



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:41 PM UTC

PDB ID : 4PW8 / pdb_00004pw8
Title : Human tryptophan 2,3-dioxygenase
Authors : Meng, B.; Wu, D.; Gu, J.H.; Ouyang, S.Y.; Ding, W.; Liu, Z.J.
Deposited on : 2014-03-19
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

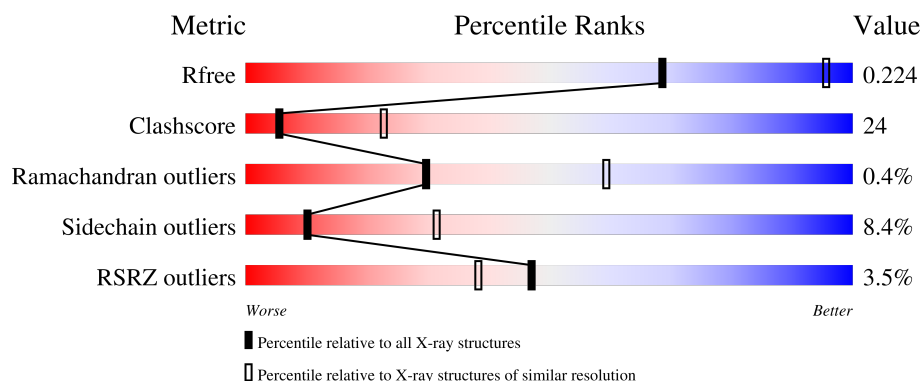
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	373	2% 54% 24% • 18%
1	B	373	3% 57% 16% 5% • 21%
1	C	373	2% 57% 20% 6% • 16%
1	D	373	3% 49% 22% 5% • 23%
1	E	373	3% 50% 22% 5% • 21%

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Mol	Chain	Length	Quality of chain
1	F	373	3% 53% 22% 5% 19%
1	G	373	4% 50% 24% 6% 18%
1	H	373	3% 61% 18% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20451 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2592	1669	447	466	10			
1	B	296	Total	C	N	O	S	0	0	0
			2510	1627	432	441	10			
1	C	313	Total	C	N	O	S	0	0	0
			2660	1711	463	475	11			
1	D	288	Total	C	N	O	S	0	0	0
			2449	1587	424	428	10			
1	E	293	Total	C	N	O	S	0	0	0
			2481	1604	428	439	10			
1	F	303	Total	C	N	O	S	0	0	0
			2564	1658	444	452	10			
1	G	304	Total	C	N	O	S	0	0	0
			2582	1668	446	458	10			
1	H	301	Total	C	N	O	S	0	0	0
			2557	1651	441	455	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	SER	-	expression tag	UNP P48775
A	17	ASN	-	expression tag	UNP P48775
A	18	ALA	-	expression tag	UNP P48775
B	16	SER	-	expression tag	UNP P48775
B	17	ASN	-	expression tag	UNP P48775
B	18	ALA	-	expression tag	UNP P48775
C	16	SER	-	expression tag	UNP P48775
C	17	ASN	-	expression tag	UNP P48775
C	18	ALA	-	expression tag	UNP P48775
D	16	SER	-	expression tag	UNP P48775
D	17	ASN	-	expression tag	UNP P48775
D	18	ALA	-	expression tag	UNP P48775
E	16	SER	-	expression tag	UNP P48775

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Chain	Residue	Modelled	Actual	Comment	Reference
E	17	ASN	-	expression tag	UNP P48775
E	18	ALA	-	expression tag	UNP P48775
F	16	SER	-	expression tag	UNP P48775
F	17	ASN	-	expression tag	UNP P48775
F	18	ALA	-	expression tag	UNP P48775
G	16	SER	-	expression tag	UNP P48775
G	17	ASN	-	expression tag	UNP P48775
G	18	ALA	-	expression tag	UNP P48775
H	16	SER	-	expression tag	UNP P48775
H	17	ASN	-	expression tag	UNP P48775
H	18	ALA	-	expression tag	UNP P48775

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Co 1 1	0	0

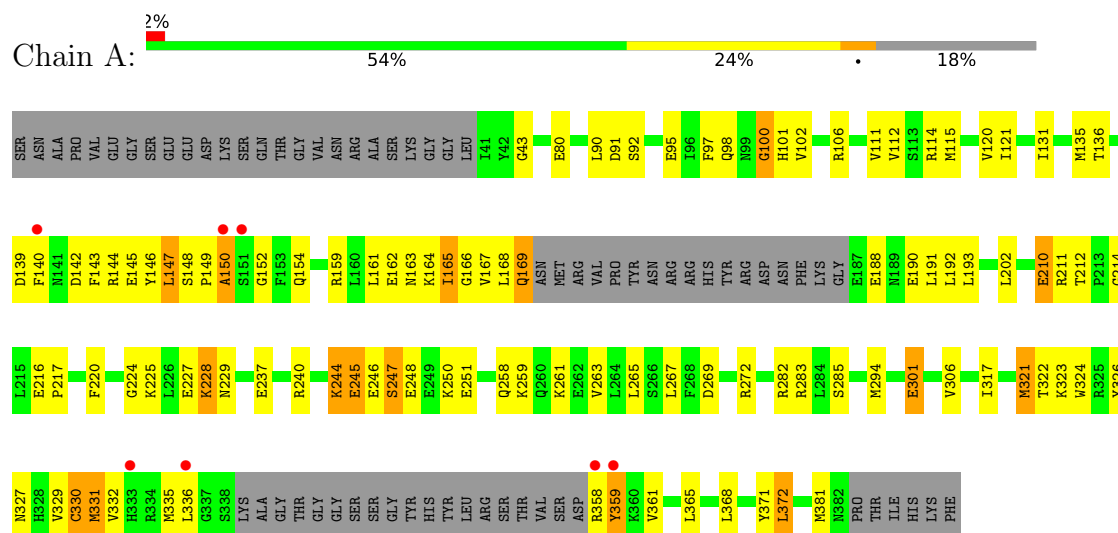
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	5	Total O 5 5	0	0
3	C	5	Total O 5 5	0	0
3	E	13	Total O 13 13	0	0
3	F	7	Total O 7 7	0	0
3	G	2	Total O 2 2	0	0
3	H	12	Total O 12 12	0	0

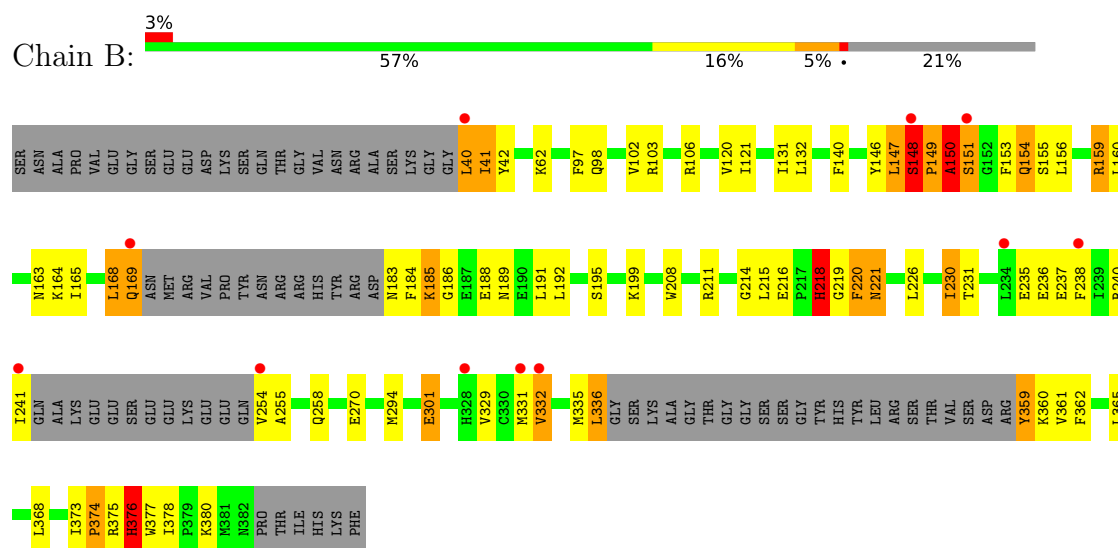
3 Residue-property plots

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

• Molecule 1: Tryptophan 2,3-dioxygenase

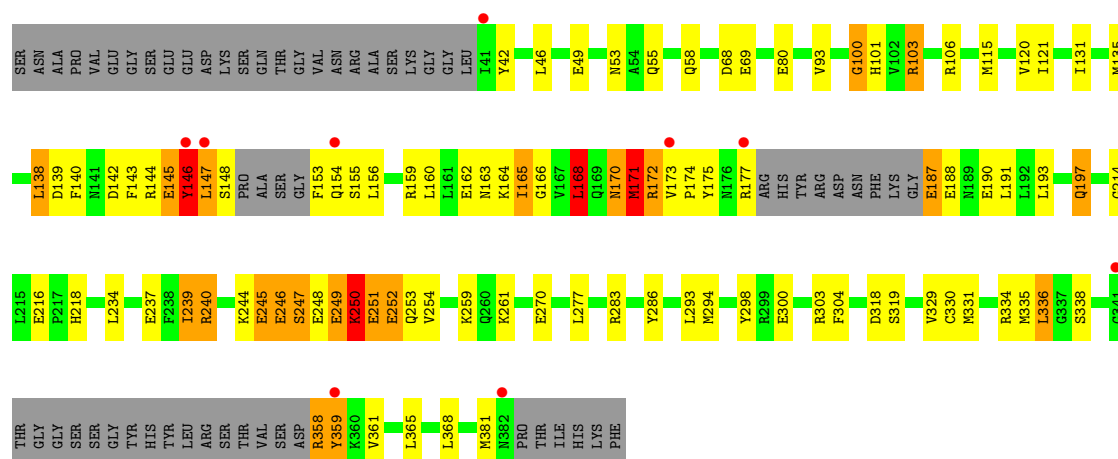


• Molecule 1: Tryptophan 2,3-dioxygenase

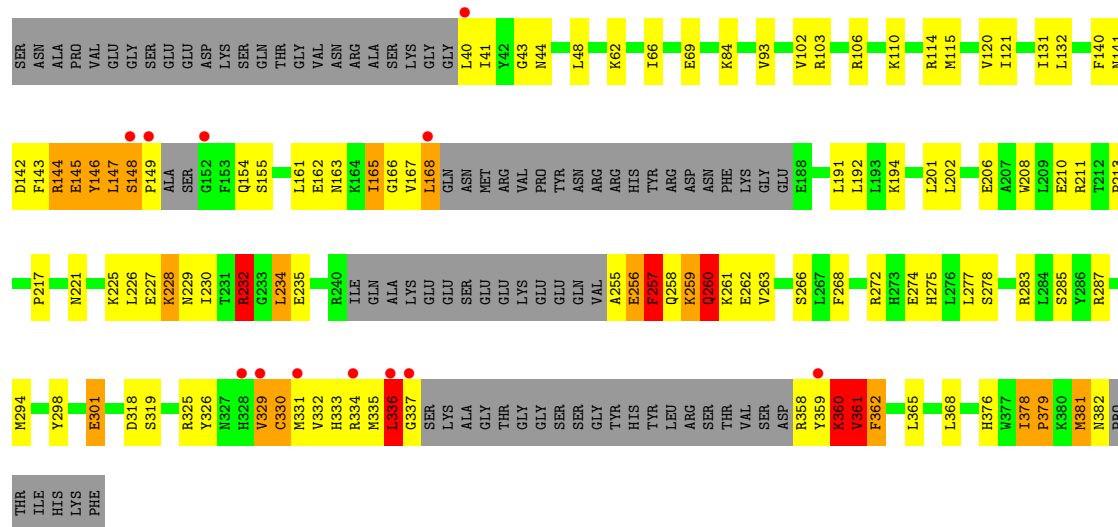


• Molecule 1: Tryptophan 2,3-dioxygenase

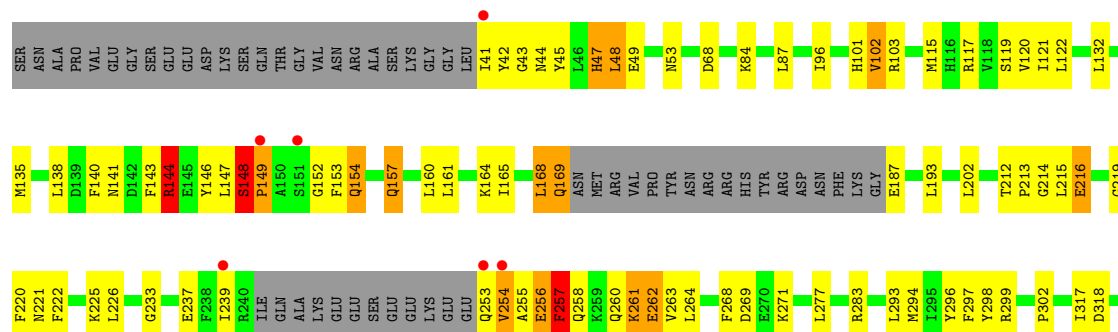


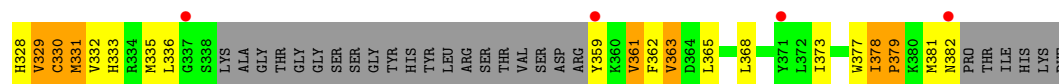


• Molecule 1: Tryptophan 2,3-dioxygenase

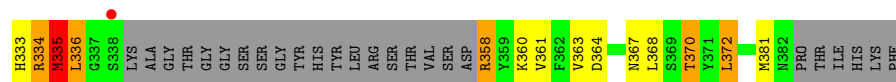
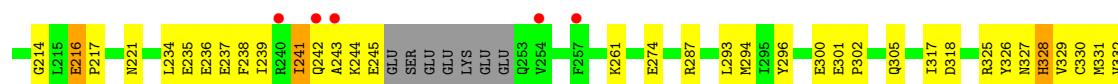
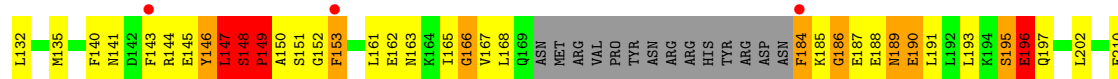


• Molecule 1: Tryptophan 2,3-dioxygenase

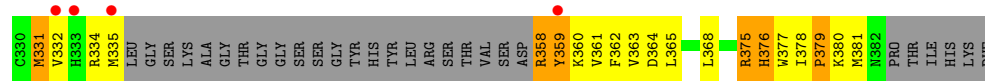
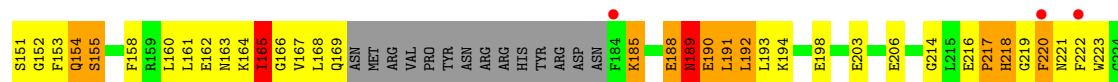




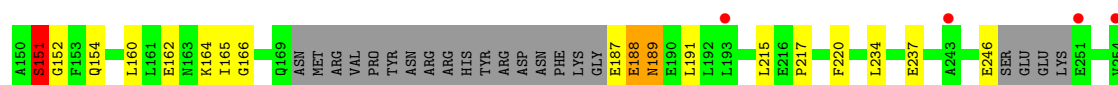
- Molecule 1: Tryptophan 2,3-dioxygenase

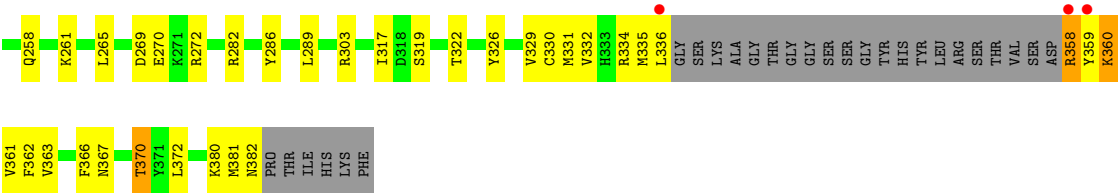


- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.33Å 156.92Å 160.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 2.90 49.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.73-2.90) 96.0 (49.73-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.204 , 0.222 0.208 , 0.224	Depositor DCC
R_{free} test set	2006 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20451	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	2/2648 (0.1%)	1.00	13/3561 (0.4%)
1	B	0.84	4/2566 (0.2%)	1.06	15/3452 (0.4%)
1	C	0.88	0/2716	1.01	15/3649 (0.4%)
1	D	0.76	2/2503 (0.1%)	1.01	17/3365 (0.5%)
1	E	0.83	7/2536 (0.3%)	0.98	14/3412 (0.4%)
1	F	0.77	1/2620 (0.0%)	1.02	19/3522 (0.5%)
1	G	0.82	1/2638 (0.0%)	0.98	7/3545 (0.2%)
1	H	0.68	0/2612	0.91	5/3513 (0.1%)
All	All	0.84	17/20839 (0.1%)	1.00	105/28019 (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	C	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	379	PRO	N-CD	7.18	1.57	1.47
1	F	149	PRO	N-CD	5.71	1.55	1.47
1	E	148	SER	C-N	5.62	1.40	1.33
1	A	163	ASN	C-O	-5.56	1.17	1.24
1	E	379	PRO	N-CD	-5.54	1.40	1.47
1	E	47	HIS	CA-C	-5.48	1.46	1.53
1	A	324	TRP	C-O	-5.42	1.17	1.24
1	B	149	PRO	N-CD	5.37	1.55	1.47
1	E	361	VAL	C-O	-5.35	1.18	1.24
1	E	149	PRO	N-CD	5.28	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	PRO	N-CD	5.18	1.55	1.47
1	E	378	ILE	C-N	5.17	1.40	1.33
1	E	47	HIS	CG-ND1	-5.13	1.32	1.38
1	B	373	ILE	C-N	5.04	1.40	1.33
1	D	378	ILE	C-N	5.04	1.40	1.33
1	B	373	ILE	C-O	-5.01	1.20	1.24
1	D	379	PRO	N-CD	5.00	1.54	1.47

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	GLY	N-CA-C	11.32	125.63	112.50
1	H	151	SER	N-CA-C	10.84	122.84	111.14
1	B	150	ALA	N-CA-C	-10.43	88.59	110.80
1	H	165	ILE	N-CA-C	10.36	120.27	110.53
1	B	218	HIS	N-CA-C	-10.25	97.31	110.53
1	C	156	LEU	N-CA-C	-9.94	99.46	111.69
1	B	376	HIS	N-CA-C	-8.95	101.44	111.82
1	A	359	TYR	N-CA-C	8.91	123.44	108.20
1	F	328	HIS	N-CA-C	-8.61	99.82	110.41
1	B	153	PHE	N-CA-C	-8.56	96.47	108.54
1	C	165	ILE	N-CA-C	8.44	118.46	110.53
1	C	171	MET	N-CA-C	8.41	123.73	113.38
1	B	220	PHE	N-CA-C	-8.35	99.38	110.24
1	B	148	SER	C-N-CD	8.07	138.36	120.60
1	C	146	TYR	N-CA-C	8.06	120.96	108.96
1	A	165	ILE	N-CA-C	8.04	119.77	111.00
1	F	148	SER	C-N-CD	7.97	138.13	120.60
1	A	100	GLY	N-CA-C	-7.64	98.83	112.58
1	E	219	GLY	N-CA-C	7.42	121.46	112.49
1	B	255	ALA	N-CA-C	7.32	119.26	111.28
1	D	226	LEU	N-CA-C	-7.20	103.37	111.07
1	F	44	ASN	N-CA-C	-7.18	103.50	112.90
1	C	146	TYR	N-CA-CB	-7.12	100.31	111.56
1	F	146	TYR	N-CA-C	7.01	119.00	111.36
1	H	188	GLU	N-CA-C	-6.84	105.49	114.31
1	G	328	HIS	N-CA-C	6.72	118.26	111.07
1	D	301	GLU	CA-C-N	6.63	128.13	119.84
1	D	301	GLU	C-N-CA	6.63	128.13	119.84
1	C	245	GLU	N-CA-C	-6.58	102.03	110.19
1	C	336	LEU	N-CA-C	6.58	118.53	111.36
1	D	378	ILE	CA-C-N	-6.45	113.31	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	378	ILE	C-N-CA	-6.45	113.31	119.76
1	E	378	ILE	CA-C-N	-6.33	113.24	119.76
1	E	378	ILE	C-N-CA	-6.33	113.24	119.76
1	B	361	VAL	N-CA-C	6.31	117.05	110.62
1	E	148	SER	CA-C-N	-6.28	113.15	119.56
1	E	148	SER	C-N-CA	-6.28	113.15	119.56
1	H	361	VAL	N-CA-C	6.16	117.72	111.00
1	E	257	PHE	N-CA-C	-6.16	104.57	111.28
1	C	246	GLU	N-CA-C	6.15	120.79	113.16
1	F	41	ILE	N-CA-C	6.07	118.64	108.81
1	C	100	GLY	N-CA-C	-6.05	101.69	112.58
1	C	249	GLU	N-CA-C	-6.05	102.12	110.35
1	E	216	GLU	CA-C-N	-5.98	112.41	119.05
1	E	216	GLU	C-N-CA	-5.98	112.41	119.05
1	A	188	GLU	N-CA-C	-5.96	106.54	113.88
1	F	186	GLY	CA-C-O	-5.96	114.88	121.37
1	B	373	ILE	CA-C-N	-5.95	113.49	119.56
1	B	373	ILE	C-N-CA	-5.95	113.49	119.56
1	F	63	GLY	N-CA-C	5.93	123.23	115.40
1	F	188	GLU	N-CA-C	-5.92	104.83	111.28
1	F	301	GLU	CA-C-N	5.89	127.20	119.84
1	F	301	GLU	C-N-CA	5.89	127.20	119.84
1	G	149	PRO	CA-N-CD	-5.87	103.78	112.00
1	F	186	GLY	N-CA-C	-5.85	100.61	111.14
1	C	250	LYS	N-CA-C	-5.79	98.48	110.80
1	F	335	MET	N-CA-C	5.74	117.62	111.36
1	D	146	TYR	N-CA-C	-5.70	105.91	112.92
1	G	222	PHE	N-CA-C	-5.67	105.18	111.36
1	D	260	GLN	N-CA-C	-5.67	105.11	111.28
1	B	184	PHE	N-CA-C	5.66	117.64	108.41
1	A	361	VAL	N-CA-C	5.62	117.12	111.00
1	A	247	SER	N-CA-C	5.61	115.95	108.38
1	A	212	THR	CA-C-N	5.55	125.73	119.90
1	A	212	THR	C-N-CA	5.55	125.73	119.90
1	D	232	ARG	N-CA-C	-5.51	105.27	111.28
1	E	260	GLN	N-CA-C	-5.51	105.28	111.28
1	D	330	CYS	N-CA-C	-5.50	105.28	111.28
1	D	361	VAL	N-CA-C	5.47	119.10	112.80
1	D	165	ILE	N-CA-C	5.47	116.20	110.62
1	D	336	LEU	N-CA-C	5.46	117.97	109.52
1	E	144	ARG	N-CA-C	-5.44	105.35	111.28
1	C	168	LEU	CA-C-N	5.43	128.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	LEU	C-N-CA	5.43	128.10	120.28
1	B	373	ILE	N-CA-C	5.41	115.12	109.01
1	C	251	GLU	N-CA-C	-5.40	105.40	111.28
1	F	381	MET	N-CA-C	5.39	117.42	108.20
1	G	165	ILE	N-CA-C	5.35	116.83	111.00
1	A	301	GLU	CA-C-N	5.33	126.50	119.84
1	A	301	GLU	C-N-CA	5.33	126.50	119.84
1	F	166	GLY	N-CA-C	-5.32	97.86	113.30
1	G	189	ASN	N-CA-C	-5.29	98.59	108.02
1	G	42	TYR	N-CA-C	-5.25	105.55	111.28
1	F	241	ILE	N-CA-C	5.24	116.01	110.72
1	F	196	GLU	N-CA-C	5.21	117.05	111.36
1	D	256	GLU	CA-C-N	5.21	127.69	120.29
1	D	256	GLU	C-N-CA	5.21	127.69	120.29
1	B	301	GLU	CA-C-N	5.21	126.35	119.84
1	B	301	GLU	C-N-CA	5.21	126.35	119.84
1	E	379	PRO	N-CD-CG	5.21	111.01	103.20
1	A	43	GLY	N-CA-C	-5.19	106.42	113.37
1	D	360	LYS	N-CA-C	5.19	116.99	110.24
1	E	261	LYS	N-CA-C	-5.16	105.65	111.28
1	D	362	PHE	N-CA-C	-5.14	104.46	111.56
1	G	359	TYR	N-CA-C	5.13	120.95	113.40
1	F	147	LEU	N-CA-C	-5.10	103.20	110.59
1	D	257	PHE	N-CA-C	5.09	116.91	111.36
1	E	48	LEU	N-CA-C	-5.08	107.04	113.18
1	A	150	ALA	N-CA-C	5.07	116.50	111.07
1	A	147	LEU	N-CA-C	5.07	116.80	111.28
1	F	149	PRO	CA-N-CD	-5.07	104.41	111.50
1	E	154	GLN	N-CA-C	5.05	117.83	109.85
1	C	252	GLU	N-CA-C	-5.03	105.80	111.28
1	H	102	VAL	CB-CA-C	-5.02	104.38	112.16
1	F	190	GLU	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	146	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2592	0	2588	86	0
1	B	2510	0	2520	97	0
1	C	2660	0	2660	132	0
1	D	2449	0	2460	151	0
1	E	2481	0	2483	139	0
1	F	2564	0	2575	146	0
1	G	2582	0	2587	197	0
1	H	2557	0	2560	67	0
2	H	1	0	0	0	0
3	A	11	0	0	2	0
3	B	5	0	0	0	0
3	C	5	0	0	3	0
3	E	13	0	0	5	0
3	F	7	0	0	2	0
3	G	2	0	0	1	0
3	H	12	0	0	1	0
All	All	20451	0	20433	962	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 24.

All (962) 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:145:GLU:O	1:C:146:TYR:CD1	1.83	1.29
1:G:146:TYR:C	1:G:147:LEU:HD23	1.63	1.22
1:H:187:GLU:HG3	1:H:188:GLU:H	1.02	1.16
1:B:375:ARG:HA	1:B:378:ILE:HD12	1.15	1.13
1:E:144:ARG:NH1	1:E:336:LEU:HD11	1.65	1.11
1:D:336:LEU:HD23	1:D:337:GLY:H	0.98	1.10
1:G:194:LYS:HE3	1:G:198:GLU:OE2	1.48	1.07
1:C:187:GLU:N	1:C:187:GLU:OE1	1.88	1.06
1:F:184:PHE:O	1:F:185:LYS:HD2	1.56	1.05
1:A:159:ARG:HH22	1:A:169:GLN:HG3	1.14	1.04
1:E:144:ARG:HH12	1:E:336:LEU:CD1	1.71	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ARG:HA	1:D:147:LEU:HD22	1.37	1.03
1:C:358:ARG:HA	1:C:359:TYR:CD1	1.93	1.02
1:D:168:LEU:H	1:D:168:LEU:HD12	1.19	1.02
1:C:247:SER:HB3	1:C:248:GLU:HA	1.40	1.02
1:E:144:ARG:HH12	1:E:336:LEU:HD11	0.88	1.02
1:G:191:LEU:HD12	1:G:191:LEU:H	1.22	1.02
1:D:260:GLN:HE21	1:D:260:GLN:HA	1.22	1.01
1:D:360:LYS:HB2	1:D:360:LYS:NZ	1.76	1.01
1:D:361:VAL:HG23	1:D:361:VAL:O	1.60	1.01
1:C:168:LEU:HD23	1:C:168:LEU:H	1.25	1.01
1:D:144:ARG:O	1:D:147:LEU:HB2	1.61	1.01
1:E:147:LEU:HB3	1:E:149:PRO:HD2	1.43	0.99
1:B:154:GLN:HE21	1:B:155:SER:H	1.10	0.99
1:G:40:LEU:HB2	1:G:41:ILE:HD12	1.41	0.99
1:F:358:ARG:HG2	1:F:358:ARG:HH11	1.28	0.97
1:G:140:PHE:CE2	1:G:335:MET:HB3	2.00	0.97
1:B:147:LEU:HB2	1:B:148:SER:HA	1.47	0.95
1:D:336:LEU:HD23	1:D:337:GLY:N	1.80	0.95
1:D:360:LYS:NZ	1:D:360:LYS:CB	2.30	0.95
1:D:154:GLN:OE1	1:D:155:SER:N	1.99	0.95
1:B:375:ARG:HA	1:B:378:ILE:CD1	1.96	0.94
1:C:187:GLU:HG2	1:C:188:GLU:H	1.33	0.93
1:D:227:GLU:HG3	1:D:268:PHE:CE1	2.02	0.93
1:H:160:LEU:O	1:H:164:LYS:HG3	1.68	0.93
1:H:187:GLU:CG	1:H:188:GLU:H	1.81	0.92
1:E:138:LEU:HB3	1:G:375:ARG:NH1	1.85	0.91
1:D:255:ALA:HA	1:D:256:GLU:CG	2.00	0.91
1:G:146:TYR:O	1:G:147:LEU:HD23	1.70	0.90
1:D:260:GLN:O	1:D:263:VAL:HG12	1.68	0.90
1:F:162:GLU:O	1:F:166:GLY:HA2	1.70	0.90
1:G:380:LYS:H	1:G:380:LYS:HD2	1.36	0.89
1:H:358:ARG:HG2	1:H:358:ARG:HH21	1.34	0.89
1:F:328:HIS:O	1:F:329:VAL:HG22	1.72	0.89
1:G:190:GLU:N	1:G:190:GLU:OE1	2.05	0.89
1:B:156:LEU:CD2	1:B:188:GLU:HG2	2.02	0.89
1:D:227:GLU:HG3	1:D:268:PHE:CD1	2.07	0.89
1:H:187:GLU:HG3	1:H:188:GLU:N	1.86	0.88
1:D:232:ARG:NH1	1:D:232:ARG:HB3	1.89	0.87
1:E:216:GLU:OE1	1:E:216:GLU:N	2.07	0.87
1:F:300:GLU:HG3	1:G:106:ARG:HH12	1.39	0.87
1:G:217:PRO:HA	1:G:221:ASN:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:GLY:HA2	1:E:153:PHE:HB3	1.55	0.86
1:B:154:GLN:HE21	1:B:155:SER:N	1.71	0.86
1:D:259:LYS:NZ	1:D:260:GLN:HG2	1.89	0.86
1:F:147:LEU:HD12	1:F:147:LEU:H	1.40	0.86
1:C:103:ARG:HG2	3:C:404:HOH:O	1.75	0.86
1:E:148:SER:HB3	1:F:40:LEU:N	1.90	0.86
1:E:149:PRO:CB	1:E:153:PHE:HB2	2.05	0.86
1:A:372:LEU:HD13	1:A:372:LEU:O	1.75	0.85
1:B:159:ARG:NH2	1:B:169:GLN:HE22	1.73	0.85
1:D:255:ALA:HA	1:D:256:GLU:CB	2.05	0.85
1:D:362:PHE:HB3	1:D:365:LEU:HD12	1.58	0.85
1:F:147:LEU:O	1:F:148:SER:OG	1.95	0.85
1:D:360:LYS:CB	1:D:360:LYS:HZ3	1.89	0.85
1:F:42:TYR:CD1	1:F:42:TYR:O	2.30	0.85
1:D:259:LYS:HE2	1:D:259:LYS:C	2.02	0.84
1:C:249:GLU:O	1:C:250:LYS:HB2	1.75	0.84
1:G:358:ARG:CB	1:G:358:ARG:HH11	1.90	0.84
1:D:360:LYS:HB2	1:D:360:LYS:HZ2	1.38	0.84
1:D:168:LEU:HD11	1:D:283:ARG:NH1	1.93	0.84
1:D:259:LYS:HZ1	1:D:260:GLN:HG2	1.43	0.84
1:A:159:ARG:NH2	1:A:169:GLN:HG3	1.93	0.83
1:F:329:VAL:HA	1:F:332:VAL:HB	1.61	0.83
1:D:230:ILE:O	1:D:234:LEU:HD23	1.78	0.82
1:C:246:GLU:O	1:C:247:SER:OG	1.95	0.82
1:F:193:LEU:HA	1:F:196:GLU:HG3	1.61	0.82
1:B:185:LYS:HB2	1:B:188:GLU:OE1	1.78	0.82
1:D:255:ALA:HA	1:D:256:GLU:HG3	1.62	0.82
1:G:221:ASN:O	1:G:221:ASN:OD1	1.96	0.81
1:B:98:GLN:HE21	1:B:199:LYS:HD2	1.45	0.81
1:F:162:GLU:O	1:F:166:GLY:CA	2.28	0.81
1:F:62:LYS:HD2	1:F:146:TYR:HD1	1.46	0.81
1:F:184:PHE:O	1:F:185:LYS:CD	2.29	0.81
1:D:336:LEU:CD2	1:D:337:GLY:H	1.87	0.81
1:G:251:GLU:O	1:G:254:VAL:HG12	1.80	0.81
1:G:190:GLU:HA	1:G:192:LEU:N	1.96	0.81
1:D:260:GLN:O	1:D:263:VAL:CG1	2.28	0.80
1:B:374:PRO:HD2	1:B:377:TRP:CD2	2.17	0.80
1:E:144:ARG:NH1	1:E:336:LEU:HD21	1.96	0.80
1:E:149:PRO:HB3	1:E:153:PHE:CB	2.12	0.80
1:G:190:GLU:CB	1:G:194:LYS:H	1.95	0.80
1:C:170:ASN:HD22	1:C:170:ASN:H	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:ARG:NH1	1:F:335:MET:HE1	1.97	0.80
1:A:372:LEU:O	1:A:372:LEU:CD1	2.29	0.80
1:D:163:ASN:O	1:D:166:GLY:HA3	1.82	0.80
1:C:42:TYR:CE1	1:C:46:LEU:HD11	2.17	0.79
1:E:149:PRO:HB3	1:E:153:PHE:HB2	1.64	0.79
1:G:154:GLN:HE21	1:G:154:GLN:HA	1.47	0.79
1:B:154:GLN:NE2	1:B:155:SER:H	1.80	0.79
1:F:144:ARG:HA	1:F:147:LEU:HD11	1.65	0.79
1:D:361:VAL:HG22	1:D:362:PHE:CD2	2.18	0.78
1:G:140:PHE:CE2	1:G:335:MET:CB	2.66	0.78
1:D:234:LEU:HD12	1:D:261:LYS:HG3	1.66	0.78
1:B:168:LEU:HD12	1:B:168:LEU:H	1.49	0.78
1:G:190:GLU:HA	1:G:193:LEU:H	1.47	0.78
1:G:331:MET:HE2	1:G:332:VAL:N	1.99	0.77
1:C:247:SER:HB3	1:C:248:GLU:CA	2.14	0.77
1:F:186:GLY:HA2	1:F:189:ASN:H	1.49	0.77
1:G:161:LEU:O	1:G:165:ILE:HG12	1.84	0.77
1:G:188:GLU:OE2	1:G:188:GLU:HA	1.84	0.77
1:C:334:ARG:HH21	1:C:335:MET:CE	1.96	0.77
1:D:232:ARG:HB3	1:D:232:ARG:HH11	1.50	0.77
1:D:361:VAL:O	1:D:361:VAL:CG2	2.30	0.77
1:E:168:LEU:HD12	1:E:168:LEU:O	1.85	0.77
1:F:163:ASN:O	1:F:166:GLY:HA3	1.85	0.77
1:E:148:SER:CB	1:F:40:LEU:N	2.46	0.77
1:A:224:GLY:O	1:A:228:LYS:HE2	1.83	0.77
1:E:68:ASP:HB3	1:E:135:MET:HE3	1.65	0.77
1:B:149:PRO:HG2	1:B:150:ALA:O	1.85	0.77
1:H:187:GLU:HG3	1:H:189:ASN:H	1.48	0.77
1:F:148:SER:HB3	1:F:149:PRO:CA	2.14	0.77
1:C:145:GLU:C	1:C:146:TYR:CG	2.63	0.76
1:E:149:PRO:CG	1:E:153:PHE:HD1	1.97	0.76
1:F:185:LYS:O	1:F:189:ASN:HB2	1.85	0.76
1:E:144:ARG:NH1	1:E:336:LEU:CD1	2.39	0.76
1:F:336:LEU:N	1:F:336:LEU:HD22	1.99	0.76
1:H:319:SER:OG	1:H:359:TYR:CE1	2.38	0.76
1:E:144:ARG:HD2	1:E:144:ARG:O	1.86	0.76
1:H:358:ARG:HG2	1:H:358:ARG:NH2	1.96	0.76
1:E:141:ASN:HA	1:E:144:ARG:HB3	1.66	0.76
1:C:358:ARG:HA	1:C:359:TYR:CG	2.21	0.75
1:G:154:GLN:NE2	1:G:155:SER:H	1.85	0.75
1:A:224:GLY:O	1:A:228:LYS:CE	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:PHE:O	1:D:144:ARG:C	2.30	0.75
1:F:140:PHE:CD2	1:F:335:MET:HG3	2.21	0.75
1:F:184:PHE:C	1:F:185:LYS:HD2	2.10	0.75
1:B:219:GLY:O	1:B:220:PHE:C	2.30	0.74
1:C:172:ARG:HH11	1:C:172:ARG:HG3	1.52	0.74
1:F:318:ASP:OD2	1:F:360:LYS:HB3	1.87	0.74
1:C:187:GLU:N	1:C:190:GLU:OE1	2.20	0.74
1:E:41:ILE:HG21	1:F:148:SER:O	1.87	0.74
1:F:62:LYS:CD	1:F:146:TYR:HD1	2.00	0.74
1:F:329:VAL:O	1:F:333:HIS:N	2.20	0.74
1:B:147:LEU:CB	1:B:148:SER:HA	2.17	0.74
1:D:148:SER:OG	1:D:149:PRO:HD2	1.87	0.74
1:G:40:LEU:N	1:G:40:LEU:HD23	2.02	0.74
1:F:193:LEU:HD12	1:F:196:GLU:HG3	1.69	0.74
1:A:372:LEU:HD12	1:A:372:LEU:N	2.02	0.73
1:C:154:GLN:OE1	1:C:173:VAL:HB	1.88	0.73
1:B:148:SER:HB3	1:B:150:ALA:N	2.03	0.73
1:G:332:VAL:O	1:G:335:MET:HG2	1.89	0.73
1:G:194:LYS:CE	1:G:198:GLU:OE2	2.34	0.73
1:G:380:LYS:HD2	1:G:380:LYS:N	2.04	0.73
1:B:154:GLN:NE2	1:B:154:GLN:HA	2.03	0.73
1:C:168:LEU:H	1:C:168:LEU:CD2	2.02	0.72
1:C:244:LYS:HB3	1:C:244:LYS:HZ2	1.54	0.72
1:C:248:GLU:HG2	1:C:249:GLU:H	1.55	0.72
1:E:149:PRO:HG2	1:E:153:PHE:CD1	2.23	0.72
1:D:360:LYS:HB2	1:D:360:LYS:HZ3	1.50	0.72
1:G:190:GLU:HB3	1:G:194:LYS:H	1.54	0.72
1:G:41:ILE:HD12	1:G:41:ILE:N	2.05	0.72
1:C:145:GLU:C	1:C:146:TYR:CD1	2.66	0.72
1:G:189:ASN:HA	1:G:192:LEU:HB2	1.71	0.72
1:G:216:GLU:C	1:G:218:HIS:H	1.94	0.72
1:G:149:PRO:O	1:G:152:GLY:N	2.23	0.72
1:C:145:GLU:O	1:C:146:TYR:CG	2.43	0.71
1:G:332:VAL:O	1:G:335:MET:CG	2.38	0.71
1:G:358:ARG:HH11	1:G:358:ARG:HB3	1.54	0.71
1:F:217:PRO:O	1:F:221:ASN:HB2	1.90	0.71
1:E:120:VAL:HG12	1:F:131:ILE:HD13	1.71	0.71
1:C:170:ASN:HD22	1:C:170:ASN:N	1.89	0.71
1:G:150:ALA:HA	1:G:152:GLY:N	2.04	0.71
1:C:303:ARG:HH21	1:C:381:MET:HE1	1.56	0.71
1:E:149:PRO:CB	1:E:153:PHE:CD1	2.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ILE:N	1:B:41:ILE:HD13	2.04	0.71
1:B:147:LEU:HD13	1:B:147:LEU:N	2.05	0.71
1:C:135:MET:HE1	1:C:143:PHE:CZ	2.26	0.71
1:C:153:PHE:N	1:C:154:GLN:HA	2.05	0.71
1:G:140:PHE:HE2	1:G:335:MET:CB	2.02	0.71
1:C:103:ARG:NH1	3:C:404:HOH:O	2.24	0.71
1:E:263:VAL:HG13	1:E:264:LEU:N	2.06	0.71
1:C:160:LEU:O	1:C:164:LYS:HG3	1.91	0.70
1:B:301:GLU:OE2	1:C:106:ARG:NH2	2.23	0.70
1:F:161:LEU:O	1:F:165:ILE:HG12	1.90	0.70
1:B:376:HIS:CD2	1:B:376:HIS:H	2.10	0.70
1:E:138:LEU:HD13	1:G:375:ARG:HH12	1.56	0.70
1:E:43:GLY:HA2	1:E:48:LEU:HD12	1.72	0.70
1:D:332:VAL:O	1:D:336:LEU:HB2	1.92	0.70
1:A:106:ARG:NH2	1:D:301:GLU:OE2	2.22	0.70
1:G:155:SER:OG	1:G:158:PHE:CB	2.40	0.70
1:A:161:LEU:O	1:A:165:ILE:HG12	1.91	0.70
1:B:156:LEU:HD11	1:B:192:LEU:HD13	1.74	0.70
1:C:334:ARG:HH21	1:C:335:MET:HE3	1.57	0.70
1:D:62:LYS:HB2	1:D:146:TYR:CE2	2.26	0.70
1:E:152:GLY:HA2	1:E:153:PHE:CB	2.22	0.70
1:F:140:PHE:CG	1:F:335:MET:HG3	2.27	0.70
1:C:69:GLU:HG3	1:C:143:PHE:CD2	2.27	0.69
1:F:300:GLU:HG3	1:G:106:ARG:NH1	2.05	0.69
1:A:322:THR:HB	1:A:359:TYR:CD1	2.28	0.69
1:C:145:GLU:O	1:C:146:TYR:CE1	2.44	0.69
1:A:301:GLU:OE1	1:D:106:ARG:NH2	2.25	0.69
1:B:150:ALA:HB1	1:B:151:SER:HA	1.74	0.69
1:E:138:LEU:HD22	1:G:375:ARG:HH11	1.58	0.69
1:E:144:ARG:HD2	1:E:144:ARG:C	2.17	0.69
1:F:147:LEU:HD12	1:F:147:LEU:N	2.01	0.69
1:F:148:SER:HB3	1:F:149:PRO:HA	1.74	0.69
1:D:255:ALA:HA	1:D:256:GLU:HB2	1.72	0.69
1:G:147:LEU:HD23	1:G:147:LEU:N	2.04	0.68
1:E:214:GLY:HA3	1:E:294:MET:HE1	1.75	0.68
1:F:358:ARG:HG2	1:F:358:ARG:NH1	2.05	0.68
1:B:188:GLU:O	1:B:191:LEU:N	2.26	0.68
1:D:260:GLN:HA	1:D:260:GLN:NE2	1.97	0.68
1:E:149:PRO:HB2	1:E:153:PHE:HB2	1.76	0.68
1:G:162:GLU:O	1:G:166:GLY:HA2	1.92	0.68
1:F:328:HIS:O	1:F:329:VAL:CG2	2.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:ARG:HH11	1:F:335:MET:HE1	1.56	0.68
1:E:149:PRO:CB	1:E:153:PHE:HD1	2.07	0.68
1:F:184:PHE:C	1:F:185:LYS:CD	2.67	0.67
1:G:214:GLY:O	1:G:220:PHE:HD2	1.78	0.67
1:A:144:ARG:O	1:A:147:LEU:N	2.28	0.67
1:C:135:MET:HE1	1:C:143:PHE:CE1	2.29	0.67
1:G:140:PHE:HE2	1:G:335:MET:HB3	1.56	0.67
1:G:358:ARG:O	1:G:359:TYR:HB2	1.95	0.67
1:A:149:PRO:HD2	1:B:40:LEU:HG	1.76	0.67
1:D:259:LYS:HE2	1:D:260:GLN:N	2.10	0.67
1:G:220:PHE:CE1	1:G:225:LYS:HE3	2.30	0.67
1:F:372:LEU:HD21	1:H:141:ASN:HD21	1.60	0.67
1:D:255:ALA:CA	1:D:256:GLU:HG3	2.25	0.67
1:A:372:LEU:CD1	1:A:372:LEU:C	2.67	0.66
1:G:150:ALA:HA	1:G:151:SER:C	2.18	0.66
1:F:99:ASN:O	1:F:99:ASN:ND2	2.24	0.66
1:C:246:GLU:C	1:C:247:SER:HG	2.01	0.66
1:E:147:LEU:HB3	1:E:149:PRO:CD	2.21	0.66
1:E:258:GLN:O	1:E:262:GLU:N	2.29	0.66
1:G:190:GLU:HA	1:G:193:LEU:N	2.09	0.66
1:H:154:GLN:OE1	1:H:154:GLN:HA	1.96	0.66
1:E:149:PRO:CG	1:E:153:PHE:CD1	2.78	0.66
1:C:131:ILE:HD13	1:D:120:VAL:HG12	1.78	0.66
1:G:191:LEU:HD12	1:G:191:LEU:N	2.04	0.66
1:G:216:GLU:C	1:G:218:HIS:N	2.48	0.66
1:G:219:GLY:O	1:G:220:PHE:HB3	1.96	0.66
1:G:190:GLU:HB2	1:G:194:LYS:H	1.61	0.65
1:C:172:ARG:HH11	1:C:172:ARG:CG	2.09	0.65
1:F:41:ILE:O	1:F:43:GLY:N	2.30	0.65
1:C:214:GLY:N	1:C:216:GLU:OE2	2.30	0.65
1:B:219:GLY:C	1:B:220:PHE:O	2.39	0.65
1:C:103:ARG:HH11	1:C:103:ARG:CG	2.09	0.65
1:A:372:LEU:HD13	1:A:372:LEU:C	2.22	0.65
1:D:143:PHE:O	1:D:145:GLU:N	2.30	0.65
1:D:168:LEU:H	1:D:168:LEU:CD1	1.96	0.65
1:G:161:LEU:O	1:G:165:ILE:CG1	2.44	0.65
1:G:216:GLU:O	1:G:218:HIS:N	2.30	0.65
1:A:144:ARG:O	1:A:147:LEU:HB2	1.95	0.64
1:A:244:LYS:HB2	1:A:250:LYS:HD2	1.79	0.64
1:A:259:LYS:O	1:A:263:VAL:HG23	1.97	0.64
1:C:172:ARG:HG3	1:C:172:ARG:NH1	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:LYS:O	1:G:229:ASN:ND2	2.23	0.64
1:D:266:SER:OG	1:D:272:ARG:NH1	2.30	0.64
1:E:160:LEU:O	1:E:164:LYS:HG3	1.98	0.64
1:E:302:PRO:HB2	3:E:406:HOH:O	1.97	0.64
1:H:234:LEU:HD13	1:H:261:LYS:HG3	1.79	0.64
1:C:193:LEU:O	1:C:197:GLN:HG2	1.97	0.64
1:D:168:LEU:CD1	1:D:283:ARG:NH1	2.61	0.64
1:E:144:ARG:NH1	1:E:336:LEU:CD2	2.61	0.64
1:G:103:ARG:NH1	3:G:401:HOH:O	2.30	0.64
1:G:163:ASN:O	1:G:166:GLY:HA3	1.97	0.64
1:G:223:TRP:CZ3	1:G:290:GLN:HG2	2.32	0.64
1:A:247:SER:OG	1:A:248:GLU:N	2.26	0.64
1:A:331:MET:HG3	1:A:332:VAL:N	2.13	0.64
1:C:250:LYS:O	1:C:254:VAL:N	2.26	0.63
1:C:216:GLU:CD	1:C:216:GLU:H	2.06	0.63
1:G:331:MET:CE	1:G:332:VAL:HA	2.28	0.63
1:D:93:VAL:HG21	1:D:115:MET:HE3	1.79	0.63
1:F:42:TYR:CD1	1:F:42:TYR:C	2.76	0.63
1:G:239:ILE:O	1:G:242:GLN:NE2	2.30	0.63
1:E:84:LYS:NZ	1:F:52:LEU:O	2.31	0.63
1:A:147:LEU:O	1:A:148:SER:C	2.41	0.63
1:D:227:GLU:HG3	1:D:268:PHE:CZ	2.33	0.63
1:E:138:LEU:HB3	1:G:375:ARG:HH12	1.63	0.63
1:G:189:ASN:HA	1:G:192:LEU:CB	2.28	0.63
1:C:168:LEU:HD22	1:C:283:ARG:NH1	2.14	0.62
1:C:187:GLU:CG	1:C:188:GLU:H	2.06	0.62
1:E:329:VAL:O	1:E:332:VAL:HB	2.00	0.62
1:D:258:GLN:O	1:D:261:LYS:HB3	2.00	0.62
1:E:335:MET:O	1:E:336:LEU:HG	1.99	0.62
1:D:259:LYS:HZ1	1:D:260:GLN:CG	2.10	0.62
1:E:87:LEU:CD1	1:E:157:GLN:HG2	2.29	0.62
1:H:359:TYR:HB3	1:H:366:PHE:CE2	2.34	0.62
1:G:214:GLY:O	1:G:220:PHE:CD2	2.52	0.62
1:B:374:PRO:O	1:B:375:ARG:HB3	1.98	0.62
1:C:120:VAL:HG12	1:D:131:ILE:HD13	1.80	0.62
1:D:144:ARG:HA	1:D:147:LEU:CD2	2.21	0.62
1:D:217:PRO:O	1:D:221:ASN:HB2	2.00	0.62
1:E:147:LEU:CB	1:E:149:PRO:HD2	2.25	0.62
1:F:62:LYS:HG3	1:F:146:TYR:CD1	2.33	0.62
1:G:223:TRP:CH2	1:G:290:GLN:HG2	2.34	0.62
1:B:160:LEU:HD23	1:B:192:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:GLN:O	1:F:242:GLN:HG3	1.99	0.62
1:A:251:GLU:HA	1:A:251:GLU:OE1	1.97	0.61
1:H:367:ASN:O	1:H:370:THR:HG23	1.99	0.61
1:D:325:ARG:O	1:D:329:VAL:HG22	2.00	0.61
1:D:261:LYS:O	1:D:262:GLU:C	2.42	0.61
1:E:253:GLN:O	1:E:254:VAL:HG22	2.01	0.61
1:G:254:VAL:O	1:G:257:PHE:HB3	2.00	0.61
1:G:155:SER:HG	1:G:158:PHE:H	1.48	0.61
1:F:40:LEU:HD22	1:F:41:ILE:H	1.65	0.61
1:F:238:PHE:O	1:F:241:ILE:HB	2.00	0.61
1:B:150:ALA:CB	1:B:151:SER:HA	2.29	0.61
1:A:327:ASN:O	1:A:330:CYS:HB2	2.01	0.61
1:B:156:LEU:HD22	1:B:188:GLU:HG2	1.81	0.61
1:F:193:LEU:HA	1:F:196:GLU:CG	2.29	0.61
1:G:334:ARG:O	1:G:335:MET:HB3	1.98	0.61
1:A:228:LYS:HD3	1:A:228:LYS:N	2.16	0.61
1:C:237:GLU:OE2	1:C:240:ARG:NH2	2.21	0.61
1:C:358:ARG:CA	1:C:359:TYR:CG	2.84	0.61
1:F:165:ILE:HB	1:F:166:GLY:HA2	1.83	0.60
1:E:161:LEU:O	1:E:165:ILE:HG12	2.01	0.60
1:G:162:GLU:HG2	1:G:167:VAL:HG21	1.83	0.60
1:G:190:GLU:HB3	1:G:194:LYS:N	2.15	0.60
1:H:40:LEU:HD12	1:H:40:LEU:O	2.00	0.60
1:H:162:GLU:O	1:H:166:GLY:HA2	2.01	0.60
1:C:42:TYR:CE1	1:C:46:LEU:CD1	2.84	0.60
1:G:150:ALA:HA	1:G:153:PHE:H	1.65	0.60
1:D:234:LEU:CD1	1:D:261:LYS:HG3	2.31	0.60
1:G:380:LYS:H	1:G:380:LYS:CD	2.12	0.60
1:C:162:GLU:O	1:C:166:GLY:HA2	2.02	0.60
1:E:138:LEU:HD22	1:G:375:ARG:NH1	2.15	0.60
1:G:191:LEU:H	1:G:191:LEU:CD1	1.94	0.60
1:G:93:VAL:HG21	1:G:115:MET:HE3	1.83	0.60
1:B:163:ASN:ND2	1:B:195:SER:OG	2.31	0.60
1:C:244:LYS:HB2	1:C:250:LYS:HE3	1.84	0.60
1:E:220:PHE:O	1:E:225:LYS:NZ	2.31	0.60
1:A:120:VAL:HG12	1:B:131:ILE:HD13	1.83	0.59
1:E:149:PRO:HG2	1:E:153:PHE:HD1	1.60	0.59
1:F:148:SER:HB3	1:F:149:PRO:HB3	1.84	0.59
1:C:187:GLU:HG2	1:C:188:GLU:N	2.13	0.59
1:H:40:LEU:HD12	1:H:40:LEU:C	2.27	0.59
1:E:381:MET:O	1:E:382:ASN:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ARG:O	1:F:147:LEU:CD1	2.50	0.59
1:C:93:VAL:HG21	1:C:115:MET:HE3	1.84	0.59
1:E:169:GLN:O	1:E:169:GLN:HG2	2.01	0.59
1:G:332:VAL:C	1:G:335:MET:HG2	2.28	0.59
1:G:358:ARG:HG2	1:G:359:TYR:H	1.67	0.59
1:B:154:GLN:HE21	1:B:154:GLN:HA	1.67	0.59
1:E:101:HIS:HB2	3:E:405:HOH:O	2.01	0.59
1:D:257:PHE:CD1	1:D:258:GLN:HA	2.38	0.59
1:E:149:PRO:HB3	1:E:153:PHE:CA	2.33	0.59
1:G:154:GLN:HG3	1:G:155:SER:N	2.18	0.59
1:D:257:PHE:HD1	1:D:258:GLN:N	2.00	0.58
1:E:138:LEU:CB	1:G:375:ARG:HH12	2.16	0.58
1:D:232:ARG:HH11	1:D:232:ARG:CB	2.15	0.58
1:F:62:LYS:HD2	1:F:146:TYR:CD1	2.34	0.58
1:B:160:LEU:CD2	1:B:192:LEU:HD12	2.34	0.58
1:H:148:SER:HA	1:H:149:PRO:C	2.28	0.58
1:H:282:ARG:NH1	3:H:507:HOH:O	2.33	0.58
1:D:257:PHE:CD1	1:D:258:GLN:N	2.71	0.58
1:B:160:LEU:O	1:B:164:LYS:HG3	2.03	0.58
1:D:232:ARG:HA	1:D:235:GLU:HG2	1.84	0.58
1:A:372:LEU:HD12	1:A:372:LEU:H	1.68	0.58
1:G:154:GLN:HE21	1:G:154:GLN:CA	2.15	0.58
1:G:246:GLU:OE1	1:G:246:GLU:N	2.30	0.58
1:B:168:LEU:HD12	1:B:168:LEU:N	2.18	0.58
1:D:168:LEU:HD12	1:D:168:LEU:N	2.04	0.58
1:D:362:PHE:O	1:D:365:LEU:HB2	2.04	0.58
1:G:239:ILE:HD12	1:G:242:GLN:NE2	2.19	0.58
1:B:220:PHE:HZ	1:B:380:LYS:O	1.87	0.57
1:C:135:MET:CE	1:C:143:PHE:HE1	2.17	0.57
1:F:329:VAL:O	1:F:332:VAL:N	2.37	0.57
1:G:331:MET:HE3	1:G:335:MET:SD	2.45	0.57
1:F:42:TYR:O	1:F:42:TYR:CG	2.56	0.57
1:F:148:SER:HB3	1:F:149:PRO:CB	2.33	0.57
1:A:322:THR:CB	1:A:359:TYR:HD1	2.18	0.57
1:C:170:ASN:H	1:C:170:ASN:ND2	2.01	0.57
1:G:189:ASN:OD1	1:G:189:ASN:N	2.32	0.57
1:G:223:TRP:O	1:G:226:LEU:HB3	2.05	0.57
1:D:165:ILE:N	1:D:166:GLY:HA2	2.20	0.57
1:G:331:MET:HE2	1:G:332:VAL:CA	2.35	0.57
1:A:144:ARG:NE	3:A:410:HOH:O	2.37	0.57
1:E:138:LEU:CB	1:G:375:ARG:NH1	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ARG:HH22	1:B:169:GLN:HE22	1.49	0.57
1:B:359:TYR:CD1	1:B:359:TYR:N	2.72	0.57
1:F:140:PHE:CG	1:F:335:MET:CG	2.88	0.57
1:F:144:ARG:O	1:F:147:LEU:HD12	2.05	0.57
1:G:254:VAL:O	1:G:257:PHE:N	2.38	0.57
1:C:103:ARG:HH11	1:C:103:ARG:HG3	1.70	0.57
1:C:248:GLU:HG2	1:C:249:GLU:N	2.19	0.57
1:C:358:ARG:N	1:C:359:TYR:CG	2.73	0.57
1:F:193:LEU:O	1:F:196:GLU:HG3	2.05	0.57
1:D:259:LYS:HZ2	1:D:260:GLN:HG2	1.70	0.56
1:H:140:PHE:CE2	1:H:335:MET:HB3	2.40	0.56
1:B:216:GLU:O	1:B:220:PHE:O	2.23	0.56
1:F:141:ASN:HD21	1:H:372:LEU:HD21	1.69	0.56
1:F:372:LEU:HD11	1:H:141:ASN:ND2	2.21	0.56
1:G:234:LEU:HD13	1:G:261:LYS:HG3	1.87	0.56
1:B:148:SER:N	1:B:149:PRO:HA	2.21	0.56
1:G:331:MET:HE3	1:G:332:VAL:HA	1.88	0.56
1:C:359:TYR:C	1:C:359:TYR:HD1	2.14	0.56
1:G:270:GLU:HG2	1:G:286:TYR:CE2	2.40	0.56
1:B:376:HIS:CD2	1:B:376:HIS:N	2.73	0.56
1:F:332:VAL:HG13	1:F:336:LEU:HD23	1.86	0.56
1:G:190:GLU:H	1:G:190:GLU:CD	2.13	0.56
1:H:220:PHE:CZ	1:H:381:MET:HA	2.41	0.56
1:B:62:LYS:HD2	1:B:146:TYR:HD1	1.69	0.56
1:F:162:GLU:O	1:F:167:VAL:N	2.38	0.56
1:A:139:ASP:O	1:A:142:ASP:HB2	2.06	0.55
1:F:140:PHE:CD2	1:F:335:MET:CG	2.88	0.55
1:G:377:TRP:N	1:G:377:TRP:CD1	2.73	0.55
1:C:249:GLU:O	1:C:250:LYS:CB	2.47	0.55
1:G:190:GLU:HA	1:G:191:LEU:C	2.31	0.55
1:B:150:ALA:CB	1:B:151:SER:CA	2.85	0.55
1:A:167:VAL:CG1	1:A:168:LEU:N	2.70	0.55
1:E:331:MET:HG3	1:E:332:VAL:N	2.21	0.55
1:A:131:ILE:HD13	1:B:120:VAL:HG12	1.86	0.55
1:E:87:LEU:HD11	1:E:157:GLN:HG2	1.88	0.55
1:G:358:ARG:HH11	1:G:358:ARG:CG	2.18	0.55
1:G:190:GLU:CA	1:G:193:LEU:H	2.17	0.55
1:D:227:GLU:HG3	1:D:268:PHE:CG	2.41	0.55
1:F:193:LEU:CA	1:F:196:GLU:HG3	2.35	0.55
1:D:257:PHE:CD1	1:D:257:PHE:C	2.85	0.55
1:F:302:PRO:HG3	1:G:105:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:MET:HE3	1:H:317:ILE:HD12	1.88	0.55
1:G:155:SER:OG	1:G:158:PHE:HB2	2.06	0.55
1:E:302:PRO:HB3	1:H:105:GLU:OE1	2.06	0.54
1:F:163:ASN:ND2	1:F:195:SER:OG	2.35	0.54
1:G:331:MET:HE2	1:G:332:VAL:HG23	1.88	0.54
1:A:90:LEU:HD22	1:A:165:ILE:HD11	1.88	0.54
1:C:135:MET:CE	1:C:143:PHE:CE1	2.90	0.54
1:C:244:LYS:HB3	1:C:244:LYS:NZ	2.17	0.54
1:D:326:TYR:O	1:D:329:VAL:HG23	2.08	0.54
1:G:188:GLU:HG3	1:G:191:LEU:CD1	2.37	0.54
1:G:363:VAL:HG13	1:G:364:ASP:N	2.22	0.54
1:H:215:LEU:O	1:H:217:PRO:HD3	2.06	0.54
1:B:150:ALA:HB1	1:B:151:SER:CA	2.38	0.54
1:A:167:VAL:HG12	1:A:168:LEU:N	2.21	0.54
1:A:169:GLN:HA	1:A:169:GLN:NE2	2.23	0.54
1:H:68:ASP:HB3	1:H:135:MET:HE3	1.90	0.54
1:C:68:ASP:HB3	1:C:135:MET:HE3	1.90	0.54
1:A:322:THR:HB	1:A:359:TYR:HD1	1.72	0.54
1:D:154:GLN:CD	1:D:155:SER:H	2.06	0.54
1:F:184:PHE:O	1:F:185:LYS:CG	2.55	0.54
1:G:219:GLY:O	1:G:220:PHE:CB	2.55	0.54
1:B:218:HIS:H	1:B:218:HIS:CD2	2.24	0.54
1:C:359:TYR:CD1	1:C:359:TYR:C	2.85	0.54
1:E:101:HIS:CA	3:E:405:HOH:O	2.56	0.54
1:B:237:GLU:O	1:B:241:ILE:HG12	2.08	0.54
1:C:100:GLY:O	1:C:101:HIS:HB2	2.07	0.54
1:C:247:SER:HA	1:C:249:GLU:O	2.08	0.54
1:E:299:ARG:HH12	1:G:138:LEU:H	1.56	0.54
1:E:328:HIS:O	1:E:332:VAL:HG23	2.07	0.54
1:F:184:PHE:C	1:F:184:PHE:CD1	2.85	0.54
1:G:331:MET:CE	1:G:332:VAL:CA	2.86	0.54
1:B:97:PHE:HA	1:B:102:VAL:CG2	2.38	0.54
1:G:141:ASN:OD1	1:G:144:ARG:HD3	2.08	0.54
1:G:332:VAL:O	1:G:335:MET:HG3	2.08	0.54
1:E:149:PRO:HB3	1:E:153:PHE:CD1	2.41	0.53
1:F:62:LYS:CD	1:F:146:TYR:CD1	2.87	0.53
1:H:322:THR:HG21	1:H:358:ARG:HA	1.90	0.53
1:B:240:ARG:O	1:B:240:ARG:HG2	2.09	0.53
1:D:360:LYS:HZ3	1:D:360:LYS:HB3	1.67	0.53
1:H:41:ILE:HG12	1:H:44:ASN:ND2	2.24	0.53
1:A:372:LEU:O	1:A:372:LEU:HD12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ILE:HD12	1:E:377:TRP:HB2	1.91	0.53
1:C:171:MET:HE2	1:C:359:TYR:HB3	1.89	0.53
1:B:147:LEU:HB2	1:B:148:SER:CA	2.28	0.53
1:D:43:GLY:HA3	1:D:48:LEU:HG	1.90	0.53
1:G:146:TYR:C	1:G:147:LEU:CD2	2.58	0.53
1:H:41:ILE:O	1:H:42:TYR:C	2.50	0.53
1:C:154:GLN:CD	1:C:173:VAL:HG21	2.33	0.53
1:B:214:GLY:HA3	1:B:294:MET:HE1	1.89	0.53
1:D:331:MET:HE2	1:D:332:VAL:HG22	1.90	0.53
1:F:144:ARG:CZ	1:F:336:LEU:HD12	2.38	0.53
1:A:150:ALA:C	1:A:152:GLY:N	2.64	0.53
1:C:154:GLN:HB2	1:C:174:PRO:O	2.08	0.53
1:C:247:SER:CB	1:C:248:GLU:HA	2.26	0.53
1:D:361:VAL:HG22	1:D:362:PHE:CE2	2.43	0.53
1:A:121:ILE:HG12	1:B:131:ILE:HD12	1.91	0.53
1:C:247:SER:HA	1:C:250:LYS:HB2	1.90	0.53
1:D:259:LYS:HZ1	1:D:260:GLN:N	2.06	0.53
1:E:263:VAL:HG13	1:E:264:LEU:H	1.70	0.53
1:E:335:MET:O	1:E:336:LEU:HD23	2.08	0.53
1:B:154:GLN:HE21	1:B:154:GLN:CA	2.22	0.53
1:E:258:GLN:O	1:E:261:LYS:HB3	2.09	0.53
1:E:318:ASP:OD2	1:E:361:VAL:N	2.36	0.53
1:F:193:LEU:HG	1:F:197:GLN:HG3	1.90	0.53
1:H:359:TYR:CG	1:H:366:PHE:CZ	2.96	0.53
1:E:233:GLY:O	1:E:237:GLU:HG2	2.08	0.52
1:F:334:ARG:HH11	1:F:335:MET:CE	2.22	0.52
1:B:148:SER:N	1:B:149:PRO:CA	2.72	0.52
1:D:162:GLU:O	1:D:166:GLY:HA2	2.09	0.52
1:H:246:GLU:N	1:H:246:GLU:OE1	2.42	0.52
1:C:58:GLN:HB3	1:C:146:TYR:CE2	2.45	0.52
1:C:214:GLY:CA	1:C:216:GLU:OE2	2.57	0.52
1:D:298:TYR:CD1	1:D:381:MET:HG3	2.43	0.52
1:G:150:ALA:CA	1:G:152:GLY:N	2.73	0.52
1:G:154:GLN:CG	1:G:155:SER:N	2.73	0.52
1:G:162:GLU:O	1:G:167:VAL:HG23	2.09	0.52
1:G:227:GLU:O	1:G:231:THR:HG23	2.10	0.52
1:E:138:LEU:CD1	1:G:375:ARG:HH12	2.22	0.52
1:B:154:GLN:NE2	1:B:154:GLN:CA	2.73	0.52
1:C:147:LEU:HD23	1:D:40:LEU:HD21	1.92	0.52
1:C:175:TYR:CD1	1:C:175:TYR:C	2.87	0.52
1:D:115:MET:HA	1:D:115:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ILE:CG2	1:F:148:SER:O	2.56	0.52
1:E:49:GLU:O	1:E:53:ASN:ND2	2.42	0.52
1:B:215:LEU:O	1:B:216:GLU:C	2.52	0.52
1:B:221:ASN:C	1:B:221:ASN:OD1	2.50	0.52
1:C:168:LEU:HD23	1:C:168:LEU:N	2.07	0.52
1:E:263:VAL:CG1	1:E:264:LEU:N	2.73	0.52
1:G:190:GLU:HB2	1:G:191:LEU:HA	1.92	0.52
1:A:92:SER:OG	1:A:114:ARG:NH1	2.43	0.52
1:C:240:ARG:HH12	1:C:253:GLN:HE22	1.57	0.52
1:E:148:SER:N	1:E:149:PRO:CD	2.73	0.52
1:F:165:ILE:N	1:F:166:GLY:HA2	2.24	0.52
1:C:187:GLU:CG	1:C:188:GLU:N	2.73	0.52
1:D:331:MET:HE2	1:D:332:VAL:CG2	2.40	0.52
1:E:335:MET:O	1:E:336:LEU:CG	2.58	0.52
1:F:144:ARG:NH2	1:F:336:LEU:HD12	2.24	0.52
1:F:148:SER:CB	1:F:149:PRO:HA	2.35	0.52
1:G:120:VAL:HG12	1:H:131:ILE:HD13	1.92	0.52
1:A:162:GLU:O	1:A:166:GLY:HA2	2.10	0.52
1:B:159:ARG:HH22	1:B:169:GLN:NE2	2.07	0.52
1:B:374:PRO:HD2	1:B:377:TRP:CE2	2.44	0.52
1:E:47:HIS:ND1	1:E:49:GLU:OE2	2.30	0.52
1:B:332:VAL:HG13	1:B:336:LEU:HD22	1.92	0.51
1:C:115:MET:HE2	1:C:115:MET:HA	1.92	0.51
1:A:80:GLU:OE2	1:B:42:TYR:OH	2.22	0.51
1:G:154:GLN:CD	1:G:155:SER:H	2.18	0.51
1:C:138:LEU:HD12	1:C:139:ASP:H	1.74	0.51
1:C:175:TYR:OH	1:C:188:GLU:OE2	2.28	0.51
1:D:257:PHE:CD1	1:D:258:GLN:CA	2.93	0.51
1:E:299:ARG:NH1	1:G:138:LEU:HB2	2.25	0.51
1:H:187:GLU:CG	1:H:189:ASN:H	2.19	0.51
1:B:103:ARG:NH2	1:B:208:TRP:O	2.43	0.51
1:E:257:PHE:CD1	1:E:258:GLN:N	2.79	0.51
1:G:84:LYS:NZ	1:H:52:LEU:O	2.43	0.51
1:C:358:ARG:N	1:C:358:ARG:CD	2.72	0.51
1:D:259:LYS:CE	1:D:260:GLN:N	2.73	0.51
1:D:336:LEU:CD2	1:D:337:GLY:N	2.61	0.51
1:E:140:PHE:CG	1:E:335:MET:SD	3.04	0.51
1:G:154:GLN:HA	1:G:154:GLN:NE2	2.21	0.51
1:G:254:VAL:HG13	1:G:255:ALA:N	2.25	0.51
1:E:101:HIS:N	3:E:405:HOH:O	2.31	0.51
1:F:333:HIS:HB2	3:F:402:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:216:GLU:O	1:G:220:PHE:O	2.29	0.51
1:G:312:THR:HA	1:G:315:MET:HE3	1.93	0.51
1:G:332:VAL:HA	1:G:335:MET:CG	2.41	0.51
1:A:322:THR:CG2	1:A:359:TYR:HD1	2.24	0.51
1:B:147:LEU:N	1:B:147:LEU:CD1	2.73	0.51
1:D:140:PHE:CD2	1:D:335:MET:HB3	2.46	0.51
1:F:372:LEU:HD11	1:H:141:ASN:HD21	1.75	0.51
1:A:322:THR:HG21	1:A:359:TYR:CD1	2.45	0.51
1:E:261:LYS:NZ	3:E:408:HOH:O	2.44	0.51
1:G:190:GLU:CA	1:G:191:LEU:C	2.84	0.50
1:G:298:TYR:OH	1:G:379:PRO:O	2.24	0.50
1:G:331:MET:HE2	1:G:332:VAL:CG2	2.41	0.50
1:A:322:THR:HG21	1:A:359:TYR:HD1	1.76	0.50
1:C:135:MET:HE1	1:C:143:PHE:HZ	1.76	0.50
1:D:255:ALA:CA	1:D:256:GLU:CB	2.84	0.50
1:C:80:GLU:OE2	1:C:155:SER:OG	2.27	0.50
1:C:147:LEU:O	1:C:148:SER:O	2.29	0.50
1:F:193:LEU:O	1:F:196:GLU:N	2.44	0.50
1:F:244:LYS:HA	1:F:245:GLU:C	2.36	0.50
1:E:226:LEU:HD23	1:E:268:PHE:HZ	1.76	0.50
1:F:318:ASP:CG	1:F:360:LYS:HB3	2.37	0.50
1:G:221:ASN:O	1:G:225:LYS:HG3	2.10	0.50
1:G:245:GLU:O	1:G:246:GLU:O	2.30	0.50
1:A:90:LEU:CD2	1:A:165:ILE:HD11	2.42	0.50
1:C:294:MET:HG3	1:C:298:TYR:HD2	1.76	0.50
1:F:162:GLU:HB3	1:F:167:VAL:HG22	1.92	0.50
1:B:97:PHE:HA	1:B:102:VAL:HG21	1.94	0.50
1:B:221:ASN:OD1	1:B:221:ASN:O	2.30	0.50
1:E:117:ARG:HD3	1:F:71:LEU:HD22	1.94	0.50
1:E:257:PHE:CD1	1:E:257:PHE:C	2.89	0.50
1:G:139:ASP:O	1:G:142:ASP:HB2	2.12	0.50
1:H:303:ARG:NH2	1:H:381:MET:HG2	2.26	0.50
1:H:322:THR:HG21	1:H:358:ARG:O	2.11	0.50
1:A:245:GLU:HG3	1:A:246:GLU:O	2.12	0.50
1:G:189:ASN:HB3	1:G:192:LEU:HD23	1.94	0.50
1:D:103:ARG:NH2	1:D:208:TRP:O	2.45	0.50
1:G:155:SER:OG	1:G:158:PHE:N	2.38	0.50
1:G:189:ASN:CB	1:G:192:LEU:HB3	2.42	0.50
1:G:376:HIS:CD2	1:G:377:TRP:CD1	3.00	0.50
1:B:156:LEU:HD21	1:B:188:GLU:HG2	1.91	0.49
1:D:62:LYS:HB2	1:D:146:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:PRO:CB	1:E:153:PHE:CB	2.77	0.49
1:F:165:ILE:N	1:F:166:GLY:CA	2.75	0.49
1:D:161:LEU:O	1:D:165:ILE:HG12	2.11	0.49
1:E:138:LEU:HD13	1:G:375:ARG:NH1	2.26	0.49
1:G:97:PHE:HA	1:G:102:VAL:HG22	1.93	0.49
1:D:376:HIS:C	1:D:378:ILE:H	2.20	0.49
1:G:190:GLU:HB3	1:G:193:LEU:HB2	1.93	0.49
1:G:303:ARG:HD3	1:G:381:MET:HE1	1.95	0.49
1:A:322:THR:CG2	1:A:359:TYR:CD1	2.95	0.49
1:E:253:GLN:NE2	1:E:253:GLN:N	2.60	0.49
1:F:327:ASN:ND2	3:F:403:HOH:O	2.42	0.49
1:G:332:VAL:HA	1:G:335:MET:SD	2.52	0.49
1:G:362:PHE:HB3	1:G:365:LEU:HD12	1.95	0.49
1:D:257:PHE:CD1	1:D:258:GLN:HG2	2.48	0.49
1:E:87:LEU:HD12	1:E:157:GLN:HG2	1.93	0.49
1:A:112:VAL:HG21	1:A:306:VAL:HG13	1.92	0.49
1:C:144:ARG:O	1:C:144:ARG:HD3	2.11	0.49
1:D:168:LEU:HD11	1:D:283:ARG:HH11	1.74	0.49
1:D:259:LYS:NZ	1:D:260:GLN:N	2.60	0.49
1:G:154:GLN:HE21	1:G:155:SER:N	2.10	0.49
1:G:331:MET:CE	1:G:332:VAL:CG2	2.90	0.49
1:A:143:PHE:O	1:A:146:TYR:HD1	1.96	0.49
1:B:219:GLY:O	1:B:220:PHE:O	2.30	0.49
1:D:298:TYR:CE1	1:D:381:MET:HG3	2.48	0.49
1:G:165:ILE:N	1:G:166:GLY:HA2	2.27	0.49
1:G:189:ASN:HB3	1:G:192:LEU:CB	2.43	0.49
1:B:62:LYS:HD2	1:B:146:TYR:CD1	2.47	0.49
1:B:148:SER:CB	1:B:149:PRO:C	2.86	0.49
1:D:144:ARG:O	1:D:147:LEU:N	2.40	0.49
1:G:358:ARG:CG	1:G:358:ARG:NH1	2.73	0.49
1:H:187:GLU:CG	1:H:188:GLU:N	2.55	0.49
1:D:232:ARG:CA	1:D:235:GLU:HG2	2.43	0.49
1:G:154:GLN:HE21	1:G:155:SER:H	1.55	0.49
1:G:220:PHE:CD1	1:G:225:LYS:HE3	2.48	0.49
1:H:140:PHE:HA	1:H:143:PHE:CE1	2.48	0.49
1:G:160:LEU:O	1:G:164:LYS:HG3	2.13	0.48
1:G:190:GLU:CA	1:G:192:LEU:N	2.73	0.48
1:A:97:PHE:HA	1:A:102:VAL:HG22	1.94	0.48
1:A:227:GLU:HB3	1:A:228:LYS:HE2	1.94	0.48
1:C:154:GLN:CD	1:C:173:VAL:CG2	2.86	0.48
1:E:335:MET:O	1:E:336:LEU:CD2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:MET:CE	1:G:335:MET:SD	3.02	0.48
1:H:41:ILE:O	1:H:41:ILE:HG13	2.10	0.48
1:H:258:GLN:HE22	1:H:261:LYS:HD3	1.77	0.48
1:A:224:GLY:O	1:A:228:LYS:HE3	2.10	0.48
1:A:322:THR:HB	1:A:359:TYR:CE1	2.48	0.48
1:B:148:SER:N	1:B:149:PRO:C	2.72	0.48
1:B:375:ARG:HG2	1:B:375:ARG:O	2.12	0.48
1:C:294:MET:HG3	1:C:298:TYR:CD2	2.49	0.48
1:C:334:ARG:NH2	1:C:335:MET:CE	2.73	0.48
1:D:260:GLN:C	1:D:263:VAL:HG12	2.37	0.48
1:F:149:PRO:O	1:F:152:GLY:HA3	2.13	0.48
1:F:234:LEU:HD13	1:F:261:LYS:HG3	1.96	0.48
1:G:141:ASN:HA	1:G:144:ARG:HD2	1.95	0.48
1:G:155:SER:OG	1:G:158:PHE:HB3	2.11	0.48
1:C:331:MET:HE3	1:C:335:MET:HG3	1.96	0.48
1:F:68:ASP:HB3	1:F:135:MET:HE3	1.95	0.48
1:F:328:HIS:O	1:F:330:CYS:N	2.43	0.48
1:G:140:PHE:HE2	1:G:335:MET:HB2	1.77	0.48
1:C:139:ASP:O	1:C:142:ASP:HB2	2.14	0.48
1:G:40:LEU:CB	1:G:41:ILE:HD12	2.30	0.48
1:E:149:PRO:HB3	1:E:153:PHE:HD1	1.78	0.48
1:G:140:PHE:CE2	1:G:335:MET:HB2	2.48	0.48
1:G:189:ASN:CB	1:G:192:LEU:CB	2.91	0.48
1:A:131:ILE:HD12	1:B:121:ILE:HG12	1.96	0.48
1:C:234:LEU:HD13	1:C:261:LYS:HG3	1.96	0.48
1:E:140:PHE:CD2	1:E:335:MET:HB3	2.49	0.48
1:G:218:HIS:HA	1:G:219:GLY:HA2	1.56	0.47
1:A:147:LEU:N	1:A:147:LEU:CD1	2.77	0.47
1:D:143:PHE:C	1:D:145:GLU:N	2.69	0.47
1:G:41:ILE:N	1:G:41:ILE:CD1	2.73	0.47
1:G:190:GLU:HB2	1:G:191:LEU:CA	2.44	0.47
1:A:91:ASP:OD1	1:A:164:LYS:NZ	2.40	0.47
1:B:156:LEU:CD1	1:B:192:LEU:HD13	2.44	0.47
1:D:103:ARG:NH2	1:D:208:TRP:CD1	2.83	0.47
1:D:298:TYR:OH	1:D:379:PRO:HG2	2.15	0.47
1:E:202:LEU:HD21	1:E:283:ARG:HB3	1.95	0.47
1:E:41:ILE:HD12	1:E:41:ILE:HA	1.80	0.47
1:F:328:HIS:C	1:F:329:VAL:HG22	2.39	0.47
1:D:41:ILE:O	1:D:44:ASN:HB2	2.14	0.47
1:E:253:GLN:C	1:E:254:VAL:CG2	2.88	0.47
1:A:282:ARG:NH2	3:A:406:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:O	1:A:336:LEU:HB2	2.13	0.47
1:D:165:ILE:O	1:D:201:LEU:HB3	2.13	0.47
1:E:103:ARG:HH22	1:E:212:THR:HA	1.78	0.47
1:E:115:MET:HE3	1:E:317:ILE:HD12	1.97	0.47
1:E:258:GLN:O	1:E:261:LYS:CB	2.61	0.47
1:F:151:SER:HA	1:F:152:GLY:HA3	1.48	0.47
1:A:237:GLU:OE2	1:A:240:ARG:NH2	2.43	0.47
1:A:317:ILE:O	1:A:321:MET:HB2	2.15	0.47
1:B:188:GLU:O	1:B:191:LEU:CB	2.63	0.47
1:D:140:PHE:HA	1:D:143:PHE:CE2	2.49	0.47
1:E:42:TYR:HD1	1:F:153:PHE:CD1	2.33	0.47
1:E:253:GLN:N	1:E:253:GLN:CD	2.73	0.47
1:G:121:ILE:HG12	1:H:131:ILE:HD12	1.97	0.47
1:G:223:TRP:O	1:G:227:GLU:N	2.38	0.47
1:B:140:PHE:CE2	1:B:335:MET:HB3	2.50	0.47
1:B:148:SER:CA	1:B:149:PRO:C	2.88	0.47
1:E:362:PHE:O	1:E:365:LEU:N	2.47	0.47
1:A:225:LYS:O	1:A:229:ASN:OD1	2.33	0.47
1:C:49:GLU:O	1:C:53:ASN:ND2	2.46	0.47
1:D:69:GLU:HG3	1:D:143:PHE:CD1	2.50	0.47
1:E:148:SER:N	1:E:149:PRO:HD3	2.29	0.47
1:E:221:ASN:O	1:E:222:PHE:C	2.58	0.47
1:F:41:ILE:C	1:F:43:GLY:H	2.23	0.47
1:F:242:GLN:HA	1:F:243:ALA:HA	1.71	0.47
1:A:220:PHE:O	1:A:225:LYS:HE3	2.15	0.46
1:C:334:ARG:HH21	1:C:335:MET:HE1	1.79	0.46
1:D:144:ARG:HG2	1:D:145:GLU:N	2.29	0.46
1:G:239:ILE:HD12	1:G:239:ILE:HA	1.78	0.46
1:G:318:ASP:OD2	1:G:361:VAL:N	2.48	0.46
1:C:250:LYS:O	1:C:253:GLN:HB2	2.15	0.46
1:F:241:ILE:O	1:F:243:ALA:HA	2.16	0.46
1:F:367:ASN:O	1:F:370:THR:OG1	2.32	0.46
1:H:270:GLU:HG2	1:H:286:TYR:CE2	2.50	0.46
1:C:165:ILE:HG22	1:C:361:VAL:HG21	1.96	0.46
1:F:62:LYS:CG	1:F:146:TYR:CD1	2.99	0.46
1:F:189:ASN:O	1:F:189:ASN:ND2	2.44	0.46
1:E:269:ASP:OD1	1:E:271:LYS:HG2	2.15	0.46
1:G:331:MET:HE1	1:G:332:VAL:HG22	1.98	0.46
1:D:228:LYS:HD2	1:D:228:LYS:HA	1.54	0.46
1:D:232:ARG:O	1:D:235:GLU:HG2	2.16	0.46
1:D:258:GLN:OE1	1:D:261:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:LYS:HZ1	1:D:260:GLN:CB	2.28	0.46
1:D:261:LYS:C	1:D:263:VAL:N	2.70	0.46
1:E:144:ARG:C	1:E:146:TYR:H	2.22	0.46
1:F:147:LEU:CD1	1:F:147:LEU:C	2.88	0.46
1:F:358:ARG:NH1	1:F:358:ARG:CG	2.71	0.46
1:H:66:ILE:HG13	1:H:143:PHE:HB3	1.97	0.46
1:B:226:LEU:HG	1:B:230:ILE:HD12	1.98	0.46
1:E:96:ILE:HG22	1:E:102:VAL:HG13	1.98	0.46
1:F:216:GLU:O	1:F:221:ASN:N	2.46	0.46
1:F:336:LEU:HD22	1:F:336:LEU:H	1.79	0.46
1:B:235:GLU:O	1:B:238:PHE:HB3	2.15	0.46
1:C:336:LEU:N	1:C:336:LEU:HD12	2.31	0.46
1:D:206:GLU:OE2	1:D:285:SER:N	2.47	0.46
1:F:237:GLU:O	1:F:241:ILE:HG13	2.15	0.46
1:B:146:TYR:C	1:B:147:LEU:HD13	2.41	0.46
1:G:332:VAL:HA	1:G:335:MET:HG2	1.97	0.46
1:C:175:TYR:HD1	1:C:175:TYR:O	2.00	0.46
1:E:298:TYR:OH	1:E:379:PRO:HG2	2.15	0.46
1:F:150:ALA:HA	1:F:151:SER:HA	1.65	0.46
1:H:381:MET:HG3	1:H:382:ASN:H	1.80	0.46
1:C:103:ARG:NH1	1:C:103:ARG:CG	2.72	0.45
1:C:163:ASN:O	1:C:166:GLY:HA3	2.16	0.45
1:C:240:ARG:HH12	1:C:253:GLN:NE2	2.14	0.45
1:F:40:LEU:HD23	1:F:40:LEU:HA	1.65	0.45
1:F:235:GLU:O	1:F:239:ILE:HG13	2.15	0.45
1:H:140:PHE:CD2	1:H:335:MET:HB3	2.51	0.45
1:H:187:GLU:OE2	1:H:189:ASN:HB2	2.16	0.45
1:B:156:LEU:HD22	1:B:188:GLU:CG	2.44	0.45
1:B:374:PRO:HA	1:D:141:ASN:HD21	1.81	0.45
1:D:259:LYS:HZ1	1:D:260:GLN:CA	2.29	0.45
1:F:358:ARG:CD	1:F:360:LYS:NZ	2.79	0.45
1:B:221:ASN:O	1:B:221:ASN:CG	2.56	0.45
1:C:135:MET:O	1:C:334:ARG:NH2	2.50	0.45
1:C:154:GLN:NE2	1:C:173:VAL:HG21	2.32	0.45
1:D:257:PHE:HD1	1:D:258:GLN:HG2	1.81	0.45
1:F:189:ASN:HD22	1:F:189:ASN:C	2.24	0.45
1:F:336:LEU:N	1:F:336:LEU:CD2	2.73	0.45
1:G:194:LYS:HE3	1:G:198:GLU:CD	2.34	0.45
1:A:267:LEU:HD13	1:A:371:TYR:CE1	2.52	0.45
1:C:121:ILE:HG12	1:D:131:ILE:HD12	1.96	0.45
1:D:66:ILE:HG13	1:D:142:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:360:LYS:HB2	1:H:360:LYS:HE3	1.41	0.45
1:A:322:THR:CB	1:A:359:TYR:CD1	2.94	0.45
1:B:132:LEU:HD23	1:B:132:LEU:HA	1.79	0.45
1:C:168:LEU:CD2	1:C:168:LEU:N	2.73	0.45
1:D:140:PHE:CE2	1:D:335:MET:HB3	2.51	0.45
1:E:103:ARG:HH12	1:E:213:PRO:HD2	1.82	0.45
1:F:148:SER:CB	1:F:149:PRO:CA	2.85	0.45
1:F:326:TYR:O	1:F:326:TYR:CD1	2.70	0.45
1:E:41:ILE:HD12	1:E:44:ASN:HB2	1.98	0.45
1:F:46:LEU:O	1:F:47:HIS:C	2.59	0.45
1:C:153:PHE:O	1:C:153:PHE:CD1	2.70	0.45
1:D:225:LYS:O	1:D:229:ASN:CG	2.60	0.45
1:E:140:PHE:HA	1:E:143:PHE:CE2	2.52	0.45
1:H:64:ASN:HB3	1:H:146:TYR:OH	2.17	0.45
1:H:151:SER:N	1:H:152:GLY:HA3	2.31	0.45
1:H:269:ASP:OD2	1:H:272:ARG:HB2	2.16	0.45
1:A:136:THR:HG23	1:A:139:ASP:HB2	1.97	0.44
1:E:153:PHE:O	1:E:153:PHE:CD2	2.70	0.44
1:G:154:GLN:CG	1:G:155:SER:H	2.30	0.44
1:A:150:ALA:O	1:A:152:GLY:N	2.50	0.44
1:E:121:ILE:HG12	1:F:131:ILE:HD12	1.99	0.44
1:A:261:LYS:HE3	1:A:265:LEU:CD1	2.48	0.44
1:C:154:GLN:CB	1:C:174:PRO:O	2.65	0.44
1:D:232:ARG:HA	1:D:235:GLU:CG	2.47	0.44
1:D:361:VAL:CG2	1:D:362:PHE:CE2	3.00	0.44
1:G:153:PHE:CD1	1:G:153:PHE:O	2.71	0.44
1:H:359:TYR:CD2	1:H:366:PHE:CE1	3.06	0.44
1:D:141:ASN:C	1:D:143:PHE:N	2.71	0.44
1:F:239:ILE:O	1:F:242:GLN:N	2.49	0.44
1:F:332:VAL:O	1:F:336:LEU:HD23	2.17	0.44
1:G:298:TYR:OH	1:G:379:PRO:HG2	2.17	0.44
1:A:214:GLY:HA3	1:A:294:MET:HE1	1.99	0.44
1:A:140:PHE:CE1	1:A:335:MET:HB3	2.53	0.44
1:C:175:TYR:CD1	1:C:175:TYR:O	2.70	0.44
1:D:165:ILE:N	1:D:166:GLY:CA	2.81	0.44
1:D:260:GLN:O	1:D:263:VAL:HG13	2.13	0.44
1:E:144:ARG:C	1:E:144:ARG:CD	2.85	0.44
1:F:326:TYR:CD1	1:F:326:TYR:C	2.93	0.44
1:G:233:GLY:O	1:G:237:GLU:HG2	2.18	0.44
1:A:210:GLU:OE2	1:A:285:SER:OG	2.26	0.44
1:G:132:LEU:HD12	1:G:132:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:254:VAL:CG1	1:G:255:ALA:N	2.81	0.44
1:A:165:ILE:HD12	1:A:165:ILE:HG23	1.60	0.44
1:B:220:PHE:CZ	1:B:380:LYS:O	2.69	0.44
1:C:172:ARG:H	1:C:172:ARG:HG2	1.56	0.44
1:F:329:VAL:HG23	1:F:330:CYS:N	2.33	0.44
1:F:363:VAL:HG13	1:F:364:ASP:N	2.32	0.44
1:A:165:ILE:N	1:A:166:GLY:HA2	2.33	0.44
1:B:140:PHE:CD2	1:B:335:MET:HB3	2.53	0.44
1:B:149:PRO:O	1:B:150:ALA:HB2	2.17	0.44
1:G:245:GLU:O	1:G:245:GLU:HG3	2.17	0.44
1:H:265:LEU:HD23	1:H:265:LEU:HA	1.84	0.44
1:H:326:TYR:CZ	1:H:330:CYS:SG	3.10	0.44
1:H:334:ARG:CZ	1:H:335:MET:HE3	2.47	0.44
1:B:159:ARG:NH2	1:B:169:GLN:NE2	2.51	0.43
1:F:293:LEU:HG	1:F:368:LEU:HD22	2.00	0.43
1:F:41:ILE:C	1:F:43:GLY:N	2.76	0.43
1:F:115:MET:HE3	1:F:317:ILE:HD12	2.01	0.43
1:G:146:TYR:O	1:G:147:LEU:CD2	2.53	0.43
1:C:239:ILE:HD13	1:C:239:ILE:HA	1.85	0.43
1:D:298:TYR:CE1	1:D:381:MET:CG	3.01	0.43
1:E:140:PHE:CE2	1:E:335:MET:HB3	2.53	0.43
1:G:141:ASN:HA	1:G:144:ARG:CD	2.48	0.43
1:G:190:GLU:N	1:G:190:GLU:CD	2.73	0.43
1:G:377:TRP:N	1:G:377:TRP:HD1	2.17	0.43
1:H:381:MET:HG3	1:H:382:ASN:N	2.34	0.43
1:D:140:PHE:CD1	1:D:143:PHE:CZ	3.07	0.43
1:D:360:LYS:CB	1:D:360:LYS:HZ2	2.08	0.43
1:A:149:PRO:HD2	1:B:40:LEU:CG	2.44	0.43
1:B:377:TRP:N	1:B:377:TRP:CD1	2.87	0.43
1:E:103:ARG:NH1	1:E:213:PRO:CD	2.81	0.43
1:E:144:ARG:C	1:E:146:TYR:N	2.75	0.43
1:F:184:PHE:O	1:F:185:LYS:HG3	2.19	0.43
1:F:210:GLU:HG2	1:F:287:ARG:HB3	2.00	0.43
1:G:203:GLU:O	1:G:206:GLU:HB3	2.19	0.43
1:H:358:ARG:HH21	1:H:358:ARG:CG	2.14	0.43
1:C:153:PHE:O	1:C:153:PHE:HD1	2.02	0.43
1:D:211:ARG:O	1:D:213:PRO:HD3	2.19	0.43
1:E:330:CYS:O	1:E:333:HIS:HB3	2.18	0.43
1:F:329:VAL:C	1:F:332:VAL:H	2.26	0.43
1:G:216:GLU:CD	1:G:216:GLU:H	2.27	0.43
1:A:100:GLY:O	1:A:101:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:O	1:A:115:MET:HG2	2.19	0.43
1:D:275:HIS:O	1:D:278:SER:OG	2.28	0.43
1:F:296:TYR:HB2	1:F:368:LEU:HD13	2.00	0.43
1:G:294:MET:HG3	1:G:298:TYR:CD2	2.54	0.43
1:H:380:LYS:HE2	1:H:380:LYS:HB2	1.77	0.43
1:D:41:ILE:O	1:D:44:ASN:N	2.51	0.43
1:E:140:PHE:CE2	1:E:144:ARG:HB2	2.54	0.43
1:F:147:LEU:C	1:F:148:SER:HG	2.09	0.43
1:F:214:GLY:HA3	1:F:294:MET:HE1	2.00	0.43
1:G:293:LEU:HD13	1:G:368:LEU:HD22	2.00	0.43
1:G:329:VAL:O	1:G:332:VAL:N	2.52	0.43
1:C:162:GLU:O	1:C:166:GLY:CA	2.66	0.42
1:E:152:GLY:CA	1:E:153:PHE:CB	2.96	0.42
1:E:293:LEU:HD22	1:E:297:PHE:CE2	2.55	0.42
1:E:362:PHE:O	1:E:363:VAL:C	2.60	0.42
1:F:58:GLN:O	1:F:62:LYS:HG2	2.19	0.42
1:G:331:MET:CE	1:G:332:VAL:N	2.74	0.42
1:H:286:TYR:O	1:H:289:LEU:HB3	2.19	0.42
1:A:229:ASN:OD1	1:A:229:ASN:N	2.52	0.42
1:C:131:ILE:HD12	1:D:121:ILE:HG12	2.01	0.42
1:D:194:LYS:HE3	1:D:194:LYS:HB2	1.72	0.42
1:E:215:LEU:O	1:E:216:GLU:C	2.60	0.42
1:F:132:LEU:HD12	1:F:132:LEU:HA	1.76	0.42
1:C:55:GLN:OE1	1:D:84:LYS:NZ	2.45	0.42
1:C:193:LEU:O	1:C:197:GLN:CG	2.66	0.42
1:E:147:LEU:C	1:E:149:PRO:CD	2.93	0.42
1:E:293:LEU:HG	1:E:368:LEU:HD22	2.02	0.42
1:E:373:ILE:HD11	1:E:378:ILE:HG12	2.02	0.42
1:G:358:ARG:HG2	1:G:359:TYR:N	2.32	0.42
1:H:220:PHE:CZ	1:H:381:MET:SD	3.12	0.42
1:D:259:LYS:C	1:D:259:LYS:CE	2.85	0.42
1:D:274:GLU:O	1:D:277:LEU:HB3	2.20	0.42
1:E:148:SER:OG	1:F:40:LEU:O	2.30	0.42
1:E:257:PHE:O	1:E:258:GLN:C	2.63	0.42
1:E:335:MET:C	1:E:336:LEU:HG	2.44	0.42
1:F:332:VAL:O	1:F:336:LEU:CD2	2.67	0.42
1:D:232:ARG:C	1:D:235:GLU:HG2	2.44	0.42
1:E:41:ILE:O	1:E:45:TYR:N	2.46	0.42
1:E:256:GLU:H	1:E:256:GLU:HG2	1.57	0.42
1:C:244:LYS:HB2	1:C:250:LYS:CE	2.50	0.42
1:E:144:ARG:HH11	1:E:336:LEU:HD21	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:LEU:HD23	1:E:193:LEU:HA	1.91	0.42
1:F:217:PRO:HA	1:F:221:ASN:OD1	2.19	0.42
1:A:165:ILE:HG13	1:A:321:MET:HE1	2.02	0.42
1:B:106:ARG:NH2	1:C:300:GLU:OE1	2.53	0.42
1:C:298:TYR:O	1:C:304:PHE:HB2	2.20	0.42
1:D:144:ARG:O	1:D:147:LEU:CB	2.50	0.42
1:E:140:PHE:CD1	1:E:335:MET:SD	3.12	0.42
1:D:318:ASP:O	1:D:319:SER:C	2.62	0.42
1:E:361:VAL:O	1:E:361:VAL:HG12	2.19	0.42
1:B:156:LEU:CD2	1:B:188:GLU:CG	2.88	0.41
1:F:141:ASN:HD21	1:H:372:LEU:CD2	2.30	0.41
1:G:138:LEU:HD12	1:G:138:LEU:HA	1.84	0.41
1:H:362:PHE:O	1:H:366:PHE:HD2	2.03	0.41
1:B:236:GLU:CD	1:B:236:GLU:C	2.88	0.41
1:C:140:PHE:HA	1:C:143:PHE:CE1	2.54	0.41
1:C:153:PHE:N	1:C:154:GLN:CA	2.81	0.41
1:C:270:GLU:HG2	1:C:286:TYR:CE2	2.56	0.41
1:C:365:LEU:HA	1:C:368:LEU:HG	2.02	0.41
1:E:122:LEU:HD23	1:E:122:LEU:HA	1.92	0.41
1:E:132:LEU:HD23	1:E:132:LEU:HA	1.78	0.41
1:F:109:LEU:HD11	1:G:305:GLN:NE2	2.36	0.41
1:G:190:GLU:HB2	1:G:191:LEU:C	2.44	0.41
1:H:106:ARG:HG3	1:H:107:ASN:N	2.35	0.41
1:H:358:ARG:HH21	1:H:358:ARG:N	2.18	0.41
1:C:103:ARG:HA	1:C:103:ARG:HD3	1.74	0.41
1:C:259:LYS:HD2	1:C:259:LYS:HA	1.94	0.41
1:E:254:VAL:HG12	1:E:255:ALA:H	1.85	0.41
1:G:148:SER:HB2	1:H:40:LEU:HD13	2.01	0.41
1:E:103:ARG:NH1	1:E:213:PRO:HD2	2.34	0.41
1:E:263:VAL:CG1	1:E:264:LEU:H	2.31	0.41
1:F:186:GLY:HA2	1:F:189:ASN:HB2	2.03	0.41
1:H:41:ILE:HG13	1:H:44:ASN:H	1.86	0.41
1:B:146:TYR:C	1:B:147:LEU:CD1	2.93	0.41
1:D:141:ASN:C	1:D:143:PHE:H	2.29	0.41
1:D:362:PHE:O	1:D:365:LEU:N	2.54	0.41
1:F:144:ARG:CA	1:F:147:LEU:HD11	2.43	0.41
1:A:190:GLU:HG3	1:A:191:LEU:N	2.34	0.41
1:B:362:PHE:HB3	1:B:365:LEU:HD12	2.03	0.41
1:D:210:GLU:HG2	1:D:287:ARG:HB3	2.02	0.41
1:G:189:ASN:HB3	1:G:192:LEU:HB2	2.03	0.41
1:G:245:GLU:C	1:G:246:GLU:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:HA	1:A:217:PRO:HD3	1.93	0.41
1:B:218:HIS:CD2	1:B:218:HIS:N	2.88	0.41
1:B:365:LEU:HA	1:B:368:LEU:HG	2.03	0.41
1:C:358:ARG:N	1:C:359:TYR:CD2	2.89	0.41
1:D:110:LYS:HD3	1:D:114:ARG:NH2	2.36	0.41
1:D:202:LEU:HD21	1:D:283:ARG:HB3	2.03	0.41
1:D:225:LYS:O	1:D:229:ASN:ND2	2.53	0.41
1:E:153:PHE:O	1:E:153:PHE:CG	2.70	0.41
1:E:296:TYR:HB2	1:E:368:LEU:HD13	2.01	0.41
1:F:358:ARG:HD2	1:F:360:LYS:NZ	2.35	0.41
1:G:115:MET:HA	1:G:115:MET:HE2	2.02	0.41
1:G:163:ASN:O	1:G:166:GLY:CA	2.69	0.41
1:G:376:HIS:C	1:G:378:ILE:N	2.78	0.41
1:A:269:ASP:OD2	1:A:272:ARG:HB2	2.21	0.41
1:C:293:LEU:HD23	1:C:293:LEU:HA	1.95	0.41
1:C:358:ARG:N	1:C:358:ARG:HD2	2.35	0.41
1:D:154:GLN:OE1	1:D:154:GLN:HA	2.20	0.41
1:D:259:LYS:HE2	1:D:260:GLN:CA	2.50	0.41
1:F:85:GLN:O	1:F:88:TRP:HB3	2.20	0.41
1:F:143:PHE:CD1	1:F:143:PHE:C	2.99	0.41
1:F:245:GLU:H	1:F:245:GLU:HG2	1.56	0.41
1:A:326:TYR:O	1:A:329:VAL:HG22	2.21	0.41
1:F:326:TYR:O	1:F:328:HIS:O	2.39	0.41
1:G:185:LYS:HE2	1:G:192:LEU:HD21	2.02	0.41
1:A:165:ILE:HA	1:A:165:ILE:HD13	1.85	0.40
1:A:202:LEU:HD21	1:A:283:ARG:HB3	2.03	0.40
1:A:365:LEU:HA	1:A:368:LEU:HG	2.03	0.40
1:A:150:ALA:C	1:A:152:GLY:H	2.29	0.40
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.81	0.40
1:D:140:PHE:CG	1:D:335:MET:SD	3.15	0.40
1:G:162:GLU:CA	1:G:167:VAL:HG23	2.51	0.40
1:G:304:PHE:C	1:G:307:PRO:HD2	2.47	0.40
1:G:332:VAL:CA	1:G:335:MET:HG2	2.51	0.40
1:C:103:ARG:CG	3:C:404:HOH:O	2.49	0.40
1:D:147:LEU:HD12	1:D:147:LEU:HA	1.80	0.40
1:D:294:MET:HG3	1:D:298:TYR:CD2	2.56	0.40
1:G:168:LEU:O	1:G:169:GLN:CB	2.70	0.40
1:G:189:ASN:CA	1:G:192:LEU:HB2	2.44	0.40
1:C:144:ARG:O	1:C:144:ARG:CG	2.69	0.40
1:C:159:ARG:NH1	1:C:172:ARG:NH2	2.69	0.40
1:F:149:PRO:O	1:F:149:PRO:CD	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:PRO:O	1:G:152:GLY:CA	2.70	0.40
1:A:192:LEU:HD12	1:A:192:LEU:HA	1.91	0.40
1:C:143:PHE:O	1:C:145:GLU:N	2.54	0.40
1:D:257:PHE:CE1	1:D:258:GLN:HA	2.57	0.40
1:D:333:HIS:O	1:D:334:ARG:C	2.63	0.40
1:F:149:PRO:O	1:F:152:GLY:CA	2.69	0.40
1:F:202:LEU:HD22	1:F:361:VAL:HG13	2.03	0.40
1:H:332:VAL:O	1:H:336:LEU:HB2	2.22	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	300/373 (80%)	294 (98%)	6 (2%)	0	100	100
1	B	288/373 (77%)	279 (97%)	8 (3%)	1 (0%)	36	65
1	C	305/373 (82%)	297 (97%)	6 (2%)	2 (1%)	18	48
1	D	278/373 (74%)	269 (97%)	9 (3%)	0	100	100
1	E	285/373 (76%)	278 (98%)	7 (2%)	0	100	100
1	F	295/373 (79%)	287 (97%)	5 (2%)	3 (1%)	12	39
1	G	296/373 (79%)	285 (96%)	8 (3%)	3 (1%)	12	39
1	H	293/373 (79%)	287 (98%)	6 (2%)	0	100	100
All	All	2340/2984 (78%)	2276 (97%)	55 (2%)	9 (0%)	30	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	150	ALA
1	C	247	SER

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Mol	Chain	Res	Type
1	C	250	LYS
1	F	42	TYR
1	F	148	SER
1	G	149	PRO
1	G	220	PHE
1	G	217	PRO
1	F	149	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	285/340 (84%)	265 (93%)	20 (7%)	14	40
1	B	276/340 (81%)	248 (90%)	28 (10%)	7	24
1	C	292/340 (86%)	265 (91%)	27 (9%)	8	27
1	D	269/340 (79%)	244 (91%)	25 (9%)	8	27
1	E	273/340 (80%)	253 (93%)	20 (7%)	13	38
1	F	281/340 (83%)	252 (90%)	29 (10%)	7	23
1	G	283/340 (83%)	258 (91%)	25 (9%)	9	29
1	H	281/340 (83%)	266 (95%)	15 (5%)	20	52
All	All	2240/2720 (82%)	2051 (92%)	189 (8%)	10	31

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	98	GLN
1	A	135	MET
1	A	145	GLU
1	A	154	GLN
1	A	169	GLN
1	A	193	LEU
1	A	210	GLU

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Mol	Chain	Res	Type
1	A	211	ARG
1	A	228	LYS
1	A	244	LYS
1	A	245	GLU
1	A	258	GLN
1	A	321	MET
1	A	323	LYS
1	A	330	CYS
1	A	331	MET
1	A	358	ARG
1	A	372	LEU
1	A	381	MET
1	B	40	LEU
1	B	41	ILE
1	B	147	LEU
1	B	148	SER
1	B	151	SER
1	B	154	GLN
1	B	159	ARG
1	B	165	ILE
1	B	168	LEU
1	B	169	GLN
1	B	183	ASN
1	B	185	LYS
1	B	189	ASN
1	B	211	ARG
1	B	218	HIS
1	B	221	ASN
1	B	230	ILE
1	B	231	THR
1	B	254	VAL
1	B	258	GLN
1	B	270	GLU
1	B	329	VAL
1	B	331	MET
1	B	332	VAL
1	B	336	LEU
1	B	359	TYR
1	B	360	LYS
1	B	376	HIS
1	C	103	ARG
1	C	138	LEU

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Mol	Chain	Res	Type
1	C	145	GLU
1	C	147	LEU
1	C	168	LEU
1	C	170	ASN
1	C	171	MET
1	C	172	ARG
1	C	177	ARG
1	C	187	GLU
1	C	191	LEU
1	C	197	GLN
1	C	218	HIS
1	C	239	ILE
1	C	240	ARG
1	C	245	GLU
1	C	250	LYS
1	C	251	GLU
1	C	252	GLU
1	C	277	LEU
1	C	318	ASP
1	C	319	SER
1	C	329	VAL
1	C	330	CYS
1	C	338	SER
1	C	358	ARG
1	C	359	TYR
1	D	102	VAL
1	D	144	ARG
1	D	145	GLU
1	D	147	LEU
1	D	148	SER
1	D	167	VAL
1	D	168	LEU
1	D	191	LEU
1	D	192	LEU
1	D	228	LYS
1	D	232	ARG
1	D	234	LEU
1	D	257	PHE
1	D	259	LYS
1	D	260	GLN
1	D	329	VAL
1	D	330	CYS

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Mol	Chain	Res	Type
1	D	336	LEU
1	D	358	ARG
1	D	359	TYR
1	D	360	LYS
1	D	361	VAL
1	D	368	LEU
1	D	381	MET
1	D	382	ASN
1	E	102	VAL
1	E	119	SER
1	E	144	ARG
1	E	148	SER
1	E	154	GLN
1	E	157	GLN
1	E	168	LEU
1	E	169	GLN
1	E	187	GLU
1	E	239	ILE
1	E	254	VAL
1	E	256	GLU
1	E	257	PHE
1	E	262	GLU
1	E	277	LEU
1	E	329	VAL
1	E	330	CYS
1	E	331	MET
1	E	359	TYR
1	E	363	VAL
1	F	40	LEU
1	F	41	ILE
1	F	102	VAL
1	F	110	LYS
1	F	113	SER
1	F	145	GLU
1	F	147	LEU
1	F	149	PRO
1	F	153	PHE
1	F	168	LEU
1	F	184	PHE
1	F	187	GLU
1	F	189	ASN
1	F	190	GLU

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Mol	Chain	Res	Type
1	F	191	LEU
1	F	195	SER
1	F	196	GLU
1	F	216	GLU
1	F	236	GLU
1	F	274	GLU
1	F	305	GLN
1	F	325	ARG
1	F	331	MET
1	F	334	ARG
1	F	335	MET
1	F	336	LEU
1	F	358	ARG
1	F	370	THR
1	F	372	LEU
1	G	40	LEU
1	G	41	ILE
1	G	102	VAL
1	G	138	LEU
1	G	145	GLU
1	G	147	LEU
1	G	149	PRO
1	G	154	GLN
1	G	155	SER
1	G	165	ILE
1	G	185	LYS
1	G	188	GLU
1	G	189	ASN
1	G	190	GLU
1	G	191	LEU
1	G	192	LEU
1	G	218	HIS
1	G	250	LYS
1	G	253	GLN
1	G	293	LEU
1	G	331	MET
1	G	358	ARG
1	G	360	LYS
1	G	375	ARG
1	G	376	HIS
1	H	41	ILE
1	H	102	VAL

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Mol	Chain	Res	Type
1	H	106	ARG
1	H	145	GLU
1	H	147	LEU
1	H	151	SER
1	H	189	ASN
1	H	191	LEU
1	H	237	GLU
1	H	329	VAL
1	H	331	MET
1	H	358	ARG
1	H	360	LYS
1	H	363	VAL
1	H	370	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	275	HIS
1	A	382	ASN
1	B	55	GLN
1	B	98	GLN
1	B	99	ASN
1	B	128	GLN
1	B	154	GLN
1	B	169	GLN
1	B	183	ASN
1	B	197	GLN
1	B	218	HIS
1	B	260	GLN
1	B	328	HIS
1	B	376	HIS
1	C	170	ASN
1	C	253	GLN
1	D	116	HIS
1	D	128	GLN
1	D	260	GLN
1	E	128	GLN
1	E	169	GLN
1	E	253	GLN
1	E	333	HIS
1	F	58	GLN

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Mol	Chain	Res	Type
1	F	260	GLN
1	F	290	GLN
1	F	382	ASN
1	G	127	GLN
1	G	128	GLN
1	G	154	GLN
1	G	221	ASN
1	H	127	GLN
1	H	141	ASN
1	H	258	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	306/373 (82%)	-0.22	7 (2%) 61 52	24, 44, 97, 131	0
1	B	296/373 (79%)	0.12	11 (3%) 45 37	29, 65, 129, 148	0
1	C	313/373 (83%)	-0.08	9 (2%) 53 45	36, 59, 101, 138	0
1	D	288/373 (77%)	0.29	12 (4%) 40 32	42, 76, 129, 147	0
1	E	293/373 (78%)	0.09	10 (3%) 48 39	33, 67, 125, 155	0
1	F	303/373 (81%)	0.10	10 (3%) 49 40	31, 66, 119, 143	0
1	G	304/373 (81%)	0.30	14 (4%) 37 29	32, 74, 126, 140	0
1	H	301/373 (80%)	-0.07	10 (3%) 49 40	27, 51, 103, 142	0
All	All	2404/2984 (80%)	0.06	83 (3%) 47 38	24, 62, 120, 155	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	GLY	6.8
1	B	254	VAL	4.4
1	G	335	MET	4.2
1	C	41	ILE	3.8
1	H	336	LEU	3.8
1	C	341	GLY	3.7
1	C	154	GLN	3.6
1	F	243	ALA	3.6
1	D	148	SER	3.3
1	D	152	GLY	3.3
1	F	338	SER	3.0
1	G	299	ARG	3.0
1	H	40	LEU	3.0
1	A	359	TYR	2.9
1	C	359	TYR	2.9
1	G	333	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	147	LEU	2.9
1	G	220	PHE	2.9
1	D	359	TYR	2.9
1	D	168	LEU	2.9
1	H	359	TYR	2.9
1	E	41	ILE	2.8
1	D	336	LEU	2.8
1	G	250	LYS	2.8
1	D	40	LEU	2.8
1	D	334	ARG	2.7
1	E	371	TYR	2.7
1	G	359	TYR	2.7
1	E	337	GLY	2.7
1	F	257	PHE	2.6
1	B	40	LEU	2.6
1	E	239	ILE	2.6
1	B	331	MET	2.6
1	F	153	PHE	2.6
1	G	332	VAL	2.6
1	G	184	PHE	2.6
1	A	333	HIS	2.5
1	E	359	TYR	2.5
1	A	336	LEU	2.5
1	H	251	GLU	2.4
1	F	242	GLN	2.4
1	F	40	LEU	2.4
1	B	241	ILE	2.4
1	E	151	SER	2.4
1	D	329	VAL	2.4
1	C	173	VAL	2.4
1	G	329	VAL	2.4
1	G	222	PHE	2.3
1	H	243	ALA	2.3
1	H	358	ARG	2.3
1	B	328	HIS	2.3
1	D	149	PRO	2.3
1	F	254	VAL	2.3
1	B	234	LEU	2.3
1	D	328	HIS	2.3
1	C	177	ARG	2.3
1	D	331	MET	2.2
1	C	382	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	382	ASN	2.2
1	F	240	ARG	2.2
1	F	143	PHE	2.2
1	F	184	PHE	2.2
1	G	241	ILE	2.2
1	B	151	SER	2.2
1	G	40	LEU	2.2
1	E	253	GLN	2.2
1	G	328	HIS	2.2
1	E	254	VAL	2.2
1	A	150	ALA	2.2
1	G	150	ALA	2.2
1	H	254	VAL	2.1
1	H	142	ASP	2.1
1	B	169	GLN	2.1
1	H	149	PRO	2.1
1	H	193	LEU	2.1
1	A	140	PHE	2.1
1	A	151	SER	2.0
1	A	358	ARG	2.0
1	C	146	TYR	2.0
1	B	148	SER	2.0
1	E	149	PRO	2.0
1	B	238	PHE	2.0
1	B	332	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO	H	401	1/1	0.97	0.13	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.