.21	0.40
1:A:406:GLU:OE2	1:B:376:HIS:ND1	2.44	0.40
1:B:290:ARG:HA	1:B:291:PRO:HD3	1.88	0.40
1:D:434:LEU:HB2	1:D:452:ASN:HB2	2.03	0.40
1:E:131:ASP:HA	1:E:132:PRO:HD3	1.92	0.40
1:E:352:ARG:NH1	1:E:352:ARG:HG3	2.35	0.40
1:A:260:GLU:HG2	1:A:265:LYS:HG3	2.03	0.40
1:B:311:PRO:HA	1:B:313:GLN:HE21	1.78	0.40
1:B:312:HIS:HD2	3:B:792:HOH:O	2.05	0.40
1:C:224:TYR:O	1:C:227:HIS:HB2	2.21	0.40
1:D:527:ASN:HD22	1:D:529:ASN:N	2.08	0.40
1:A:331:PRO:HB3	1:A:360:LYS:O	2.21	0.40
1:C:140:LEU:HD12	1:C:140:LEU:HA	1.91	0.40
1:F:338:CYS:SG	1:F:364:CYS:CB	3.10	0.40
1:F:645:PRO:O	1:F:646:ARG:HD2	2.22	0.40
1:A:191:ASP:OD1	1:A:212:ARG:NH1	2.54	0.40
1:C:211:ARG:NH2	1:C:435:GLY:HA3	2.37	0.40
1:D:157:THR:C	1:D:159:GLY:N	2.75	0.40
1:F:128:ILE:HG13	1:F:129:ARG:N	2.34	0.40
1:F:319:ASP:HB3	1:F:328:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	652/655 (100%)	616 (94%)	33 (5%)	3 (0%)	24	37
1	B	652/655 (100%)	616 (94%)	34 (5%)	2 (0%)	36	50
1	C	652/655 (100%)	616 (94%)	32 (5%)	4 (1%)	21	32
1	D	652/655 (100%)	617 (95%)	32 (5%)	3 (0%)	24	37
1	E	652/655 (100%)	619 (95%)	30 (5%)	3 (0%)	24	37
1	F	652/655 (100%)	613 (94%)	36 (6%)	3 (0%)	24	37
All	All	3912/3930 (100%)	3697 (94%)	197 (5%)	18 (0%)	24	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	512	LEU
1	E	468	ILE
1	E	512	LEU
1	A	512	LEU
1	D	333	SER
1	D	512	LEU
1	E	333	SER
1	F	512	LEU
1	A	333	SER
1	A	468	ILE
1	B	333	SER
1	B	468	ILE
1	C	333	SER
1	F	333	SER
1	C	468	ILE
1	F	468	ILE
1	D	468	ILE
1	C	441	GLY

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	565/565 (100%)	511 (90%)	54 (10%)	8	12
1	B	565/565 (100%)	510 (90%)	55 (10%)	8	12
1	C	565/565 (100%)	509 (90%)	56 (10%)	7	11
1	D	565/565 (100%)	512 (91%)	53 (9%)	8	13
1	E	565/565 (100%)	509 (90%)	56 (10%)	7	11
1	F	565/565 (100%)	512 (91%)	53 (9%)	8	13
All	All	3390/3390 (100%)	3063 (90%)	327 (10%)	8	12

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	50	SER
1	A	62	LYS
1	A	68	LYS
1	A	84	LEU
1	A	88	LYS
1	A	109	LEU
1	A	112	VAL
1	A	118	VAL
1	A	120	ASP
1	A	127	VAL
1	A	140	LEU
1	A	146	ASN
1	A	157	THR
1	A	158	ILE
1	A	170	LEU
1	A	202	LYS
1	A	212	ARG
1	A	213	ARG
1	A	215	VAL
1	A	230	GLU
1	A	245	THR
1	A	262	SER
1	A	313	GLN
1	A	329	THR
1	A	332	LEU
1	A	334	LEU
1	A	338	CYS

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Mol	Chain	Res	Type
1	A	359	VAL
1	A	360	LYS
1	A	364	CYS
1	A	368	GLU
1	A	369	ASP
1	A	392	THR
1	A	394	LEU
1	A	406	GLU
1	A	421	LEU
1	A	430	ASN
1	A	462	LEU
1	A	467	ARG
1	A	487	LEU
1	A	504	THR
1	A	507	THR
1	A	527	ASN
1	A	531	VAL
1	A	546	THR
1	A	554	LYS
1	A	567	SER
1	A	576	LYS
1	A	633	LEU
1	A	641	LEU
1	A	644	ARG
1	A	663	MET
1	A	664	THR
1	B	47	LYS
1	B	62	LYS
1	B	68	LYS
1	B	84	LEU
1	B	88	LYS
1	B	109	LEU
1	B	112	VAL
1	B	118	VAL
1	B	120	ASP
1	B	127	VAL
1	B	140	LEU
1	B	146	ASN
1	B	157	THR
1	B	158	ILE
1	B	170	LEU
1	B	179	SER

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Mol	Chain	Res	Type
1	B	199	GLU
1	B	202	LYS
1	B	212	ARG
1	B	213	ARG
1	B	215	VAL
1	B	217	LYS
1	B	230	GLU
1	B	245	THR
1	B	262	SER
1	B	313	GLN
1	B	329	THR
1	B	332	LEU
1	B	334	LEU
1	B	352	ARG
1	B	359	VAL
1	B	360	LYS
1	B	364	CYS
1	B	369	ASP
1	B	392	THR
1	B	394	LEU
1	B	406	GLU
1	B	421	LEU
1	B	430	ASN
1	B	462	LEU
1	B	467	ARG
1	B	481	LYS
1	B	487	LEU
1	B	504	THR
1	B	506	LYS
1	B	507	THR
1	B	546	THR
1	B	554	LYS
1	B	558	LEU
1	B	567	SER
1	B	576	LYS
1	B	633	LEU
1	B	641	LEU
1	B	663	MET
1	B	664	THR
1	C	47	LYS
1	C	62	LYS
1	C	68	LYS

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Mol	Chain	Res	Type
1	C	84	LEU
1	C	88	LYS
1	C	109	LEU
1	C	112	VAL
1	C	118	VAL
1	C	120	ASP
1	C	127	VAL
1	C	140	LEU
1	C	146	ASN
1	C	157	THR
1	C	158	ILE
1	C	170	LEU
1	C	202	LYS
1	C	212	ARG
1	C	213	ARG
1	C	215	VAL
1	C	230	GLU
1	C	245	THR
1	C	262	SER
1	C	313	GLN
1	C	329	THR
1	C	332	LEU
1	C	334	LEU
1	C	338	CYS
1	C	357	ILE
1	C	359	VAL
1	C	360	LYS
1	C	364	CYS
1	C	368	GLU
1	C	369	ASP
1	C	392	THR
1	C	394	LEU
1	C	406	GLU
1	C	421	LEU
1	C	430	ASN
1	C	452	ASN
1	C	462	LEU
1	C	467	ARG
1	C	481	LYS
1	C	487	LEU
1	C	504	THR
1	C	506	LYS

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Mol	Chain	Res	Type
1	C	507	THR
1	C	527	ASN
1	C	531	VAL
1	C	546	THR
1	C	554	LYS
1	C	567	SER
1	C	576	LYS
1	C	633	LEU
1	C	641	LEU
1	C	664	THR
1	C	665	THR
1	D	50	SER
1	D	62	LYS
1	D	68	LYS
1	D	84	LEU
1	D	88	LYS
1	D	109	LEU
1	D	112	VAL
1	D	118	VAL
1	D	120	ASP
1	D	127	VAL
1	D	140	LEU
1	D	146	ASN
1	D	157	THR
1	D	170	LEU
1	D	202	LYS
1	D	212	ARG
1	D	213	ARG
1	D	215	VAL
1	D	230	GLU
1	D	245	THR
1	D	262	SER
1	D	313	GLN
1	D	329	THR
1	D	332	LEU
1	D	334	LEU
1	D	338	CYS
1	D	357	ILE
1	D	359	VAL
1	D	360	LYS
1	D	364	CYS
1	D	368	GLU

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Mol	Chain	Res	Type
1	D	369	ASP
1	D	392	THR
1	D	394	LEU
1	D	406	GLU
1	D	421	LEU
1	D	430	ASN
1	D	462	LEU
1	D	481	LYS
1	D	487	LEU
1	D	504	THR
1	D	507	THR
1	D	527	ASN
1	D	531	VAL
1	D	546	THR
1	D	554	LYS
1	D	567	SER
1	D	576	LYS
1	D	633	LEU
1	D	641	LEU
1	D	644	ARG
1	D	663	MET
1	D	664	THR
1	E	47	LYS
1	E	50	SER
1	E	62	LYS
1	E	68	LYS
1	E	84	LEU
1	E	88	LYS
1	E	91	VAL
1	E	109	LEU
1	E	112	VAL
1	E	118	VAL
1	E	120	ASP
1	E	127	VAL
1	E	140	LEU
1	E	146	ASN
1	E	157	THR
1	E	158	ILE
1	E	170	LEU
1	E	202	LYS
1	E	212	ARG
1	E	213	ARG

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Mol	Chain	Res	Type
1	E	215	VAL
1	E	230	GLU
1	E	245	THR
1	E	262	SER
1	E	313	GLN
1	E	329	THR
1	E	332	LEU
1	E	334	LEU
1	E	338	CYS
1	E	357	ILE
1	E	359	VAL
1	E	360	LYS
1	E	364	CYS
1	E	368	GLU
1	E	369	ASP
1	E	375	LYS
1	E	392	THR
1	E	394	LEU
1	E	406	GLU
1	E	421	LEU
1	E	430	ASN
1	E	462	LEU
1	E	467	ARG
1	E	487	LEU
1	E	504	THR
1	E	507	THR
1	E	531	VAL
1	E	546	THR
1	E	554	LYS
1	E	567	SER
1	E	576	LYS
1	E	633	LEU
1	E	641	LEU
1	E	644	ARG
1	E	663	MET
1	E	664	THR
1	F	47	LYS
1	F	50	SER
1	F	62	LYS
1	F	68	LYS
1	F	84	LEU
1	F	88	LYS

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Mol	Chain	Res	Type
1	F	109	LEU
1	F	112	VAL
1	F	118	VAL
1	F	120	ASP
1	F	127	VAL
1	F	140	LEU
1	F	146	ASN
1	F	157	THR
1	F	158	ILE
1	F	170	LEU
1	F	199	GLU
1	F	212	ARG
1	F	213	ARG
1	F	215	VAL
1	F	230	GLU
1	F	245	THR
1	F	262	SER
1	F	313	GLN
1	F	329	THR
1	F	332	LEU
1	F	334	LEU
1	F	338	CYS
1	F	359	VAL
1	F	360	LYS
1	F	364	CYS
1	F	368	GLU
1	F	369	ASP
1	F	392	THR
1	F	394	LEU
1	F	406	GLU
1	F	421	LEU
1	F	430	ASN
1	F	462	LEU
1	F	467	ARG
1	F	487	LEU
1	F	504	THR
1	F	507	THR
1	F	527	ASN
1	F	531	VAL
1	F	546	THR
1	F	554	LYS
1	F	567	SER

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Mol	Chain	Res	Type
1	F	576	LYS
1	F	633	LEU
1	F	641	LEU
1	F	644	ARG
1	F	664	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	66	GLN
1	A	70	GLN
1	A	146	ASN
1	A	149	HIS
1	A	218	HIS
1	A	288	ASN
1	A	294	HIS
1	A	312	HIS
1	A	313	GLN
1	A	330	ASN
1	A	382	ASN
1	A	450	ASN
1	A	452	ASN
1	A	457	GLN
1	A	473	ASN
1	A	527	ASN
1	A	547	GLN
1	B	23	HIS
1	B	66	GLN
1	B	146	ASN
1	B	246	GLN
1	B	288	ASN
1	B	294	HIS
1	B	312	HIS
1	B	313	GLN
1	B	330	ASN
1	B	382	ASN
1	B	450	ASN
1	B	452	ASN
1	B	457	GLN
1	B	473	ASN
1	B	527	ASN

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Mol	Chain	Res	Type
1	B	529	ASN
1	B	547	GLN
1	B	611	ASN
1	C	23	HIS
1	C	66	GLN
1	C	70	GLN
1	C	146	ASN
1	C	218	HIS
1	C	243	ASN
1	C	257	ASN
1	C	286	HIS
1	C	288	ASN
1	C	294	HIS
1	C	312	HIS
1	C	313	GLN
1	C	330	ASN
1	C	382	ASN
1	C	450	ASN
1	C	452	ASN
1	C	457	GLN
1	C	473	ASN
1	C	527	ASN
1	C	547	GLN
1	C	568	HIS
1	C	578	ASN
1	D	23	HIS
1	D	66	GLN
1	D	70	GLN
1	D	146	ASN
1	D	149	HIS
1	D	218	HIS
1	D	243	ASN
1	D	246	GLN
1	D	286	HIS
1	D	288	ASN
1	D	294	HIS
1	D	312	HIS
1	D	313	GLN
1	D	330	ASN
1	D	382	ASN
1	D	450	ASN
1	D	452	ASN

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Mol	Chain	Res	Type
1	D	457	GLN
1	D	473	ASN
1	D	527	ASN
1	D	529	ASN
1	D	547	GLN
1	D	611	ASN
1	E	23	HIS
1	E	66	GLN
1	E	70	GLN
1	E	146	ASN
1	E	149	HIS
1	E	218	HIS
1	E	243	ASN
1	E	246	GLN
1	E	286	HIS
1	E	288	ASN
1	E	294	HIS
1	E	312	HIS
1	E	313	GLN
1	E	330	ASN
1	E	382	ASN
1	E	450	ASN
1	E	452	ASN
1	E	457	GLN
1	E	473	ASN
1	E	527	ASN
1	E	529	ASN
1	E	547	GLN
1	E	611	ASN
1	F	23	HIS
1	F	52	ASN
1	F	66	GLN
1	F	70	GLN
1	F	146	ASN
1	F	149	HIS
1	F	243	ASN
1	F	246	GLN
1	F	288	ASN
1	F	294	HIS
1	F	312	HIS
1	F	313	GLN
1	F	330	ASN

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Mol	Chain	Res	Type
1	F	382	ASN
1	F	450	ASN
1	F	452	ASN
1	F	457	GLN
1	F	473	ASN
1	F	527	ASN
1	F	547	GLN
1	F	578	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	TPQ	D	405	1	13,14,15	2.71	7 (53%)	13,19,21	1.03	1 (7%)
1	TPQ	E	405	1	13,14,15	2.41	6 (46%)	13,19,21	0.90	0
1	TPQ	F	405	1	13,14,15	2.65	4 (30%)	13,19,21	1.01	0
1	TPQ	B	405	1	13,14,15	2.59	5 (38%)	13,19,21	0.94	0
1	TPQ	C	405	1	13,14,15	2.59	7 (53%)	13,19,21	1.00	0
1	TPQ	A	405	1	13,14,15	2.53	6 (46%)	13,19,21	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	D	405	1	-	4/5/22/24	0/1/1/1
1	TPQ	E	405	1	-	4/5/22/24	0/1/1/1
1	TPQ	F	405	1	-	4/5/22/24	0/1/1/1
1	TPQ	B	405	1	-	3/5/22/24	0/1/1/1
1	TPQ	C	405	1	-	4/5/22/24	0/1/1/1
1	TPQ	A	405	1	-	4/5/22/24	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	TPQ	C1-C2	-7.27	1.39	1.49
1	D	405	TPQ	C1-C2	-7.01	1.39	1.49
1	C	405	TPQ	C1-C2	-6.91	1.39	1.49
1	F	405	TPQ	C1-C2	-6.85	1.39	1.49
1	A	405	TPQ	C1-C2	-6.81	1.39	1.49
1	E	405	TPQ	C1-C2	-5.88	1.41	1.49
1	F	405	TPQ	O5-C5	3.81	1.34	1.24
1	D	405	TPQ	C3-C4	2.98	1.41	1.36
1	E	405	TPQ	C6-C1	2.98	1.42	1.34
1	D	405	TPQ	O5-C5	2.93	1.32	1.24
1	E	405	TPQ	C3-C4	2.88	1.41	1.36
1	F	405	TPQ	C6-C1	2.70	1.41	1.34
1	A	405	TPQ	C3-C4	2.66	1.40	1.36
1	C	405	TPQ	O5-C5	2.63	1.31	1.24
1	C	405	TPQ	C3-C4	2.62	1.40	1.36
1	F	405	TPQ	C3-C4	2.61	1.40	1.36
1	D	405	TPQ	C6-C1	2.58	1.41	1.34
1	A	405	TPQ	C6-C1	2.57	1.41	1.34
1	B	405	TPQ	C3-C4	2.47	1.40	1.36
1	C	405	TPQ	C6-C1	2.42	1.40	1.34
1	A	405	TPQ	O5-C5	2.35	1.30	1.24
1	B	405	TPQ	C4-C5	-2.34	1.40	1.47
1	A	405	TPQ	C4-C5	-2.33	1.40	1.47
1	B	405	TPQ	O5-C5	2.30	1.30	1.24
1	B	405	TPQ	C6-C1	2.28	1.40	1.34
1	A	405	TPQ	C3-C2	-2.19	1.39	1.44
1	E	405	TPQ	O5-C5	2.19	1.30	1.24
1	C	405	TPQ	C4-C5	-2.18	1.41	1.47
1	E	405	TPQ	C4-C5	-2.18	1.41	1.47
1	C	405	TPQ	O4-C4	2.12	1.39	1.33
1	C	405	TPQ	C3-C2	-2.12	1.39	1.44
1	D	405	TPQ	C4-C5	-2.09	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	405	TPQ	O4-C4	2.05	1.39	1.33
1	E	405	TPQ	C3-C2	-2.04	1.39	1.44
1	D	405	TPQ	C6-C5	-2.02	1.39	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	TPQ	C6-C1-C2	2.17	120.20	118.66

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	405	TPQ	N-CA-CB-C1
1	A	405	TPQ	C-CA-CB-C1
1	B	405	TPQ	N-CA-CB-C1
1	B	405	TPQ	C-CA-CB-C1
1	C	405	TPQ	N-CA-CB-C1
1	C	405	TPQ	C-CA-CB-C1
1	D	405	TPQ	N-CA-CB-C1
1	D	405	TPQ	C-CA-CB-C1
1	E	405	TPQ	N-CA-CB-C1
1	E	405	TPQ	C-CA-CB-C1
1	F	405	TPQ	N-CA-CB-C1
1	F	405	TPQ	C-CA-CB-C1
1	F	405	TPQ	C2-C1-CB-CA
1	A	405	TPQ	C2-C1-CB-CA
1	B	405	TPQ	C2-C1-CB-CA
1	C	405	TPQ	C2-C1-CB-CA
1	D	405	TPQ	C2-C1-CB-CA
1	E	405	TPQ	C2-C1-CB-CA
1	F	405	TPQ	C6-C1-CB-CA
1	A	405	TPQ	C6-C1-CB-CA
1	C	405	TPQ	C6-C1-CB-CA
1	D	405	TPQ	C6-C1-CB-CA
1	E	405	TPQ	C6-C1-CB-CA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	405	TPQ	1	0
1	C	405	TPQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.