



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 PM UTC

PDB ID : 3SYV / pdb_00003syv
Title : Crystal structure of mPACSIN 3 F-BAR domain mutant
Authors : Bai, X.
Deposited on : 2011-07-18
Resolution : 3.10 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

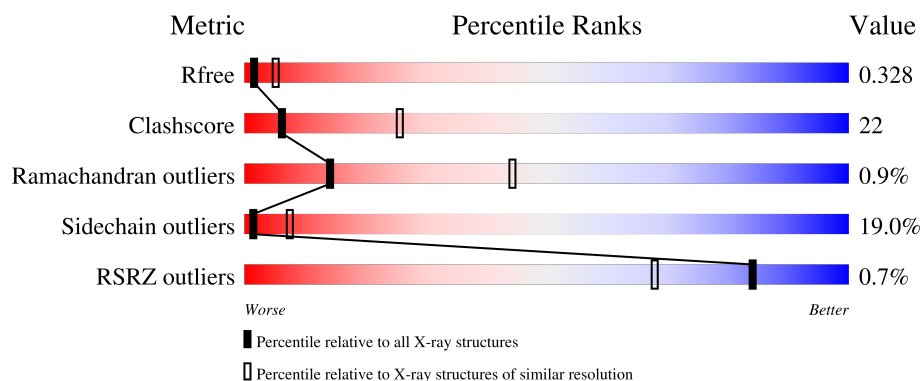
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	347	2% 37% 29% 6% 28%
1	B	347	% 41% 27% 7% 26%
1	C	347	38% 29% 6% 26%
1	D	347	35% 31% 7% 27%
1	E	347	% 33% 32% 8% 27%

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Mol	Chain	Length	Quality of chain
1	F	347	40%24%9%•27%
1	G	347	37%26%9%•27%
1	H	347	38%26%7%29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16470 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 Protein kinase C and casein kinase II substrate protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2047	1284	384	372	7			
1	B	257	Total	C	N	O	S	0	0	0
			2115	1317	403	387	8			
1	C	257	Total	C	N	O	S	0	0	0
			2061	1284	390	379	8			
1	D	255	Total	C	N	O	S	0	0	0
			2085	1304	396	378	7			
1	E	255	Total	C	N	O	S	0	0	1
			2044	1278	387	374	5			
1	F	255	Total	C	N	O	S	0	0	0
			2050	1283	392	369	6			
1	G	254	Total	C	N	O	S	0	0	0
			1978	1231	374	368	5			
1	H	247	Total	C	N	O	S	0	0	0
			1981	1236	378	364	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q99JB8
A	-4	HIS	-	expression tag	UNP Q99JB8
A	-3	HIS	-	expression tag	UNP Q99JB8
A	-2	HIS	-	expression tag	UNP Q99JB8
A	-1	HIS	-	expression tag	UNP Q99JB8
A	0	HIS	-	expression tag	UNP Q99JB8
A	121	GLN	PRO	engineered mutation	UNP Q99JB8
B	-5	HIS	-	expression tag	UNP Q99JB8
B	-4	HIS	-	expression tag	UNP Q99JB8
B	-3	HIS	-	expression tag	UNP Q99JB8
B	-2	HIS	-	expression tag	UNP Q99JB8
B	-1	HIS	-	expression tag	UNP Q99JB8
B	0	HIS	-	expression tag	UNP Q99JB8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	121	GLN	PRO	engineered mutation	UNP Q99JB8
C	-5	HIS	-	expression tag	UNP Q99JB8
C	-4	HIS	-	expression tag	UNP Q99JB8
C	-3	HIS	-	expression tag	UNP Q99JB8
C	-2	HIS	-	expression tag	UNP Q99JB8
C	-1	HIS	-	expression tag	UNP Q99JB8
C	0	HIS	-	expression tag	UNP Q99JB8
C	121	GLN	PRO	engineered mutation	UNP Q99JB8
D	-5	HIS	-	expression tag	UNP Q99JB8
D	-4	HIS	-	expression tag	UNP Q99JB8
D	-3	HIS	-	expression tag	UNP Q99JB8
D	-2	HIS	-	expression tag	UNP Q99JB8
D	-1	HIS	-	expression tag	UNP Q99JB8
D	0	HIS	-	expression tag	UNP Q99JB8
D	121	GLN	PRO	engineered mutation	UNP Q99JB8
E	-5	HIS	-	expression tag	UNP Q99JB8
E	-4	HIS	-	expression tag	UNP Q99JB8
E	-3	HIS	-	expression tag	UNP Q99JB8
E	-2	HIS	-	expression tag	UNP Q99JB8
E	-1	HIS	-	expression tag	UNP Q99JB8
E	0	HIS	-	expression tag	UNP Q99JB8
E	121	GLN	PRO	engineered mutation	UNP Q99JB8
F	-5	HIS	-	expression tag	UNP Q99JB8
F	-4	HIS	-	expression tag	UNP Q99JB8
F	-3	HIS	-	expression tag	UNP Q99JB8
F	-2	HIS	-	expression tag	UNP Q99JB8
F	-1	HIS	-	expression tag	UNP Q99JB8
F	0	HIS	-	expression tag	UNP Q99JB8
F	121	GLN	PRO	engineered mutation	UNP Q99JB8
G	-5	HIS	-	expression tag	UNP Q99JB8
G	-4	HIS	-	expression tag	UNP Q99JB8
G	-3	HIS	-	expression tag	UNP Q99JB8
G	-2	HIS	-	expression tag	UNP Q99JB8
G	-1	HIS	-	expression tag	UNP Q99JB8
G	0	HIS	-	expression tag	UNP Q99JB8
G	121	GLN	PRO	engineered mutation	UNP Q99JB8
H	-5	HIS	-	expression tag	UNP Q99JB8
H	-4	HIS	-	expression tag	UNP Q99JB8
H	-3	HIS	-	expression tag	UNP Q99JB8
H	-2	HIS	-	expression tag	UNP Q99JB8
H	-1	HIS	-	expression tag	UNP Q99JB8
H	0	HIS	-	expression tag	UNP Q99JB8

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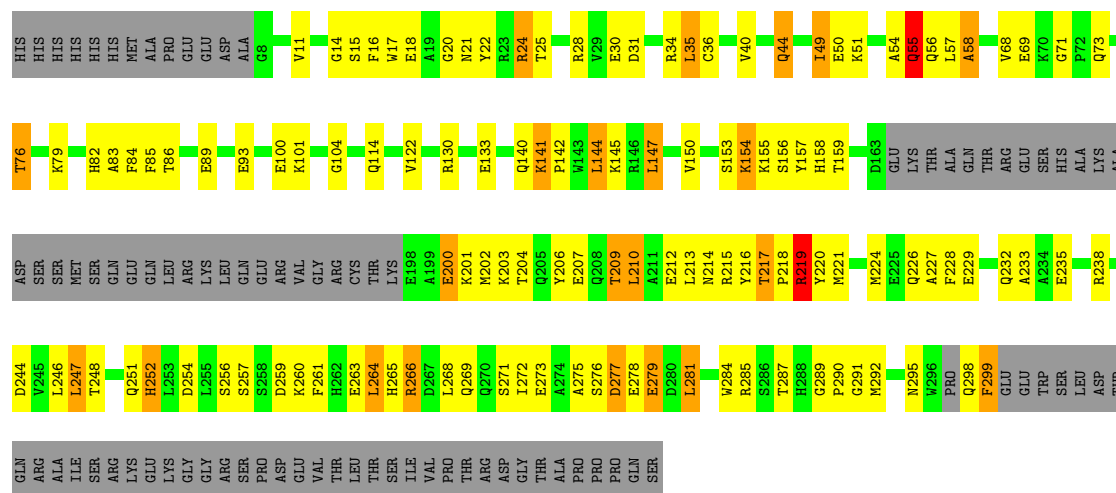
Chain	Residue	Modelled	Actual	Comment	Reference
H	121	GLN	PRO	engineered mutation	UNP Q99JB8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	13	Total O 13 13	0	0
2	C	19	Total O 19 19	0	0
2	D	12	Total O 12 12	0	0
2	E	12	Total O 12 12	0	0
2	F	16	Total O 16 16	0	0
2	G	10	Total O 10 10	0	0
2	H	13	Total O 13 13	0	0

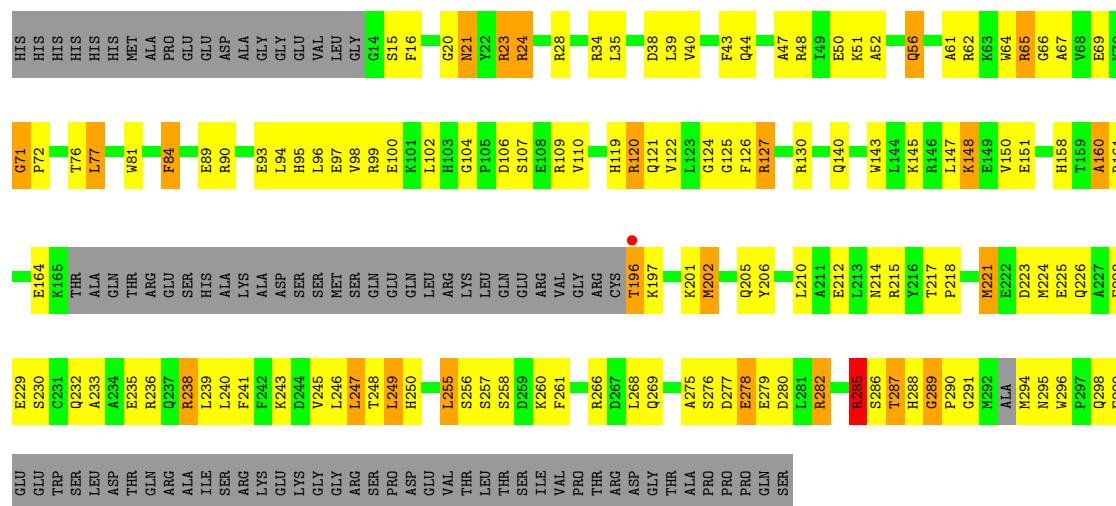
- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain C: 38% 29% 6% • 26%

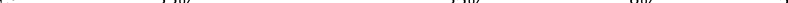


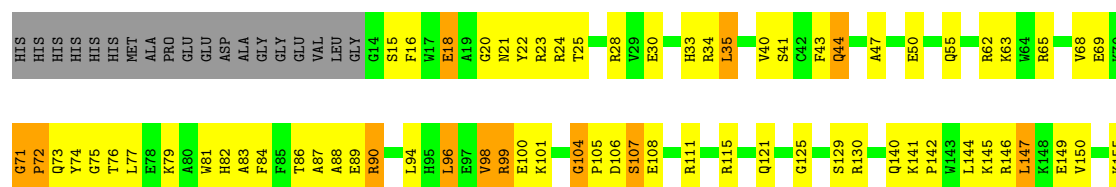
- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

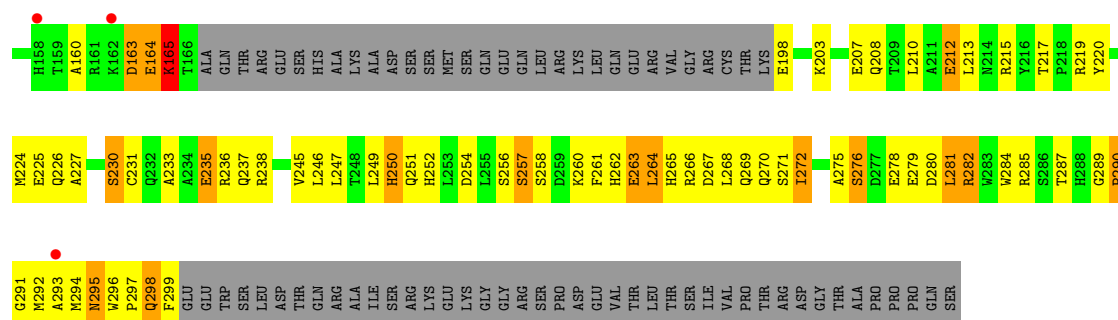
Chain D: 35% 31% 7% 27%



- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

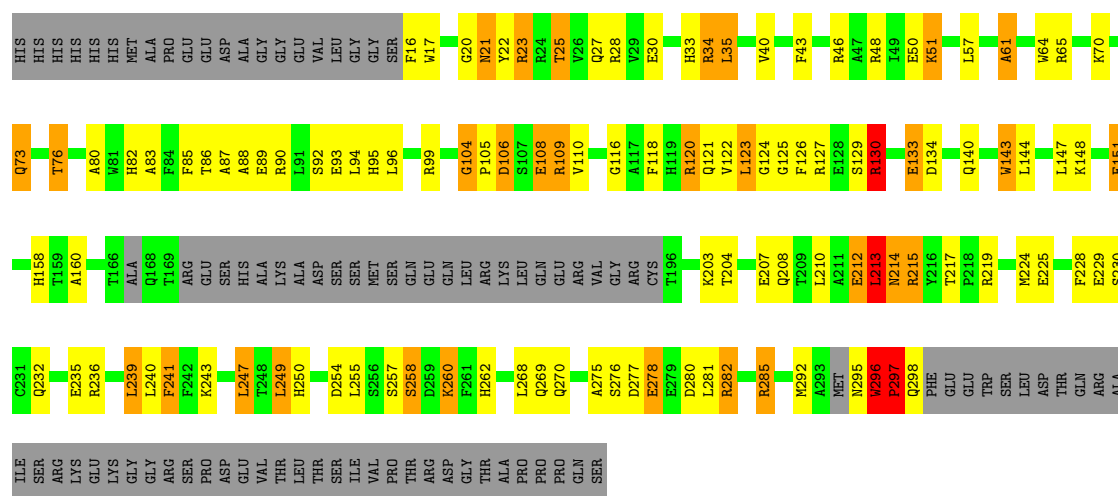
Chain E: 





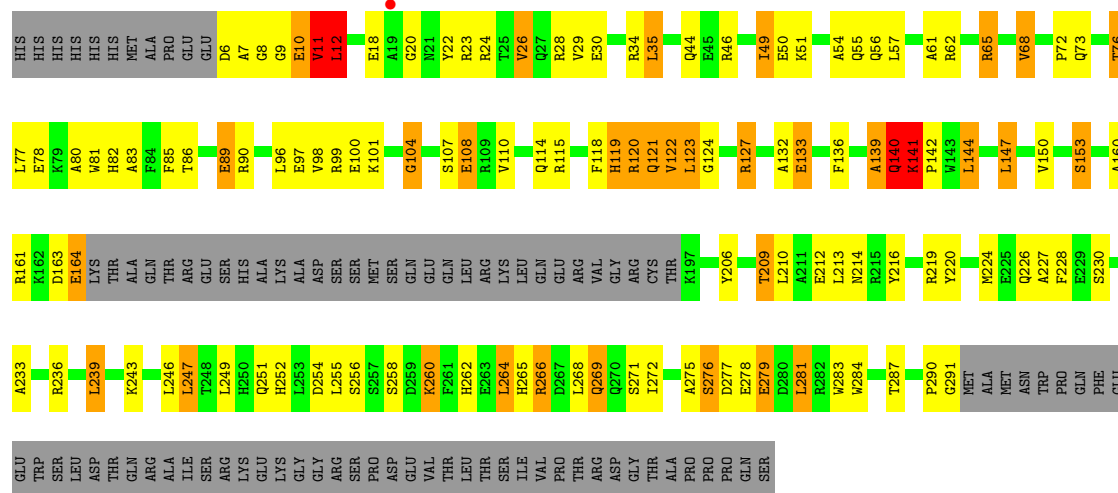
- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain F: 40% 24% 9% 27%



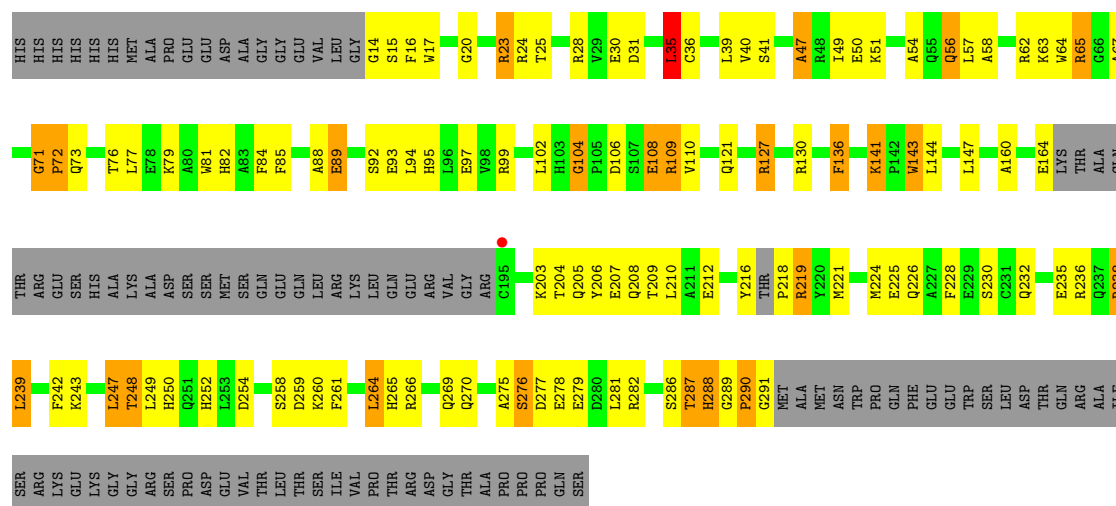
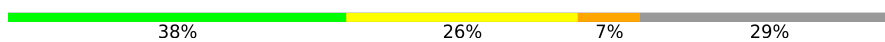
- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain G: 37% 26% 9% 27%



- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.57Å 108.90Å 222.32Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	48.90 – 3.10 48.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.90-3.10) 98.5 (48.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.281 , 0.337 0.274 , 0.328	Depositor DCC
R_{free} test set	5196 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16470	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1201e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.28	7/2094 (0.3%)	1.32	6/2811 (0.2%)
1	B	1.33	7/2160 (0.3%)	1.41	18/2895 (0.6%)
1	C	1.33	9/2104 (0.4%)	1.35	13/2821 (0.5%)
1	D	1.50	14/2133 (0.7%)	1.41	14/2862 (0.5%)
1	E	1.38	14/2092 (0.7%)	1.40	19/2813 (0.7%)
1	F	1.42	9/2097 (0.4%)	1.46	19/2821 (0.7%)
1	G	1.39	15/2021 (0.7%)	1.41	16/2724 (0.6%)
1	H	1.49	13/2025 (0.6%)	1.50	16/2725 (0.6%)
All	All	1.39	88/16726 (0.5%)	1.41	121/22472 (0.5%)

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 (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	160	ALA	C-O	14.15	1.42	1.24
1	H	160	ALA	C-O	10.18	1.37	1.24
1	F	160	ALA	C-O	9.18	1.36	1.24
1	C	156	SER	C-O	9.13	1.35	1.24
1	H	290	PRO	N-CA	8.87	1.58	1.47
1	F	61	ALA	CA-CB	-8.79	1.39	1.53
1	B	61	ALA	CA-CB	-8.31	1.40	1.53
1	B	290	PRO	N-CA	8.31	1.57	1.47
1	H	54	ALA	CA-CB	-7.68	1.41	1.53
1	F	296	TRP	CA-C	7.64	1.60	1.52
1	D	161	ARG	CZ-NH1	7.40	1.43	1.32
1	D	285	ARG	CD-NE	7.33	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	THR	CA-CB	7.25	1.62	1.53
1	D	196	THR	CB-CG2	7.23	1.76	1.52
1	G	160	ALA	C-O	7.01	1.32	1.24
1	C	290	PRO	CA-C	6.97	1.62	1.52
1	E	88	ALA	CA-C	-6.97	1.44	1.52
1	E	121	GLN	CA-CB	6.96	1.64	1.53
1	A	47	ALA	CA-CB	-6.91	1.42	1.53
1	C	68	VAL	CA-CB	6.91	1.63	1.54
1	G	123	LEU	CA-C	6.67	1.61	1.52
1	H	63	LYS	N-CA	-6.52	1.38	1.46
1	H	47	ALA	CA-CB	-6.44	1.42	1.53
1	E	121	GLN	CA-C	6.40	1.61	1.52
1	H	290	PRO	CA-C	6.34	1.61	1.52
1	E	231	CYS	CA-C	6.34	1.60	1.52
1	E	233	ALA	CA-CB	-6.30	1.43	1.53
1	F	108	GLU	CG-CD	6.24	1.67	1.52
1	G	12	LEU	N-CA	6.17	1.54	1.46
1	D	52	ALA	CA-CB	-6.16	1.43	1.53
1	G	124	GLY	N-CA	6.12	1.55	1.45
1	D	289	GLY	N-CA	6.08	1.53	1.44
1	H	108	GLU	CG-CD	6.04	1.67	1.52
1	D	65	ARG	N-CA	-6.01	1.38	1.46
1	E	245	VAL	CA-CB	-5.98	1.47	1.54
1	A	292	MET	N-CA	5.96	1.53	1.45
1	B	43	PHE	CA-C	-5.96	1.44	1.52
1	H	97	GLU	CG-CD	5.92	1.66	1.52
1	A	233	ALA	CA-CB	-5.87	1.44	1.53
1	C	299	PHE	N-CA	5.80	1.57	1.46
1	D	61	ALA	CA-CB	-5.79	1.44	1.53
1	A	59	ASP	CA-C	-5.78	1.45	1.52
1	G	133	GLU	N-CA	-5.78	1.39	1.46
1	B	290	PRO	CA-C	5.71	1.60	1.52
1	E	87	ALA	N-CA	5.71	1.53	1.46
1	F	88	ALA	CA-CB	-5.70	1.44	1.53
1	E	163	ASP	C-O	5.61	1.30	1.24
1	B	290	PRO	C-O	5.61	1.31	1.24
1	G	164	GLU	CA-CB	5.59	1.64	1.53
1	C	68	VAL	N-CA	5.58	1.53	1.46
1	H	164	GLU	C-O	5.58	1.34	1.23
1	C	233	ALA	CA-CB	-5.57	1.44	1.53
1	F	215	ARG	CZ-NH2	5.55	1.40	1.33
1	D	71	GLY	N-CA	5.54	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	123	LEU	N-CA	5.54	1.52	1.46
1	D	233	ALA	CA-CB	-5.51	1.44	1.53
1	H	84	PHE	CA-C	-5.47	1.45	1.52
1	C	58	ALA	CA-CB	-5.46	1.44	1.53
1	E	165	LYS	C-N	5.44	1.41	1.33
1	G	68	VAL	CA-CB	5.43	1.63	1.54
1	G	119	HIS	C-O	5.40	1.29	1.23
1	H	35	LEU	CB-CG	5.37	1.64	1.53
1	G	290	PRO	CA-C	5.36	1.60	1.52
1	G	11	VAL	CA-C	5.36	1.59	1.52
1	G	68	VAL	N-CA	5.34	1.53	1.46
1	A	88	ALA	CA-CB	-5.34	1.45	1.53
1	G	233	ALA	CA-CB	-5.34	1.44	1.53
1	D	84	PHE	CA-C	-5.33	1.45	1.52
1	F	120	ARG	CG-CD	5.32	1.68	1.52
1	F	110	VAL	CA-CB	-5.31	1.48	1.54
1	A	88	ALA	CA-C	-5.28	1.46	1.52
1	B	288	HIS	C-O	5.28	1.30	1.23
1	D	285	ARG	CG-CD	5.27	1.68	1.52
1	E	299	PHE	CA-CB	-5.26	1.43	1.53
1	C	11	VAL	CA-CB	5.26	1.61	1.54
1	E	198	GLU	CA-CB	5.24	1.64	1.53
1	H	291	GLY	N-CA	5.19	1.53	1.45
1	E	250	HIS	CA-C	-5.19	1.46	1.52
1	D	148	LYS	CE-NZ	5.15	1.64	1.49
1	A	87	ALA	CA-CB	-5.13	1.45	1.53
1	B	110	VAL	CA-CB	-5.12	1.47	1.54
1	D	295	ASN	CA-C	5.12	1.60	1.52
1	C	24	ARG	CG-CD	5.12	1.67	1.52
1	G	11	VAL	N-CA	5.11	1.52	1.46
1	E	98	VAL	CA-C	-5.11	1.46	1.52
1	E	291	GLY	CA-C	5.10	1.59	1.51
1	H	72	PRO	N-CA	-5.09	1.43	1.47
1	G	139	ALA	CA-CB	-5.01	1.45	1.53

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	289	GLY	CA-C-N	15.15	138.77	119.84
1	H	289	GLY	C-N-CA	15.15	138.77	119.84
1	B	289	GLY	CA-C-N	11.81	134.61	119.84
1	B	289	GLY	C-N-CA	11.81	134.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	118	PHE	N-CA-C	-11.52	96.94	112.03
1	F	282	ARG	N-CA-C	-9.96	100.39	111.14
1	B	130	ARG	N-CA-C	-9.54	102.15	113.88
1	G	122	VAL	N-CA-C	-9.22	93.74	108.95
1	F	296	TRP	CA-C-N	8.64	130.64	119.84
1	F	296	TRP	C-N-CA	8.64	130.64	119.84
1	G	127	ARG	N-CA-C	-8.11	102.40	111.07
1	B	44	GLN	N-CA-C	-7.92	102.63	111.82
1	G	123	LEU	N-CA-C	7.92	121.64	108.73
1	G	107	SER	N-CA-C	-7.73	102.86	111.28
1	D	104	GLY	CA-C-N	7.63	128.32	119.47
1	D	104	GLY	C-N-CA	7.63	128.32	119.47
1	C	141	LYS	CA-C-N	-7.50	110.46	119.84
1	C	141	LYS	C-N-CA	-7.50	110.46	119.84
1	H	71	GLY	CA-C-N	-7.44	112.04	121.04
1	H	71	GLY	C-N-CA	-7.44	112.04	121.04
1	E	296	TRP	CA-C-N	7.40	129.09	119.84
1	E	296	TRP	C-N-CA	7.40	129.09	119.84
1	D	71	GLY	CA-C-N	-7.38	110.62	119.84
1	D	71	GLY	C-N-CA	-7.38	110.62	119.84
1	F	21	ASN	N-CA-C	7.31	121.89	113.19
1	G	104	GLY	CA-C-N	7.20	128.84	119.84
1	G	104	GLY	C-N-CA	7.20	128.84	119.84
1	B	225	GLU	N-CA-C	-7.09	103.24	110.97
1	G	120	ARG	N-CA-C	-7.05	102.05	113.19
1	B	75	GLY	N-CA-C	7.03	125.09	112.02
1	F	257	SER	N-CA-C	-6.88	103.17	112.26
1	F	104	GLY	CA-C-N	6.85	128.41	119.84
1	F	104	GLY	C-N-CA	6.85	128.41	119.84
1	G	8	GLY	N-CA-C	-6.83	104.37	112.64
1	E	98	VAL	N-CA-C	-6.78	103.88	110.72
1	E	165	LYS	O-C-N	6.72	132.24	122.43
1	A	113	TRP	N-CA-C	-6.69	103.91	111.07
1	E	68	VAL	CB-CA-C	-6.68	102.99	112.22
1	C	104	GLY	CA-C-N	6.63	128.13	119.84
1	C	104	GLY	C-N-CA	6.63	128.13	119.84
1	F	297	PRO	N-CA-C	-6.61	98.84	112.47
1	F	130	ARG	N-CA-C	-6.55	105.92	114.04
1	D	229	GLU	N-CA-C	-6.54	104.14	111.28
1	D	21	ASN	N-CA-C	6.47	120.78	113.01
1	F	214	ASN	N-CA-C	-6.43	104.53	112.38
1	C	219	ARG	N-CA-C	-6.41	104.21	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	VAL	N-CA-C	6.38	117.13	110.62
1	H	127	ARG	N-CA-CB	6.37	119.43	109.94
1	A	104	GLY	CA-C-N	6.36	127.79	119.84
1	A	104	GLY	C-N-CA	6.36	127.79	119.84
1	H	58	ALA	N-CA-C	6.32	118.25	111.36
1	E	104	GLY	CA-C-N	6.21	125.70	119.24
1	E	104	GLY	C-N-CA	6.21	125.70	119.24
1	B	71	GLY	CA-C-N	6.17	127.29	120.45
1	B	71	GLY	C-N-CA	6.17	127.29	120.45
1	F	270	GLN	N-CA-C	6.14	118.78	111.71
1	B	282	ARG	N-CA-C	-6.13	104.52	111.14
1	H	79	LYS	N-CA-C	6.13	118.46	111.11
1	D	127	ARG	N-CA-C	-6.09	104.72	111.36
1	B	229	GLU	N-CA-C	-6.07	104.35	110.97
1	F	90	ARG	N-CA-C	-6.03	104.79	111.36
1	H	136	PHE	N-CA-C	6.02	118.64	111.71
1	F	127	ARG	N-CA-C	-6.00	104.75	111.28
1	G	276	SER	N-CA-C	5.96	118.11	108.34
1	A	123	LEU	N-CA-C	5.93	117.44	110.97
1	H	127	ARG	N-CA-C	-5.89	104.04	111.11
1	G	140	GLN	N-CA-C	5.87	118.15	111.11
1	E	267	ASP	N-CA-C	5.87	117.34	111.07
1	D	48	ARG	N-CA-C	-5.81	105.03	111.71
1	D	122	VAL	N-CA-C	5.81	116.55	110.62
1	E	33	HIS	N-CA-C	-5.73	104.95	111.14
1	E	257	SER	N-CA-C	-5.66	105.69	112.59
1	F	116	GLY	N-CA-C	5.65	120.88	114.67
1	B	104	GLY	CA-C-N	5.64	125.75	119.32
1	B	104	GLY	C-N-CA	5.64	125.75	119.32
1	G	141	LYS	CA-C-N	-5.63	113.22	119.19
1	G	141	LYS	C-N-CA	-5.63	113.22	119.19
1	G	26	VAL	CB-CA-C	-5.63	104.46	112.22
1	F	82	HIS	N-CA-CB	5.58	118.96	110.14
1	E	289	GLY	CA-C-N	5.53	126.75	119.84
1	E	289	GLY	C-N-CA	5.53	126.75	119.84
1	F	134	ASP	N-CA-C	5.52	116.99	110.97
1	C	224	MET	N-CA-C	5.46	117.23	111.28
1	B	43	PHE	N-CA-C	-5.46	107.27	114.31
1	D	291	GLY	N-CA-C	5.45	126.10	113.18
1	H	212	GLU	N-CA-C	5.42	117.94	111.71
1	E	71	GLY	CA-C-N	-5.41	114.49	121.04
1	E	71	GLY	C-N-CA	-5.41	114.49	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	65	ARG	N-CA-C	-5.38	104.46	111.02
1	A	42	CYS	N-CA-C	5.38	117.56	111.11
1	B	89	GLU	N-CA-C	5.36	117.12	111.28
1	D	126	PHE	N-CA-C	5.34	117.78	108.76
1	A	245	VAL	CB-CA-C	-5.34	105.05	112.04
1	B	244	ASP	N-CA-C	5.31	117.48	111.11
1	E	25	THR	N-CA-C	-5.31	105.94	112.90
1	C	85	PHE	N-CA-C	-5.30	105.42	111.14
1	G	122	VAL	CA-C-O	-5.29	116.11	121.67
1	B	90	ARG	N-CA-C	-5.29	105.69	111.82
1	F	285	ARG	N-CA-C	-5.28	105.42	111.07
1	B	72	PRO	N-CA-C	5.26	120.93	114.35
1	C	55	GLN	N-CA-CB	5.26	117.85	110.12
1	E	72	PRO	N-CA-C	-5.23	107.35	114.98
1	H	270	GLN	N-CA-C	5.22	116.66	111.07
1	C	252	HIS	N-CA-C	5.21	117.70	111.71
1	H	276	SER	N-CA-C	5.21	116.90	108.26
1	D	285	ARG	N-CA-CB	5.20	117.69	109.94
1	E	129	SER	N-CA-C	5.18	116.93	111.28
1	E	282	ARG	N-CA-C	-5.17	105.64	111.28
1	F	40	VAL	N-CA-C	-5.15	105.08	112.35
1	D	230	SER	N-CA-C	5.15	117.29	111.11
1	H	282	ARG	N-CA-C	-5.12	105.61	111.14
1	C	122	VAL	N-CA-C	5.10	115.31	110.42
1	B	265	HIS	N-CA-C	-5.09	106.24	112.90
1	D	69	GLU	N-CA-CB	5.05	117.33	110.01
1	G	239	LEU	N-CA-C	5.03	116.76	111.28
1	E	272	ILE	N-CA-C	-5.02	105.60	110.42
1	C	141	LYS	O-C-N	5.02	124.34	120.38
1	F	241	PHE	N-CA-C	-5.01	105.09	111.11
1	C	229	GLU	N-CA-C	5.01	116.43	111.07
1	H	104	GLY	CA-C-N	5.01	125.03	119.32
1	H	104	GLY	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	160	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2047	0	1943	94	0
1	B	2115	0	2020	80	0
1	C	2061	0	1930	106	0
1	D	2085	0	1982	115	0
1	E	2044	0	1900	117	0
1	F	2050	0	1898	96	0
1	G	1978	0	1807	95	0
1	H	1981	0	1827	93	0
2	A	14	0	0	1	0
2	B	13	0	0	2	0
2	C	19	0	0	0	0
2	D	12	0	0	3	0
2	E	12	0	0	0	0
2	F	16	0	0	2	0
2	G	10	0	0	0	0
2	H	13	0	0	1	0
All	All	16470	0	15307	709	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 22.

All (709) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:THR:CB	1:D:196:THR:CG2	1.76	1.59
1:D:121:GLN:HE22	1:D:130:ARG:CD	1.42	1.33
1:D:121:GLN:NE2	1:D:130:ARG:HD3	1.46	1.30
1:E:76:THR:CG2	1:E:275:ALA:HA	1.69	1.23
1:A:76:THR:CG2	1:A:275:ALA:HA	1.74	1.18
1:G:276:SER:HB3	1:G:279:GLU:HB2	1.21	1.14
1:B:229:GLU:OE1	1:B:229:GLU:OE2	1.69	1.10
1:D:120:ARG:H	1:D:120:ARG:HD3	1.08	1.09
1:E:76:THR:HG21	1:E:275:ALA:HA	1.28	1.08
1:H:216:TYR:C	1:H:218:PRO:HD2	1.78	1.06
1:H:76:THR:CG2	1:H:275:ALA:HA	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:GLN:HE22	1:H:130:ARG:HD2	1.21	1.04
1:H:76:THR:HG21	1:H:275:ALA:HA	1.36	1.02
1:A:76:THR:HG22	1:A:275:ALA:HA	1.41	1.01
1:A:247:LEU:O	1:A:251:GLN:HG2	1.60	1.00
1:F:260:LYS:HB2	1:F:260:LYS:NZ	1.78	0.99
1:A:76:THR:HG21	1:A:275:ALA:HA	1.45	0.98
1:G:272:ILE:HG21	1:H:247:LEU:HD13	1.44	0.97
1:D:120:ARG:HA	1:D:125:GLY:O	1.64	0.97
1:H:121:GLN:HE22	1:H:130:ARG:CD	1.78	0.97
1:A:235:GLU:CG	1:A:238:ARG:HH21	1.77	0.96
1:C:35:LEU:HD11	1:D:72:PRO:HD2	1.42	0.96
1:D:121:GLN:HE22	1:D:130:ARG:HD3	0.79	0.95
1:D:120:ARG:H	1:D:120:ARG:CD	1.79	0.93
1:E:76:THR:HG22	1:E:275:ALA:HA	1.47	0.92
1:G:276:SER:CB	1:G:279:GLU:HB2	2.00	0.91
1:F:296:TRP:HE3	1:F:296:TRP:N	1.70	0.90
1:H:121:GLN:NE2	1:H:130:ARG:HD2	1.87	0.90
1:C:268:LEU:HD23	1:D:250:HIS:CD2	2.06	0.90
1:F:260:LYS:HB2	1:F:260:LYS:HZ3	1.34	0.90
1:G:65:ARG:NH2	1:G:82:HIS:HB3	1.87	0.90
1:G:136:PHE:HD1	1:G:224:MET:HE3	1.34	0.89
1:F:151:GLU:OE2	1:F:151:GLU:HA	1.73	0.88
1:C:266:ARG:HH11	1:C:269:GLN:NE2	1.71	0.88
1:F:296:TRP:HE3	1:F:296:TRP:H	0.92	0.88
1:G:20:GLY:HA2	1:G:22:TYR:CE1	2.10	0.87
1:C:292:MET:H	1:C:292:MET:HE2	1.40	0.85
1:H:31:ASP:O	1:H:35:LEU:HD23	1.76	0.85
1:C:101:LYS:HD2	1:C:252:HIS:CD2	2.12	0.85
1:H:261:PHE:O	1:H:264:LEU:CD2	2.25	0.84
1:C:76:THR:HB	1:C:275:ALA:HA	1.56	0.84
1:F:76:THR:HG23	1:F:275:ALA:HA	1.58	0.84
1:H:264:LEU:HD23	1:H:265:HIS:H	1.43	0.84
1:E:76:THR:HG21	1:E:275:ALA:CA	2.06	0.83
1:C:295:ASN:O	1:C:298:GLN:N	2.11	0.83
1:D:202:MET:HE2	1:D:202:MET:HA	1.59	0.83
1:G:276:SER:HB3	1:G:279:GLU:CB	2.08	0.83
1:E:73:GLN:HE21	1:E:81:TRP:HE3	1.27	0.82
1:C:276:SER:HB3	1:C:279:GLU:HB2	1.61	0.82
1:E:235:GLU:HA	1:E:235:GLU:OE1	1.78	0.82
1:G:163:ASP:CB	1:G:164:GLU:CB	2.59	0.81
1:A:290:PRO:C	1:A:292:MET:H	1.85	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ARG:CG	1:D:24:ARG:HH11	1.92	0.81
1:C:228:PHE:HE2	1:C:232:GLN:HE21	1.26	0.81
1:D:282:ARG:HG2	1:D:282:ARG:HH11	1.45	0.80
1:F:123:LEU:H	1:F:123:LEU:HD23	1.46	0.80
1:G:11:VAL:O	1:G:12:LEU:C	2.25	0.80
1:D:120:ARG:HD3	1:D:120:ARG:N	1.94	0.79
1:E:268:LEU:HD23	1:F:250:HIS:CD2	2.17	0.79
1:F:76:THR:HB	1:F:280:ASP:OD1	1.83	0.79
1:B:254:ASP:OD1	1:B:256:SER:HB3	1.82	0.78
1:G:163:ASP:CA	1:G:164:GLU:CB	2.61	0.78
1:G:101:LYS:HD2	1:G:252:HIS:CD2	2.18	0.78
1:D:94:LEU:O	1:D:98:VAL:HG23	1.83	0.78
1:D:277:ASP:OD2	1:D:278:GLU:N	2.17	0.78
1:E:71:GLY:HA2	2:F:345:HOH:O	1.82	0.78
1:F:212:GLU:OE2	1:F:212:GLU:C	2.26	0.78
1:C:24:ARG:HD3	1:D:288:HIS:ND1	1.99	0.78
1:E:65:ARG:CZ	1:E:82:HIS:HB3	2.14	0.77
1:B:40:VAL:O	1:B:44:GLN:HG3	1.83	0.77
1:G:76:THR:HB	1:G:275:ALA:HA	1.67	0.77
1:A:290:PRO:C	1:A:292:MET:N	2.42	0.77
1:G:163:ASP:HA	1:G:164:GLU:CB	2.15	0.76
1:G:216:TYR:O	1:G:219:ARG:HB3	1.86	0.76
1:C:266:ARG:NH1	1:C:269:GLN:NE2	2.33	0.76
1:F:123:LEU:H	1:F:123:LEU:CD2	1.99	0.76
1:D:121:GLN:NE2	1:D:130:ARG:CD	2.23	0.76
1:G:281:LEU:HD23	1:H:236:ARG:NH2	2.01	0.76
1:H:264:LEU:HD23	1:H:265:HIS:N	2.00	0.76
1:H:51:LYS:HB2	1:H:99:ARG:HG3	1.66	0.75
1:A:293:ALA:O	1:B:15:SER:HA	1.86	0.75
1:C:16:PHE:CD1	1:D:289:GLY:HA2	2.22	0.75
1:B:258:SER:O	1:B:262:HIS:HD2	1.69	0.75
1:E:76:THR:HG21	1:E:276:SER:N	2.02	0.74
1:C:268:LEU:CD2	1:D:250:HIS:CD2	2.71	0.73
1:F:76:THR:CG2	1:F:275:ALA:HA	2.18	0.73
1:C:141:LYS:O	1:C:142:PRO:C	2.30	0.73
1:E:76:THR:HG21	1:E:276:SER:H	1.52	0.73
1:C:49:ILE:HG23	1:D:56:GLN:HG2	1.70	0.73
1:H:287:THR:HB	1:H:288:HIS:HD2	1.53	0.73
1:C:28:ARG:NH1	1:C:235:GLU:HG2	2.04	0.73
1:B:43:PHE:CZ	1:B:249:LEU:HD13	2.23	0.73
1:F:296:TRP:N	1:F:296:TRP:CE3	2.49	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:THR:HG22	1:H:275:ALA:HA	1.69	0.73
1:C:14:GLY:O	1:C:18:GLU:HB2	1.89	0.73
1:E:264:LEU:HD12	1:E:264:LEU:C	2.14	0.72
1:C:200:GLU:OE1	1:C:200:GLU:HA	1.90	0.72
1:E:235:GLU:OE1	1:E:235:GLU:CA	2.38	0.72
1:E:295:ASN:O	1:E:297:PRO:HD3	1.90	0.72
1:G:73:GLN:NE2	1:G:81:TRP:HE3	1.88	0.71
1:A:235:GLU:CG	1:A:238:ARG:NH2	2.51	0.71
1:D:121:GLN:HE22	1:D:130:ARG:HD2	1.50	0.71
1:F:27:GLN:HA	1:F:30:GLU:OE2	1.90	0.71
1:A:258:SER:O	1:A:262:HIS:CD2	2.43	0.71
1:E:96:LEU:O	1:E:96:LEU:HD12	1.90	0.70
1:G:85:PHE:O	1:G:89:GLU:HG2	1.91	0.70
1:G:140:GLN:HG2	1:G:220:TYR:HE1	1.55	0.70
1:A:99:ARG:NH1	1:A:103:HIS:CD2	2.58	0.70
1:F:258:SER:O	1:F:262:HIS:HD2	1.74	0.70
1:H:89:GLU:O	1:H:92:SER:HB3	1.91	0.70
1:A:270:GLN:HG2	2:A:347:HOH:O	1.90	0.70
1:C:285:ARG:CZ	1:D:225:GLU:OE2	2.40	0.70
1:D:202:MET:HE2	1:D:202:MET:CA	2.22	0.70
1:C:28:ARG:HH11	1:C:235:GLU:HG2	1.57	0.70
1:E:40:VAL:O	1:E:44:GLN:HB2	1.92	0.70
1:A:268:LEU:HD23	1:B:250:HIS:CD2	2.26	0.70
1:D:24:ARG:HH11	1:D:24:ARG:HG2	1.56	0.70
1:H:216:TYR:O	1:H:218:PRO:HD2	1.92	0.69
1:E:264:LEU:HD12	1:E:265:HIS:N	2.07	0.69
1:F:20:GLY:O	1:F:23:ARG:HD2	1.92	0.69
1:A:24:ARG:HD2	1:B:288:HIS:ND1	2.08	0.69
1:B:285:ARG:C	1:B:288:HIS:O	2.36	0.69
1:C:14:GLY:C	1:C:18:GLU:HB2	2.17	0.69
1:F:235:GLU:HG3	1:F:239:LEU:HD22	1.75	0.69
1:H:136:PHE:HD1	1:H:224:MET:HE3	1.58	0.69
1:F:121:GLN:CD	1:F:130:ARG:HE	2.00	0.68
1:A:76:THR:N	1:A:280:ASP:OD1	2.21	0.68
1:C:299:PHE:C	1:D:214:ASN:OD1	2.36	0.68
1:F:76:THR:HG21	1:F:276:SER:H	1.59	0.68
1:F:213:LEU:HD12	1:F:213:LEU:C	2.17	0.68
1:G:150:VAL:HG22	1:G:209:THR:HG23	1.76	0.68
1:G:115:ARG:O	1:G:119:HIS:CB	2.41	0.68
1:D:40:VAL:HG13	1:D:107:SER:HB3	1.74	0.68
1:H:235:GLU:OE1	1:H:238:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLN:HE22	1:B:130:ARG:HD2	1.59	0.68
1:F:212:GLU:OE2	1:F:212:GLU:CA	2.41	0.68
1:E:76:THR:N	1:E:280:ASP:OD1	2.26	0.68
1:G:266:ARG:NH1	1:G:269:GLN:HE21	1.90	0.68
1:F:260:LYS:NZ	1:F:260:LYS:CB	2.57	0.67
1:C:247:LEU:O	1:C:251:GLN:HG3	1.95	0.67
1:D:39:LEU:HD21	1:D:245:VAL:HG11	1.75	0.67
1:B:20:GLY:HA2	1:B:22:TYR:CE1	2.30	0.67
1:D:282:ARG:HH11	1:D:282:ARG:CG	2.08	0.67
1:C:281:LEU:HD21	1:D:236:ARG:HB2	1.77	0.66
1:E:272:ILE:CG2	1:F:247:LEU:HD13	2.25	0.66
1:C:228:PHE:CE2	1:C:232:GLN:NE2	2.63	0.66
1:F:120:ARG:HA	1:F:125:GLY:O	1.95	0.66
1:H:143:TRP:CD1	1:H:143:TRP:C	2.74	0.66
1:A:18:GLU:OE1	1:B:294:MET:SD	2.53	0.66
1:E:101:LYS:HD3	1:E:252:HIS:CE1	2.30	0.66
1:A:238:ARG:HH12	1:B:73:GLN:HE22	1.44	0.66
1:E:62:ARG:HG3	1:E:63:LYS:N	2.10	0.66
1:F:213:LEU:C	1:F:213:LEU:CD1	2.69	0.66
1:C:28:ARG:NH1	1:C:235:GLU:CG	2.58	0.65
1:H:287:THR:HB	1:H:288:HIS:CD2	2.30	0.65
1:A:292:MET:HG2	1:A:293:ALA:N	2.11	0.65
1:B:222:GLU:OE2	1:B:222:GLU:HA	1.96	0.65
1:C:254:ASP:OD2	1:C:254:ASP:C	2.39	0.65
1:A:260:LYS:O	1:A:263:GLU:HG2	1.96	0.65
1:A:26:VAL:O	1:A:29:VAL:HG23	1.96	0.65
1:E:76:THR:O	1:E:79:LYS:HB2	1.97	0.65
1:G:73:GLN:HE21	1:G:81:TRP:HE3	1.43	0.65
1:F:203:LYS:O	1:F:207:GLU:HG2	1.96	0.65
1:D:34:ARG:NH2	2:D:348:HOH:O	2.30	0.65
1:D:147:LEU:HD23	1:D:147:LEU:O	1.97	0.65
1:D:294:MET:O	1:D:294:MET:SD	2.53	0.65
1:F:204:THR:O	1:F:208:GLN:HG3	1.97	0.65
1:C:140:GLN:HG3	1:C:220:TYR:HE1	1.61	0.65
1:C:292:MET:HE2	1:C:292:MET:N	2.09	0.65
1:C:28:ARG:HH11	1:C:235:GLU:CG	2.10	0.65
1:C:266:ARG:HH11	1:C:269:GLN:HE21	1.43	0.64
1:A:99:ARG:HH12	1:A:103:HIS:CD2	2.15	0.64
1:H:248:THR:HG22	1:H:252:HIS:CE1	2.33	0.64
1:A:259:ASP:O	1:A:260:LYS:C	2.39	0.64
1:C:141:LYS:HD3	1:C:142:PRO:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:GLN:NE2	1:G:81:TRP:CE3	2.66	0.64
1:F:147:LEU:HD12	1:F:147:LEU:O	1.98	0.64
1:H:99:ARG:C	1:H:99:ARG:HD3	2.23	0.64
1:D:99:ARG:HD3	1:D:99:ARG:C	2.23	0.64
1:F:225:GLU:OE1	1:F:229:GLU:OE2	2.16	0.63
1:F:121:GLN:NE2	1:F:130:ARG:HE	1.94	0.63
1:G:120:ARG:O	1:G:121:GLN:C	2.39	0.63
1:D:76:THR:CG2	1:D:275:ALA:HA	2.28	0.63
1:G:6:ASP:HA	1:G:214:ASN:HD22	1.63	0.63
1:G:147:LEU:HD13	1:G:147:LEU:O	1.99	0.63
1:D:24:ARG:CG	1:D:24:ARG:NH1	2.57	0.63
1:C:235:GLU:CD	1:C:238:ARG:HH21	2.07	0.62
1:B:73:GLN:OE1	1:B:77:LEU:HD23	2.00	0.62
1:C:232:GLN:HE21	1:D:285:ARG:HG3	1.64	0.62
1:G:254:ASP:OD1	1:G:256:SER:N	2.33	0.62
1:G:51:LYS:O	1:G:54:ALA:HB3	2.00	0.62
1:G:136:PHE:CD1	1:G:224:MET:HE3	2.26	0.62
1:H:216:TYR:O	1:H:218:PRO:CD	2.48	0.62
1:F:94:LEU:HD11	1:F:260:LYS:HG2	1.82	0.61
1:G:49:ILE:HD13	1:H:56:GLN:HG2	1.80	0.61
1:G:20:GLY:O	1:G:23:ARG:HG3	2.00	0.61
1:F:123:LEU:CD2	1:F:123:LEU:N	2.61	0.61
1:C:266:ARG:NH1	1:C:269:GLN:HE22	1.97	0.61
1:G:139:ALA:O	1:G:142:PRO:HD2	2.01	0.61
1:H:20:GLY:O	1:H:23:ARG:HB2	2.00	0.61
1:C:17:TRP:CZ2	1:D:290:PRO:HB3	2.36	0.61
1:C:154:LYS:HG2	1:C:206:TYR:CE1	2.35	0.61
1:E:272:ILE:HG21	1:F:247:LEU:HD13	1.82	0.60
1:G:272:ILE:CG2	1:H:247:LEU:HD13	2.27	0.60
1:G:277:ASP:OD2	1:G:277:ASP:N	2.34	0.60
1:A:96:LEU:HD12	1:A:96:LEU:O	2.02	0.60
1:B:61:ALA:O	1:B:65:ARG:HB2	2.01	0.60
1:D:65:ARG:NE	2:D:352:HOH:O	2.35	0.60
1:D:121:GLN:CD	1:D:130:ARG:HD3	2.21	0.60
1:C:140:GLN:HG3	1:C:220:TYR:CE1	2.37	0.59
1:D:235:GLU:OE2	1:D:238:ARG:HD3	2.01	0.59
1:A:157:TYR:CZ	1:A:203:LYS:HG3	2.37	0.59
1:B:202:MET:O	1:B:205:GLN:HG2	2.02	0.59
1:G:239:LEU:HD23	1:H:77:LEU:HD23	1.84	0.59
1:B:121:GLN:NE2	1:B:130:ARG:HD2	2.17	0.59
1:C:289:GLY:O	1:C:292:MET:CE	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ALA:N	1:F:16:PHE:CB	2.64	0.59
1:B:235:GLU:HG3	1:B:239:LEU:HD22	1.84	0.59
1:C:31:ASP:OD1	1:C:34:ARG:NH2	2.35	0.59
1:C:264:LEU:HD12	1:C:265:HIS:N	2.17	0.59
1:E:292:MET:O	1:E:294:MET:N	2.36	0.59
1:F:143:TRP:CD1	1:F:143:TRP:C	2.79	0.59
1:B:42:CYS:O	1:B:42:CYS:SG	2.60	0.59
1:B:222:GLU:OE2	1:B:222:GLU:CA	2.50	0.59
1:B:283:TRP:CZ2	1:B:287:THR:HG21	2.37	0.58
1:C:269:GLN:O	1:C:273:GLU:HG3	2.03	0.58
1:F:92:SER:OG	1:F:93:GLU:N	2.36	0.58
1:C:40:VAL:O	1:C:44:GLN:HB2	2.03	0.58
1:C:289:GLY:N	1:C:292:MET:HE1	2.18	0.58
1:D:39:LEU:CD2	1:D:245:VAL:HG11	2.33	0.58
1:D:51:LYS:HB2	1:D:99:ARG:HG3	1.84	0.58
1:E:96:LEU:O	1:E:96:LEU:CD1	2.51	0.58
1:H:206:TYR:CZ	1:H:210:LEU:HD12	2.38	0.58
1:E:258:SER:HB3	1:E:261:PHE:CB	2.34	0.58
1:H:204:THR:HG22	1:H:208:GLN:HE21	1.69	0.58
1:D:217:THR:O	1:D:221:MET:HG3	2.04	0.58
1:G:46:ARG:NE	1:G:50:GLU:OE2	2.31	0.58
1:G:20:GLY:O	1:G:23:ARG:CG	2.52	0.57
1:G:141:LYS:HB3	1:G:142:PRO:HD3	1.84	0.57
1:C:157:TYR:CE1	1:C:203:LYS:HB2	2.38	0.57
1:A:103:HIS:CG	1:A:103:HIS:O	2.56	0.57
1:E:106:ASP:OD1	1:E:252:HIS:CE1	2.58	0.57
1:E:163:ASP:HB3	1:E:164:GLU:OE2	2.04	0.57
1:G:80:ALA:O	1:G:83:ALA:HB3	2.04	0.57
1:H:205:GLN:O	1:H:209:THR:HG23	2.05	0.57
1:A:28:ARG:NH2	1:A:232:GLN:OE1	2.38	0.57
1:A:40:VAL:O	1:A:44:GLN:HB2	2.03	0.57
1:C:272:ILE:HG21	1:D:247:LEU:CD1	2.35	0.57
1:G:260:LYS:O	1:G:264:LEU:HB3	2.03	0.57
1:A:76:THR:HG21	1:A:275:ALA:CA	2.26	0.57
1:E:106:ASP:OD1	1:E:252:HIS:ND1	2.38	0.57
1:G:77:LEU:HD22	1:H:239:LEU:HD12	1.86	0.57
1:A:140:GLN:HG3	1:A:220:TYR:CE1	2.40	0.57
1:E:275:ALA:O	1:F:243:LYS:NZ	2.36	0.57
1:D:20:GLY:O	1:D:23:ARG:HB2	2.04	0.56
1:C:71:GLY:HA2	2:D:348:HOH:O	2.05	0.56
1:D:298:GLN:O	1:D:299:PHE:CB	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG23	1:B:56:GLN:HG2	1.88	0.56
1:D:24:ARG:NH1	1:D:24:ARG:HG3	2.20	0.56
1:G:6:ASP:CA	1:G:214:ASN:HD22	2.16	0.56
1:H:39:LEU:HD22	1:H:242:PHE:CE1	2.40	0.56
1:E:73:GLN:NE2	1:E:81:TRP:HE3	1.99	0.56
1:E:293:ALA:N	1:F:16:PHE:HB3	2.21	0.56
1:B:54:ALA:O	1:B:92:SER:HB2	2.05	0.56
1:G:68:VAL:HG21	1:G:81:TRP:CE2	2.40	0.56
1:G:72:PRO:HG2	1:H:35:LEU:HD21	1.88	0.56
1:G:35:LEU:HD11	1:H:72:PRO:HD2	1.86	0.56
1:H:136:PHE:CD1	1:H:224:MET:HE3	2.38	0.56
1:C:28:ARG:NH1	1:C:235:GLU:CB	2.69	0.56
1:F:212:GLU:OE2	1:F:212:GLU:HA	2.06	0.56
1:G:161:ARG:O	1:G:164:GLU:CB	2.54	0.56
1:C:272:ILE:HG21	1:D:247:LEU:HD13	1.89	0.56
1:B:203:LYS:HA	1:B:206:TYR:HB3	1.88	0.55
1:D:76:THR:HG21	1:D:275:ALA:HA	1.87	0.55
1:A:272:ILE:HG21	1:B:247:LEU:HD23	1.88	0.55
1:H:121:GLN:CD	1:H:130:ARG:HD2	2.31	0.55
1:B:277:ASP:OD2	1:B:278:GLU:N	2.40	0.55
1:A:51:LYS:O	1:A:55:GLN:HG2	2.07	0.55
1:D:287:THR:HB	1:D:288:HIS:HD2	1.71	0.55
1:E:15:SER:HA	1:F:292:MET:SD	2.47	0.55
1:E:35:LEU:HD23	1:F:73:GLN:HE21	1.71	0.55
1:F:23:ARG:NH2	1:F:133:GLU:OE1	2.39	0.55
1:C:147:LEU:HD12	1:C:147:LEU:O	2.07	0.55
1:E:263:GLU:HG3	1:E:264:LEU:N	2.22	0.55
1:B:264:LEU:C	1:B:264:LEU:HD23	2.31	0.55
1:E:281:LEU:HD23	1:F:236:ARG:NH2	2.22	0.55
1:E:298:GLN:H	1:E:298:GLN:HE21	1.55	0.55
1:F:121:GLN:OE1	1:F:130:ARG:NE	2.40	0.55
1:C:292:MET:HE3	1:D:16:PHE:HB2	1.88	0.54
1:G:268:LEU:HD23	1:H:250:HIS:CD2	2.42	0.54
1:H:94:LEU:HG	1:H:260:LYS:HD3	1.88	0.54
1:C:275:ALA:O	1:D:243:LYS:NZ	2.41	0.54
1:F:34:ARG:NH2	2:F:345:HOH:O	2.41	0.54
1:A:140:GLN:HG3	1:A:220:TYR:HE1	1.73	0.54
1:B:206:TYR:CD2	1:B:207:GLU:HG3	2.43	0.54
1:E:278:GLU:OE2	1:E:278:GLU:HA	2.07	0.54
1:C:153:SER:HB2	1:C:209:THR:HG21	1.89	0.54
1:H:121:GLN:HE22	1:H:130:ARG:CG	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ALA:O	1:C:228:PHE:C	2.51	0.54
1:A:35:LEU:HD13	1:B:73:GLN:HE21	1.73	0.53
1:A:96:LEU:O	1:A:96:LEU:CD1	2.56	0.53
1:G:140:GLN:OE1	1:G:144:LEU:HD11	2.07	0.53
1:C:150:VAL:HG22	1:C:209:THR:HG23	1.89	0.53
1:H:35:LEU:O	1:H:36:CYS:C	2.51	0.53
1:H:261:PHE:O	1:H:264:LEU:HD22	2.08	0.53
1:B:16:PHE:CG	1:B:16:PHE:O	2.61	0.53
1:B:242:PHE:O	1:B:243:LYS:C	2.52	0.53
1:H:89:GLU:O	1:H:93:GLU:HG3	2.08	0.53
1:D:202:MET:HA	1:D:202:MET:CE	2.36	0.53
1:F:30:GLU:OE1	1:F:129:SER:CB	2.57	0.53
1:G:264:LEU:C	1:G:264:LEU:HD23	2.33	0.53
1:B:121:GLN:OE1	1:B:130:ARG:HD2	2.08	0.53
1:H:259:ASP:O	1:H:260:LYS:C	2.52	0.53
1:E:150:VAL:HG21	1:E:213:LEU:HG	1.91	0.53
1:H:24:ARG:NH2	2:H:346:HOH:O	2.41	0.53
1:A:247:LEU:HG	1:B:272:ILE:HG21	1.90	0.53
1:F:108:GLU:O	1:F:109:ARG:C	2.51	0.53
1:G:243:LYS:NZ	1:H:275:ALA:O	2.34	0.53
1:A:94:LEU:O	1:A:98:VAL:HG23	2.08	0.53
1:A:298:GLN:O	1:A:299:PHE:CB	2.56	0.53
1:G:140:GLN:HG2	1:G:220:TYR:CE1	2.41	0.53
1:A:157:TYR:CE1	1:A:203:LYS:HG3	2.44	0.52
1:C:20:GLY:HA2	1:C:22:TYR:CE1	2.43	0.52
1:G:7:ALA:N	1:G:214:ASN:ND2	2.57	0.52
1:B:205:GLN:HG3	1:B:206:TYR:N	2.23	0.52
1:F:51:LYS:HB2	1:F:99:ARG:HG3	1.90	0.52
1:A:268:LEU:O	1:A:269:GLN:C	2.53	0.52
1:D:205:GLN:HG3	1:D:206:TYR:N	2.23	0.52
1:E:108:GLU:OE2	1:E:111:ARG:HD2	2.10	0.52
1:F:260:LYS:HB2	1:F:260:LYS:HZ2	1.68	0.52
1:A:278:GLU:HA	1:A:278:GLU:OE2	2.09	0.52
1:G:283:TRP:O	1:G:284:TRP:C	2.53	0.52
1:C:232:GLN:NE2	1:D:285:ARG:HG3	2.24	0.52
1:A:256:SER:O	1:A:262:HIS:HE1	1.93	0.52
1:C:206:TYR:O	1:C:209:THR:HG22	2.09	0.52
1:D:102:LEU:N	1:D:102:LEU:HD12	2.24	0.52
1:H:143:TRP:CD1	1:H:144:LEU:N	2.78	0.52
1:H:216:TYR:C	1:H:218:PRO:CD	2.68	0.52
1:H:254:ASP:OD1	1:H:254:ASP:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD2	1:A:252:HIS:ND1	2.41	0.52
1:C:289:GLY:C	1:C:291:GLY:H	2.18	0.52
1:C:284:TRP:O	1:C:285:ARG:C	2.51	0.51
1:E:125:GLY:H	1:E:130:ARG:HH21	1.58	0.51
1:H:47:ALA:HB1	1:H:99:ARG:HG2	1.93	0.51
1:H:261:PHE:O	1:H:264:LEU:HD23	2.09	0.51
1:H:264:LEU:HD21	1:H:265:HIS:CD2	2.45	0.51
1:D:202:MET:HE2	1:D:202:MET:N	2.25	0.51
1:D:217:THR:HB	1:D:218:PRO:HD3	1.93	0.51
1:E:258:SER:C	1:E:262:HIS:CD2	2.89	0.51
1:E:264:LEU:C	1:E:264:LEU:CD1	2.84	0.51
1:E:298:GLN:NE2	1:E:298:GLN:O	2.43	0.51
1:F:277:ASP:OD2	1:F:278:GLU:N	2.43	0.51
1:A:55:GLN:O	1:A:58:ALA:HB3	2.10	0.51
1:B:223:ASP:O	1:B:226:GLN:HB2	2.09	0.51
1:E:272:ILE:HG22	1:F:247:LEU:HD13	1.91	0.51
1:C:285:ARG:NH1	1:D:225:GLU:OE2	2.44	0.51
1:E:76:THR:HG21	1:E:275:ALA:C	2.34	0.51
1:A:290:PRO:O	1:A:292:MET:N	2.44	0.51
1:A:133:GLU:O	1:A:133:GLU:HG3	2.11	0.51
1:C:51:LYS:O	1:C:54:ALA:HB3	2.11	0.51
1:F:228:PHE:HE2	1:F:232:GLN:HE21	1.58	0.51
1:E:65:ARG:CZ	1:E:82:HIS:CG	2.93	0.51
1:B:260:LYS:O	1:B:264:LEU:HB3	2.11	0.51
1:C:299:PHE:CA	1:D:214:ASN:OD1	2.59	0.51
1:D:164:GLU:CG	1:D:196:THR:N	2.74	0.51
1:F:99:ARG:HD3	1:F:99:ARG:C	2.36	0.51
1:H:235:GLU:OE2	1:H:235:GLU:HA	2.11	0.51
1:B:43:PHE:CE2	1:B:249:LEU:HD13	2.47	0.50
1:D:64:TRP:HA	1:D:67:ALA:HB3	1.92	0.50
1:G:278:GLU:O	1:G:279:GLU:C	2.53	0.50
1:H:238:ARG:O	1:H:242:PHE:HD2	1.95	0.50
1:D:47:ALA:HB1	1:D:99:ARG:HG2	1.93	0.50
1:E:238:ARG:HH12	1:F:73:GLN:NE2	2.09	0.50
1:E:250:HIS:ND1	1:F:268:LEU:HD23	2.25	0.50
1:G:11:VAL:O	1:G:12:LEU:O	2.28	0.50
1:H:216:TYR:O	1:H:218:PRO:N	2.44	0.50
1:A:254:ASP:OD2	1:A:256:SER:N	2.44	0.50
1:A:95:HIS:CE1	1:A:255:LEU:HD11	2.46	0.50
1:E:258:SER:HB3	1:E:261:PHE:HB3	1.93	0.50
1:C:272:ILE:CG2	1:D:247:LEU:HD13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:LYS:O	1:E:149:GLU:HG3	2.11	0.50
1:A:263:GLU:O	1:A:267:ASP:OD2	2.29	0.50
1:G:100:GLU:OE2	1:G:100:GLU:HA	2.11	0.50
1:H:277:ASP:OD2	1:H:278:GLU:N	2.44	0.50
1:A:277:ASP:OD2	1:A:278:GLU:N	2.43	0.50
1:G:258:SER:O	1:G:262:HIS:HD2	1.95	0.50
1:E:15:SER:O	1:E:18:GLU:HB2	2.12	0.50
1:G:6:ASP:HB3	1:G:214:ASN:ND2	2.26	0.50
1:C:254:ASP:OD2	1:C:256:SER:OG	2.27	0.50
1:B:24:ARG:NH2	2:B:342:HOH:O	2.45	0.49
1:C:235:GLU:CD	1:C:238:ARG:HE	2.19	0.49
1:C:289:GLY:O	1:C:292:MET:HE2	2.12	0.49
1:H:85:PHE:O	1:H:88:ALA:HB3	2.12	0.49
1:B:15:SER:N	2:B:345:HOH:O	2.44	0.49
1:G:26:VAL:O	1:G:29:VAL:HG23	2.12	0.49
1:G:140:GLN:O	1:G:144:LEU:HD12	2.11	0.49
1:A:99:ARG:O	1:A:103:HIS:HB3	2.12	0.49
1:A:141:LYS:HB3	1:A:142:PRO:HD3	1.94	0.49
1:D:50:GLU:OE2	1:D:95:HIS:ND1	2.35	0.49
1:G:254:ASP:OD1	1:G:254:ASP:C	2.54	0.49
1:A:256:SER:HB3	1:B:265:HIS:CD2	2.46	0.49
1:E:258:SER:HB3	1:E:261:PHE:HB2	1.93	0.49
1:E:293:ALA:N	1:F:16:PHE:CA	2.75	0.49
1:B:164:GLU:HG3	1:B:196:THR:HA	1.94	0.49
1:D:89:GLU:O	1:D:93:GLU:HG3	2.13	0.49
1:F:61:ALA:O	1:F:65:ARG:HB2	2.11	0.49
1:F:96:LEU:HD12	1:F:96:LEU:O	2.11	0.49
1:D:151:GLU:OE2	1:D:151:GLU:HA	2.13	0.49
1:D:277:ASP:O	1:D:280:ASP:N	2.45	0.49
1:E:76:THR:CG2	1:E:276:SER:H	2.22	0.49
1:F:297:PRO:O	1:F:298:GLN:HG2	2.13	0.49
1:A:284:TRP:CD1	1:B:28:ARG:NH1	2.81	0.49
1:B:200:GLU:O	1:B:203:LYS:HD3	2.12	0.49
1:G:258:SER:O	1:G:262:HIS:CD2	2.66	0.49
1:B:147:LEU:HA	1:B:213:LEU:CD1	2.43	0.49
1:D:90:ARG:NH1	1:D:260:LYS:HE2	2.28	0.49
1:E:65:ARG:CZ	1:E:82:HIS:CB	2.89	0.48
1:G:7:ALA:H	1:G:214:ASN:ND2	2.11	0.48
1:B:64:TRP:HB3	1:B:85:PHE:CZ	2.48	0.48
1:F:255:LEU:O	1:F:258:SER:HB3	2.13	0.48
1:B:157:TYR:HB2	1:B:202:MET:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLU:HG3	1:B:235:GLU:O	2.10	0.48
1:D:201:LYS:C	1:D:202:MET:HE2	2.39	0.48
1:H:219:ARG:NH1	1:H:219:ARG:HG3	2.27	0.48
1:A:217:THR:O	1:A:221:MET:HG3	2.13	0.48
1:E:72:PRO:HG3	1:F:34:ARG:NH1	2.28	0.48
1:E:77:LEU:HD22	1:F:239:LEU:HD12	1.94	0.48
1:F:22:TYR:O	1:F:23:ARG:C	2.57	0.48
1:G:49:ILE:HG23	1:H:56:GLN:HG2	1.95	0.48
1:A:275:ALA:O	1:B:243:LYS:CE	2.61	0.48
1:F:46:ARG:NH2	1:F:50:GLU:OE1	2.37	0.48
1:E:28:ARG:CZ	1:E:235:GLU:HG2	2.44	0.48
1:E:266:ARG:O	1:E:269:GLN:HB3	2.14	0.48
1:F:151:GLU:OE2	1:F:151:GLU:CA	2.54	0.48
1:H:266:ARG:O	1:H:269:GLN:HB3	2.14	0.48
1:C:25:THR:O	1:C:28:ARG:HB3	2.13	0.48
1:E:96:LEU:CD1	1:E:96:LEU:C	2.87	0.48
1:F:121:GLN:HE22	1:F:130:ARG:HE	1.62	0.48
1:A:270:GLN:HA	1:A:273:GLU:HG3	1.96	0.47
1:B:219:ARG:O	1:B:222:GLU:HB3	2.14	0.47
1:A:83:ALA:HB1	1:A:268:LEU:HD12	1.95	0.47
1:B:203:LYS:HE3	1:B:203:LYS:C	2.40	0.47
1:E:108:GLU:OE2	1:E:111:ARG:CD	2.62	0.47
1:G:264:LEU:HD23	1:G:265:HIS:N	2.29	0.47
1:D:40:VAL:O	1:D:44:GLN:HG3	2.15	0.47
1:D:65:ARG:O	1:D:66:GLY:C	2.56	0.47
1:F:43:PHE:CD1	1:F:249:LEU:HG	2.50	0.47
1:F:212:GLU:OE2	1:F:213:LEU:N	2.48	0.47
1:H:81:TRP:O	1:H:82:HIS:C	2.57	0.47
1:C:217:THR:O	1:C:221:MET:HG3	2.15	0.47
1:C:292:MET:HB2	1:D:16:PHE:H	1.79	0.47
1:D:119:HIS:HB2	1:D:127:ARG:HG2	1.95	0.47
1:F:64:TRP:HB3	1:F:85:PHE:CZ	2.49	0.47
1:F:80:ALA:O	1:F:83:ALA:HB3	2.15	0.47
1:B:16:PHE:O	1:B:16:PHE:CD1	2.68	0.47
1:G:272:ILE:HG21	1:H:247:LEU:CD1	2.30	0.47
1:E:236:ARG:HB2	1:F:281:LEU:HD11	1.97	0.47
1:A:256:SER:O	1:A:262:HIS:CE1	2.68	0.47
1:A:269:GLN:O	1:A:273:GLU:HG2	2.15	0.47
1:E:284:TRP:O	1:E:285:ARG:C	2.57	0.47
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.83	0.46
1:E:140:GLN:HG3	1:E:220:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD12	1:A:265:HIS:N	2.30	0.46
1:E:21:ASN:C	1:E:23:ARG:H	2.22	0.46
1:H:228:PHE:CE2	1:H:232:GLN:NE2	2.83	0.46
1:D:76:THR:N	1:D:280:ASP:OD1	2.36	0.46
1:G:49:ILE:HD13	1:H:56:GLN:CG	2.46	0.46
1:A:46:ARG:HD2	1:A:46:ARG:O	2.14	0.46
1:E:40:VAL:HG13	1:E:107:SER:HB3	1.98	0.46
1:E:96:LEU:HD12	1:E:96:LEU:C	2.40	0.46
1:H:228:PHE:CE2	1:H:232:GLN:HG3	2.51	0.46
1:A:163:ASP:N	1:A:163:ASP:OD1	2.48	0.46
1:A:289:GLY:O	1:A:292:MET:HB3	2.16	0.46
1:C:278:GLU:O	1:C:279:GLU:C	2.59	0.46
1:D:20:GLY:H	1:D:140:GLN:HE22	1.64	0.46
1:E:16:PHE:C	1:E:16:PHE:CD2	2.93	0.46
1:E:165:LYS:HD2	1:E:165:LYS:N	2.31	0.46
1:E:43:PHE:CD2	1:E:249:LEU:HD13	2.51	0.46
1:B:121:GLN:CD	1:B:130:ARG:HD2	2.41	0.46
1:C:82:HIS:O	1:C:83:ALA:C	2.58	0.46
1:C:228:PHE:HE2	1:D:285:ARG:HG3	1.80	0.46
1:H:39:LEU:HD22	1:H:242:PHE:HE1	1.80	0.46
1:E:203:LYS:O	1:E:207:GLU:HB2	2.16	0.46
1:G:20:GLY:HA2	1:G:22:TYR:CD1	2.50	0.45
1:G:206:TYR:O	1:G:209:THR:HG22	2.16	0.45
1:C:264:LEU:HD12	1:C:264:LEU:C	2.41	0.45
1:F:50:GLU:OE2	1:F:95:HIS:ND1	2.45	0.45
1:B:235:GLU:OE2	1:B:238:ARG:HD3	2.16	0.45
1:D:38:ASP:O	1:D:39:LEU:C	2.57	0.45
1:G:120:ARG:CA	1:G:127:ARG:H	2.29	0.45
1:G:140:GLN:O	1:G:141:LYS:C	2.60	0.45
1:D:24:ARG:HH11	1:D:24:ARG:HG3	1.71	0.45
1:E:94:LEU:O	1:E:98:VAL:HG23	2.16	0.45
1:H:50:GLU:OE2	1:H:95:HIS:ND1	2.48	0.45
1:E:43:PHE:CG	1:E:249:LEU:HD13	2.51	0.45
1:E:254:ASP:OD2	1:E:254:ASP:C	2.59	0.45
1:D:223:ASP:O	1:D:226:GLN:HB2	2.16	0.45
1:E:101:LYS:HB3	1:E:252:HIS:ND1	2.32	0.45
1:F:213:LEU:HD12	1:F:214:ASN:N	2.31	0.45
1:F:240:LEU:O	1:F:241:PHE:C	2.60	0.45
1:G:268:LEU:CD2	1:H:250:HIS:CD2	2.99	0.45
1:B:76:THR:HA	1:B:79:LYS:HG3	1.99	0.45
1:C:86:THR:HA	1:C:89:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HH11	1:D:260:LYS:HE2	1.81	0.45
1:F:254:ASP:OD1	1:F:254:ASP:C	2.59	0.45
1:G:281:LEU:HD23	1:H:236:ARG:HH21	1.81	0.45
1:B:164:GLU:OE1	1:B:196:THR:HA	2.17	0.45
1:B:198:GLU:O	1:B:201:LYS:N	2.49	0.45
1:D:196:THR:CG2	1:D:196:THR:CA	2.85	0.45
1:F:228:PHE:CE2	1:F:232:GLN:NE2	2.83	0.45
1:E:140:GLN:HG3	1:E:220:TYR:CE1	2.52	0.45
1:H:64:TRP:O	1:H:65:ARG:C	2.60	0.45
1:A:254:ASP:OD2	1:A:254:ASP:C	2.60	0.44
1:B:121:GLN:CD	1:B:130:ARG:HH11	2.24	0.44
1:B:258:SER:O	1:B:262:HIS:CD2	2.60	0.44
1:C:17:TRP:HZ2	1:D:290:PRO:HB3	1.82	0.44
1:E:21:ASN:C	1:E:21:ASN:OD1	2.60	0.44
1:E:72:PRO:HD2	1:F:35:LEU:HD11	1.99	0.44
1:E:141:LYS:HB3	1:E:142:PRO:HD3	1.99	0.44
1:F:16:PHE:CD1	1:F:16:PHE:C	2.93	0.44
1:H:141:LYS:C	1:H:141:LYS:HE2	2.42	0.44
1:A:247:LEU:HG	1:B:272:ILE:CG2	2.47	0.44
1:A:267:ASP:OD2	1:A:267:ASP:N	2.51	0.44
1:C:15:SER:O	1:C:21:ASN:CG	2.60	0.44
1:C:69:GLU:C	1:C:71:GLY:H	2.25	0.44
1:F:121:GLN:HG2	1:F:125:GLY:HA3	1.98	0.44
1:B:141:LYS:O	1:B:144:LEU:N	2.48	0.44
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.74	0.44
1:D:106:ASP:O	1:D:110:VAL:HG23	2.17	0.44
1:D:255:LEU:O	1:D:258:SER:HB3	2.18	0.44
1:E:83:ALA:HB1	1:E:268:LEU:HD12	2.00	0.44
1:E:146:ARG:HG3	1:E:146:ARG:HH11	1.82	0.44
1:A:63:LYS:HG2	1:A:64:TRP:N	2.31	0.44
1:A:284:TRP:CG	1:B:28:ARG:HH11	2.35	0.44
1:E:62:ARG:CG	1:E:63:LYS:N	2.78	0.44
1:G:97:GLU:O	1:G:98:VAL:C	2.58	0.44
1:G:227:ALA:O	1:G:228:PHE:C	2.61	0.44
1:E:74:TYR:C	1:E:74:TYR:CD2	2.96	0.44
1:E:84:PHE:HA	1:E:268:LEU:CD1	2.48	0.44
1:G:56:GLN:OE1	1:H:49:ILE:HG12	2.17	0.44
1:C:17:TRP:HZ3	1:C:221:MET:HA	1.82	0.44
1:E:212:GLU:O	1:E:213:LEU:C	2.58	0.44
1:E:269:GLN:HA	1:E:269:GLN:OE1	2.17	0.44
1:F:204:THR:O	1:F:208:GLN:CG	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ARG:HA	1:B:125:GLY:O	2.18	0.44
1:C:216:TYR:O	1:C:219:ARG:HB3	2.18	0.44
1:A:272:ILE:HG21	1:B:247:LEU:CD2	2.47	0.44
1:D:201:LYS:HD2	1:D:202:MET:CE	2.48	0.44
1:D:240:LEU:O	1:D:241:PHE:C	2.61	0.44
1:F:106:ASP:OD1	1:F:106:ASP:N	2.50	0.44
1:B:228:PHE:CE2	1:B:232:GLN:NE2	2.86	0.43
1:B:255:LEU:O	1:B:258:SER:HB3	2.18	0.43
1:C:150:VAL:HA	1:C:209:THR:HG23	2.00	0.43
1:E:75:GLY:HA3	1:E:280:ASP:OD1	2.18	0.43
1:G:249:LEU:HA	1:G:249:LEU:HD23	1.79	0.43
1:H:17:TRP:CZ2	1:H:221:MET:HE3	2.53	0.43
1:G:275:ALA:O	1:H:243:LYS:CE	2.67	0.43
1:H:276:SER:OG	1:H:279:GLU:HB2	2.19	0.43
1:C:298:GLN:O	1:C:299:PHE:CB	2.67	0.43
1:F:140:GLN:NE2	1:F:144:LEU:HD11	2.34	0.43
1:B:101:LYS:HD3	1:B:252:HIS:CD2	2.54	0.43
1:C:150:VAL:HA	1:C:209:THR:CG2	2.48	0.43
1:C:210:LEU:HD22	1:C:214:ASN:OD1	2.19	0.43
1:C:277:ASP:OD1	1:C:277:ASP:N	2.45	0.43
1:D:99:ARG:HD3	1:D:100:GLU:N	2.34	0.43
1:B:40:VAL:HG13	1:B:107:SER:HB3	2.01	0.43
1:C:281:LEU:HD12	1:C:281:LEU:HA	1.80	0.43
1:G:291:GLY:O	1:H:15:SER:OG	2.36	0.43
1:E:227:ALA:O	1:E:230:SER:OG	2.36	0.43
1:F:104:GLY:HA3	1:F:105:PRO:HD3	1.89	0.43
1:F:268:LEU:O	1:F:269:GLN:C	2.61	0.43
1:G:9:GLY:C	1:G:10:GLU:O	2.61	0.43
1:G:65:ARG:HH22	1:G:82:HIS:HB3	1.76	0.43
1:G:239:LEU:HD23	1:H:77:LEU:CD2	2.47	0.43
1:E:101:LYS:O	1:E:105:PRO:HD2	2.18	0.43
1:E:160:ALA:HA	1:E:163:ASP:HB2	2.01	0.43
1:B:108:GLU:O	1:B:109:ARG:C	2.62	0.43
1:D:276:SER:OG	1:D:279:GLU:CB	2.67	0.43
1:E:285:ARG:NH1	1:F:225:GLU:OE2	2.48	0.43
1:F:295:ASN:N	1:F:296:TRP:CE3	2.87	0.43
1:G:73:GLN:HG3	1:G:78:GLU:HB2	2.01	0.43
1:H:219:ARG:HH11	1:H:219:ARG:CG	2.32	0.43
1:B:248:THR:CG2	1:B:252:HIS:CE1	3.01	0.43
1:D:90:ARG:NH1	1:D:260:LYS:CE	2.82	0.43
1:A:65:ARG:O	1:A:69:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:CD1	1:D:72:PRO:HD2	2.30	0.42
1:C:147:LEU:HD12	1:C:147:LEU:C	2.44	0.42
1:E:16:PHE:CD2	1:E:16:PHE:O	2.72	0.42
1:C:259:ASP:O	1:C:260:LYS:C	2.61	0.42
1:F:258:SER:O	1:F:262:HIS:CD2	2.64	0.42
1:H:121:GLN:OE1	1:H:130:ARG:HD2	2.19	0.42
1:A:15:SER:C	1:A:21:ASN:HD21	2.27	0.42
1:C:292:MET:N	1:C:292:MET:CE	2.81	0.42
1:E:65:ARG:O	1:E:69:GLU:HB3	2.19	0.42
1:E:269:GLN:OE1	1:E:269:GLN:CA	2.67	0.42
1:F:86:THR:O	1:F:87:ALA:C	2.61	0.42
1:H:64:TRP:HA	1:H:67:ALA:HB3	2.01	0.42
1:C:100:GLU:OE2	1:C:100:GLU:HA	2.18	0.42
1:E:24:ARG:HD2	1:E:24:ARG:HA	1.67	0.42
1:F:33:HIS:HB2	1:F:118:PHE:CD2	2.54	0.42
1:H:23:ARG:C	1:H:25:THR:N	2.76	0.42
1:E:260:LYS:HA	1:E:263:GLU:HG2	2.00	0.42
1:G:147:LEU:HD13	1:G:147:LEU:C	2.44	0.42
1:H:77:LEU:HD12	1:H:77:LEU:HA	1.74	0.42
1:E:99:ARG:HG3	1:E:100:GLU:N	2.34	0.42
1:A:258:SER:HB3	1:A:261:PHE:CB	2.50	0.42
1:D:39:LEU:HD21	1:D:245:VAL:CG1	2.45	0.42
1:G:61:ALA:O	1:G:65:ARG:HB3	2.19	0.42
1:A:17:TRP:HB2	1:B:294:MET:HG2	2.01	0.42
1:D:64:TRP:HA	1:D:67:ALA:CB	2.49	0.42
1:D:276:SER:HG	1:D:279:GLU:HB3	1.85	0.42
1:H:28:ARG:CZ	1:H:235:GLU:HG2	2.50	0.42
1:H:108:GLU:O	1:H:109:ARG:C	2.61	0.42
1:E:47:ALA:O	1:E:50:GLU:HB2	2.20	0.42
1:G:247:LEU:O	1:G:251:GLN:HG3	2.20	0.42
1:H:14:GLY:HA2	1:H:17:TRP:HD1	1.84	0.42
1:A:56:GLN:O	1:A:57:LEU:C	2.62	0.42
1:A:103:HIS:CD2	1:A:103:HIS:O	2.73	0.42
1:A:282:ARG:O	1:A:283:TRP:C	2.62	0.42
1:C:200:GLU:O	1:C:201:LYS:C	2.63	0.42
1:C:261:PHE:CE2	1:D:256:SER:HB3	2.55	0.42
1:D:268:LEU:O	1:D:269:GLN:C	2.62	0.42
1:E:73:GLN:NE2	1:E:81:TRP:CE3	2.84	0.42
1:E:251:GLN:HE21	1:E:251:GLN:HB3	1.72	0.42
1:H:106:ASP:O	1:H:110:VAL:HG23	2.19	0.42
1:H:276:SER:O	1:H:277:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LYS:HA	1:C:263:GLU:HG2	2.00	0.41
1:C:281:LEU:HD23	1:D:236:ARG:NH2	2.35	0.41
1:D:119:HIS:CD2	1:D:127:ARG:NH1	2.88	0.41
1:D:212:GLU:HA	1:D:215:ARG:HD2	2.02	0.41
1:E:254:ASP:OD2	1:E:256:SER:OG	2.32	0.41
1:G:120:ARG:O	1:G:122:VAL:N	2.53	0.41
1:C:266:ARG:HD3	1:C:266:ARG:HA	1.88	0.41
1:D:255:LEU:HA	1:D:255:LEU:HD12	1.68	0.41
1:E:147:LEU:HD12	1:E:147:LEU:O	2.20	0.41
1:E:225:GLU:OE2	1:F:285:ARG:NH2	2.36	0.41
1:C:215:ARG:O	1:C:218:PRO:HD2	2.21	0.41
1:E:298:GLN:HE21	1:E:298:GLN:N	2.16	0.41
1:B:115:ARG:HA	1:B:120:ARG:HH22	1.85	0.41
1:C:268:LEU:HD21	1:D:250:HIS:CD2	2.55	0.41
1:C:292:MET:HB3	1:D:15:SER:HA	2.03	0.41
1:E:20:GLY:HA2	1:E:22:TYR:CE1	2.55	0.41
1:H:64:TRP:HB3	1:H:85:PHE:CZ	2.55	0.41
1:H:121:GLN:NE2	1:H:130:ARG:CD	2.59	0.41
1:A:96:LEU:CD1	1:A:96:LEU:C	2.94	0.41
1:E:21:ASN:C	1:E:23:ARG:N	2.77	0.41
1:E:35:LEU:HD12	1:E:35:LEU:HA	1.87	0.41
1:A:21:ASN:C	1:A:23:ARG:H	2.28	0.41
1:D:97:GLU:O	1:D:98:VAL:C	2.60	0.41
1:D:120:ARG:CD	1:D:120:ARG:N	2.59	0.41
1:G:153:SER:HB2	1:G:209:THR:HG21	2.01	0.41
1:A:104:GLY:HA3	1:A:105:PRO:HD3	1.93	0.41
1:B:79:LYS:H	1:B:79:LYS:HG2	1.48	0.41
1:C:36:CYS:O	1:C:40:VAL:HG23	2.20	0.41
1:C:84:PHE:CE2	1:D:246:LEU:HD22	2.55	0.41
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.45	0.41
1:D:81:TRP:O	1:D:84:PHE:HB2	2.21	0.41
1:D:120:ARG:CA	1:D:125:GLY:O	2.53	0.41
1:D:202:MET:HA	1:D:205:GLN:HG2	2.03	0.41
1:G:6:ASP:CA	1:G:214:ASN:ND2	2.82	0.41
1:G:85:PHE:O	1:G:86:THR:C	2.59	0.41
1:H:219:ARG:NH1	1:H:219:ARG:CG	2.84	0.41
1:A:269:GLN:O	1:A:272:ILE:HB	2.20	0.41
1:E:104:GLY:HA3	1:E:105:PRO:HD3	1.88	0.41
1:G:132:ALA:O	1:G:133:GLU:C	2.61	0.41
1:A:51:LYS:HB2	1:A:99:ARG:HG2	2.02	0.41
1:A:236:ARG:HB2	1:B:281:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PHE:O	1:A:243:LYS:C	2.62	0.41
1:B:150:VAL:HG21	1:B:210:LEU:HD22	2.03	0.41
1:B:240:LEU:O	1:B:241:PHE:C	2.64	0.41
1:C:203:LYS:O	1:C:206:TYR:HB3	2.21	0.41
1:C:216:TYR:O	1:C:217:THR:C	2.64	0.41
1:D:28:ARG:CZ	1:D:235:GLU:HG2	2.50	0.41
1:E:89:GLU:O	1:E:90:ARG:C	2.61	0.41
1:E:294:MET:CA	1:F:17:TRP:HD1	2.33	0.41
1:F:124:GLY:HA3	1:F:125:GLY:HA3	1.66	0.41
1:F:260:LYS:CB	1:F:260:LYS:HZ2	2.28	0.41
1:G:266:ARG:NH1	1:G:269:GLN:NE2	2.64	0.41
1:A:240:LEU:HD21	1:B:277:ASP:OD1	2.21	0.41
1:C:247:LEU:HD13	1:C:247:LEU:HA	1.95	0.41
1:D:96:LEU:O	1:D:97:GLU:C	2.61	0.41
1:D:228:PHE:CE2	1:D:232:GLN:HG3	2.56	0.41
1:E:238:ARG:HH12	1:F:73:GLN:HE22	1.68	0.41
1:A:45:GLU:O	1:A:46:ARG:C	2.63	0.40
1:B:202:MET:O	1:B:205:GLN:CG	2.68	0.40
1:C:55:GLN:O	1:C:58:ALA:HB3	2.20	0.40
1:A:102:LEU:O	1:A:107:SER:HB2	2.21	0.40
1:A:216:TYR:O	1:A:217:THR:C	2.62	0.40
1:D:43:PHE:CE1	1:D:249:LEU:HG	2.56	0.40
1:E:101:LYS:HB3	1:E:252:HIS:HD1	1.85	0.40
1:G:104:GLY:O	1:G:108:GLU:HB3	2.21	0.40
1:H:203:LYS:O	1:H:207:GLU:HG2	2.21	0.40
1:A:89:GLU:O	1:A:90:ARG:C	2.62	0.40
1:A:273:GLU:HG2	1:A:273:GLU:H	1.67	0.40
1:B:228:PHE:HE2	1:B:232:GLN:NE2	2.19	0.40
1:B:264:LEU:HD23	1:B:265:HIS:N	2.36	0.40
1:D:258:SER:HB3	1:D:261:PHE:CB	2.52	0.40
1:E:249:LEU:HA	1:E:249:LEU:HD23	1.73	0.40
1:F:25:THR:O	1:F:25:THR:CG2	2.70	0.40
1:A:15:SER:O	1:A:16:PHE:C	2.63	0.40
1:A:62:ARG:HA	1:A:65:ARG:CZ	2.51	0.40
1:A:76:THR:HG21	1:A:276:SER:H	1.86	0.40
1:E:276:SER:HG	1:E:279:GLU:H	1.65	0.40
1:E:279:GLU:HA	1:E:282:ARG:CZ	2.52	0.40
1:D:276:SER:OG	1:D:279:GLU:HB3	2.21	0.40
1:F:126:PHE:O	1:F:130:ARG:HB2	2.21	0.40
1:G:22:TYR:O	1:G:26:VAL:HG23	2.21	0.40
1:G:236:ARG:HB2	1:H:281:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:HIS:C	1:H:82:HIS:CD2	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/347 (70%)	229 (94%)	10 (4%)	4 (2%)	7	30
1	B	253/347 (73%)	236 (93%)	14 (6%)	3 (1%)	10	37
1	C	251/347 (72%)	231 (92%)	20 (8%)	0	100	100
1	D	249/347 (72%)	230 (92%)	17 (7%)	2 (1%)	16	47
1	E	249/347 (72%)	232 (93%)	16 (6%)	1 (0%)	30	61
1	F	247/347 (71%)	224 (91%)	21 (8%)	2 (1%)	16	47
1	G	250/347 (72%)	222 (89%)	25 (10%)	3 (1%)	10	37
1	H	241/347 (70%)	224 (93%)	14 (6%)	3 (1%)	10	37
All	All	1983/2776 (71%)	1828 (92%)	137 (7%)	18 (1%)	14	44

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	213	LEU
1	F	297	PRO
1	B	290	PRO
1	D	71	GLY
1	H	71	GLY
1	H	104	GLY
1	D	124	GLY
1	G	12	LEU
1	H	290	PRO

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Mol	Chain	Res	Type
1	A	83	ALA
1	B	104	GLY
1	B	291	GLY
1	G	10	GLU
1	G	11	VAL
1	A	72	PRO
1	A	291	GLY
1	E	290	PRO
1	A	290	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	201/294 (68%)	168 (84%)	33 (16%)	2	11
1	B	210/294 (71%)	177 (84%)	33 (16%)	2	12
1	C	197/294 (67%)	152 (77%)	45 (23%)	1	4
1	D	205/294 (70%)	172 (84%)	33 (16%)	2	11
1	E	196/294 (67%)	154 (79%)	42 (21%)	1	5
1	F	193/294 (66%)	155 (80%)	38 (20%)	1	6
1	G	182/294 (62%)	138 (76%)	44 (24%)	1	3
1	H	186/294 (63%)	155 (83%)	31 (17%)	2	10
All	All	1570/2352 (67%)	1271 (81%)	299 (19%)	1	7

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	29	VAL
1	A	30	GLU
1	A	51	LYS
1	A	55	GLN
1	A	69	GLU

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	96	LEU
1	A	99	ARG
1	A	112	THR
1	A	120	ARG
1	A	123	LEU
1	A	129	SER
1	A	130	ARG
1	A	133	GLU
1	A	148	LYS
1	A	155	LYS
1	A	163	ASP
1	A	204	THR
1	A	205	GLN
1	A	212	GLU
1	A	217	THR
1	A	224	MET
1	A	230	SER
1	A	246	LEU
1	A	248	THR
1	A	251	GLN
1	A	255	LEU
1	A	256	SER
1	A	257	SER
1	A	266	ARG
1	A	269	GLN
1	A	271	SER
1	B	15	SER
1	B	21	ASN
1	B	23	ARG
1	B	30	GLU
1	B	35	LEU
1	B	55	GLN
1	B	56	GLN
1	B	62	ARG
1	B	70	LYS
1	B	79	LYS
1	B	89	GLU
1	B	120	ARG
1	B	123	LEU
1	B	127	ARG
1	B	129	SER

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Mol	Chain	Res	Type
1	B	140	GLN
1	B	148	LYS
1	B	150	VAL
1	B	158	HIS
1	B	166	THR
1	B	201	LYS
1	B	203	LYS
1	B	210	LEU
1	B	224	MET
1	B	239	LEU
1	B	258	SER
1	B	260	LYS
1	B	264	LEU
1	B	270	GLN
1	B	276	SER
1	B	278	GLU
1	B	279	GLU
1	B	298	GLN
1	C	30	GLU
1	C	35	LEU
1	C	44	GLN
1	C	49	ILE
1	C	50	GLU
1	C	55	GLN
1	C	56	GLN
1	C	57	LEU
1	C	73	GLN
1	C	76	THR
1	C	79	LYS
1	C	93	GLU
1	C	114	GLN
1	C	130	ARG
1	C	133	GLU
1	C	144	LEU
1	C	145	LYS
1	C	147	LEU
1	C	154	LYS
1	C	155	LYS
1	C	158	HIS
1	C	159	THR
1	C	200	GLU
1	C	202	MET

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Mol	Chain	Res	Type
1	C	204	THR
1	C	207	GLU
1	C	209	THR
1	C	210	LEU
1	C	212	GLU
1	C	213	LEU
1	C	217	THR
1	C	219	ARG
1	C	226	GLN
1	C	244	ASP
1	C	246	LEU
1	C	247	LEU
1	C	248	THR
1	C	257	SER
1	C	264	LEU
1	C	266	ARG
1	C	271	SER
1	C	277	ASP
1	C	279	GLU
1	C	281	LEU
1	C	287	THR
1	D	21	ASN
1	D	23	ARG
1	D	24	ARG
1	D	35	LEU
1	D	56	GLN
1	D	62	ARG
1	D	77	LEU
1	D	109	ARG
1	D	120	ARG
1	D	143	TRP
1	D	145	LYS
1	D	148	LYS
1	D	150	VAL
1	D	158	HIS
1	D	197	LYS
1	D	202	MET
1	D	210	LEU
1	D	221	MET
1	D	224	MET
1	D	238	ARG
1	D	239	LEU

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Mol	Chain	Res	Type
1	D	247	LEU
1	D	248	THR
1	D	249	LEU
1	D	255	LEU
1	D	257	SER
1	D	266	ARG
1	D	278	GLU
1	D	282	ARG
1	D	285	ARG
1	D	286	SER
1	D	287	THR
1	D	296	TRP
1	E	18	GLU
1	E	30	GLU
1	E	34	ARG
1	E	35	LEU
1	E	41	SER
1	E	44	GLN
1	E	55	GLN
1	E	86	THR
1	E	90	ARG
1	E	96	LEU
1	E	99	ARG
1	E	107	SER
1	E	115	ARG
1	E	144	LEU
1	E	147	LEU
1	E	155	LYS
1	E	164	GLU
1	E	165	LYS
1	E	208	GLN
1	E	210	LEU
1	E	212	GLU
1	E	215	ARG
1	E	217	THR
1	E	219	ARG
1	E	224	MET
1	E	226	GLN
1	E	230	SER
1	E	235	GLU
1	E	237	GLN
1	E	246	LEU

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Mol	Chain	Res	Type
1	E	247	LEU
1	E	257	SER
1	E	263	GLU
1	E	264	LEU
1	E	270	GLN
1	E	271	SER
1	E	276	SER
1	E	281	LEU
1	E	287	THR
1	E	290	PRO
1	E	295	ASN
1	E	298	GLN
1	F	21	ASN
1	F	23	ARG
1	F	25	THR
1	F	28	ARG
1	F	34	ARG
1	F	35	LEU
1	F	48	ARG
1	F	51	LYS
1	F	57	LEU
1	F	70	LYS
1	F	73	GLN
1	F	76	THR
1	F	89	GLU
1	F	106	ASP
1	F	109	ARG
1	F	122	VAL
1	F	123	LEU
1	F	130	ARG
1	F	133	GLU
1	F	143	TRP
1	F	148	LYS
1	F	151	GLU
1	F	158	HIS
1	F	210	LEU
1	F	212	GLU
1	F	213	LEU
1	F	215	ARG
1	F	219	ARG
1	F	224	MET
1	F	230	SER

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Mol	Chain	Res	Type
1	F	239	LEU
1	F	247	LEU
1	F	249	LEU
1	F	258	SER
1	F	260	LYS
1	F	278	GLU
1	F	282	ARG
1	F	296	TRP
1	G	18	GLU
1	G	24	ARG
1	G	28	ARG
1	G	30	GLU
1	G	34	ARG
1	G	35	LEU
1	G	44	GLN
1	G	49	ILE
1	G	55	GLN
1	G	57	LEU
1	G	62	ARG
1	G	65	ARG
1	G	76	THR
1	G	89	GLU
1	G	90	ARG
1	G	96	LEU
1	G	99	ARG
1	G	108	GLU
1	G	110	VAL
1	G	114	GLN
1	G	121	GLN
1	G	123	LEU
1	G	140	GLN
1	G	141	LYS
1	G	144	LEU
1	G	147	LEU
1	G	153	SER
1	G	209	THR
1	G	210	LEU
1	G	212	GLU
1	G	213	LEU
1	G	226	GLN
1	G	230	SER
1	G	246	LEU

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Mol	Chain	Res	Type
1	G	247	LEU
1	G	255	LEU
1	G	260	LYS
1	G	264	LEU
1	G	266	ARG
1	G	269	GLN
1	G	271	SER
1	G	279	GLU
1	G	281	LEU
1	G	287	THR
1	H	16	PHE
1	H	23	ARG
1	H	30	GLU
1	H	35	LEU
1	H	40	VAL
1	H	41	SER
1	H	56	GLN
1	H	57	LEU
1	H	62	ARG
1	H	73	GLN
1	H	89	GLU
1	H	102	LEU
1	H	109	ARG
1	H	127	ARG
1	H	141	LYS
1	H	143	TRP
1	H	147	LEU
1	H	219	ARG
1	H	225	GLU
1	H	226	GLN
1	H	230	SER
1	H	238	ARG
1	H	239	LEU
1	H	247	LEU
1	H	248	THR
1	H	249	LEU
1	H	258	SER
1	H	264	LEU
1	H	286	SER
1	H	287	THR
1	H	288	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	44	GLN
1	A	56	GLN
1	A	82	HIS
1	A	103	HIS
1	A	205	GLN
1	A	251	GLN
1	A	262	HIS
1	A	269	GLN
1	A	270	GLN
1	B	55	GLN
1	B	73	GLN
1	B	82	HIS
1	B	205	GLN
1	B	208	GLN
1	B	214	ASN
1	B	226	GLN
1	B	250	HIS
1	B	262	HIS
1	B	265	HIS
1	C	44	GLN
1	C	55	GLN
1	C	226	GLN
1	C	232	GLN
1	C	251	GLN
1	C	252	HIS
1	C	265	HIS
1	C	269	GLN
1	C	270	GLN
1	C	288	HIS
1	D	21	ASN
1	D	55	GLN
1	D	73	GLN
1	D	103	HIS
1	D	119	HIS
1	D	121	GLN
1	D	140	GLN
1	D	250	HIS
1	D	251	GLN
1	D	262	HIS
1	D	288	HIS
1	E	27	GLN

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Mol	Chain	Res	Type
1	E	44	GLN
1	E	73	GLN
1	E	226	GLN
1	E	237	GLN
1	E	251	GLN
1	E	262	HIS
1	E	270	GLN
1	E	298	GLN
1	F	44	GLN
1	F	55	GLN
1	F	56	GLN
1	F	73	GLN
1	F	82	HIS
1	F	140	GLN
1	F	205	GLN
1	F	226	GLN
1	F	237	GLN
1	F	250	HIS
1	F	262	HIS
1	F	288	HIS
1	F	295	ASN
1	F	298	GLN
1	G	44	GLN
1	G	82	HIS
1	G	103	HIS
1	G	214	ASN
1	G	250	HIS
1	G	251	GLN
1	G	265	HIS
1	G	269	GLN
1	H	44	GLN
1	H	55	GLN
1	H	82	HIS
1	H	119	HIS
1	H	121	GLN
1	H	140	GLN
1	H	208	GLN
1	H	237	GLN
1	H	250	HIS
1	H	251	GLN
1	H	265	HIS
1	H	270	GLN

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Mol	Chain	Res	Type
1	H	288	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/347 (72%)	-0.61	6 (2%) 59 38	37, 61, 103, 129	0
1	B	257/347 (74%)	-0.74	2 (0%) 82 65	25, 55, 120, 137	0
1	C	257/347 (74%)	-0.71	0 100 100	42, 59, 97, 112	0
1	D	255/347 (73%)	-0.72	1 (0%) 88 76	34, 54, 120, 135	0
1	E	255/347 (73%)	-0.55	3 (1%) 76 58	39, 59, 108, 127	0
1	F	255/347 (73%)	-0.76	0 100 100	32, 55, 101, 114	0
1	G	254/347 (73%)	-0.71	1 (0%) 88 76	41, 59, 83, 98	0
1	H	247/347 (71%)	-0.78	1 (0%) 88 76	35, 53, 89, 102	0
All	All	2030/2776 (73%)	-0.70	14 (0%) 84 68	25, 57, 103, 137	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	158	HIS	5.3
1	A	296	TRP	5.1
1	E	162	LYS	3.4
1	A	298	GLN	3.2
1	E	293	ALA	3.2
1	D	196	THR	3.0
1	A	158	HIS	3.0
1	H	195	CYS	2.4
1	A	123	LEU	2.3
1	G	19	ALA	2.2
1	A	164	GLU	2.2
1	B	292	MET	2.1
1	A	293	ALA	2.1
1	B	197	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.