



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:39 AM UTC

PDB ID : 1K1D / pdb_00001k1d
Title : Crystal structure of D-hydantoinase
Authors : Cheon, Y.H.; Kim, H.S.; Han, K.H.; Abendroth, J.; Niefind, K.; Schomburg, D.; Wang, J.; Kim, Y.
Deposited on : 2001-09-25
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

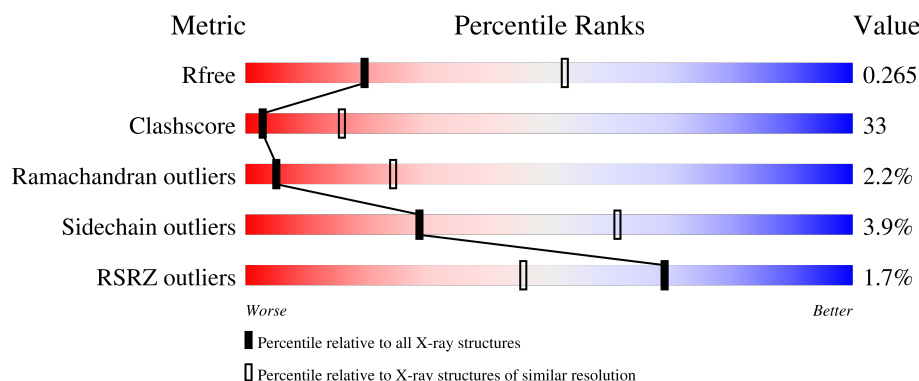
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	460	2% 49% 45% 5%
1	B	460	0% 50% 44% 5%
1	C	460	2% 50% 45% 5%
1	D	460	2% 49% 45% 5%
1	E	460	2% 51% 43% 6%

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Mol	Chain	Length	Quality of chain
1	F	460	3% 48% 47% 5%
1	G	460	2% 50% 45% 5%
1	H	460	% 48% 47% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 28496 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 D-hydantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			
1	B	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			
1	C	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			
1	D	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			
1	E	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			
1	F	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			
1	G	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			
1	H	460	Total	C	N	O	S	0	0	0
			3560	2271	591	682	16			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

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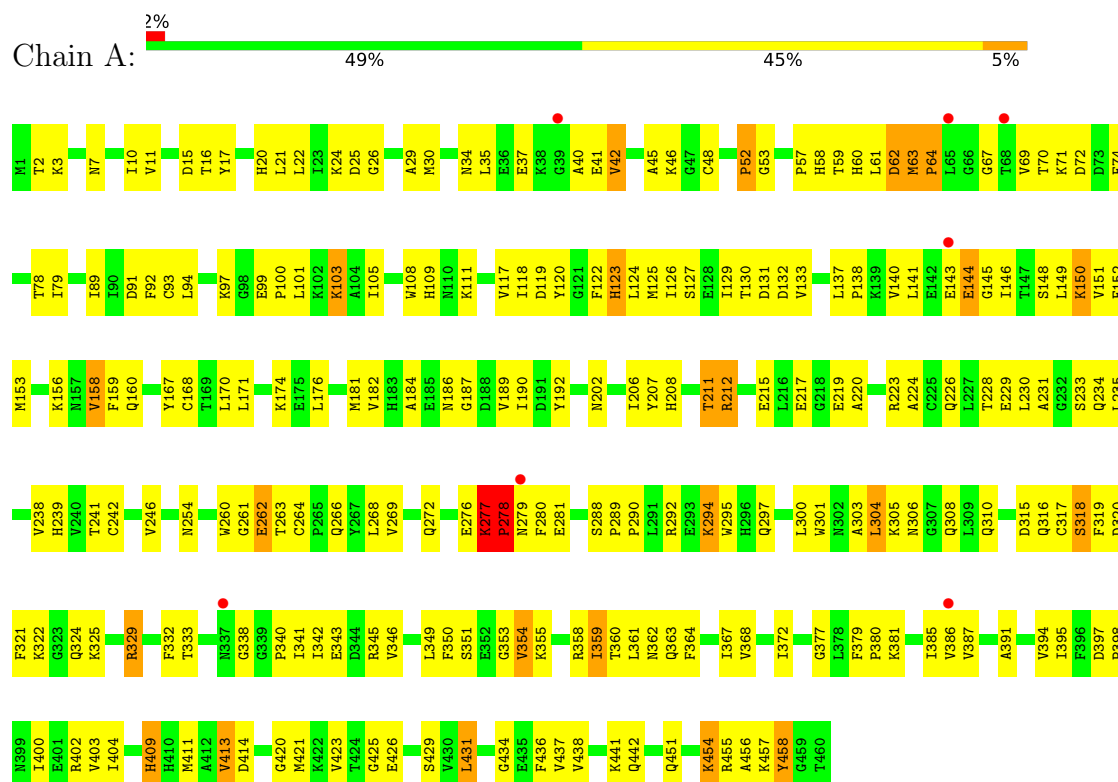
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0

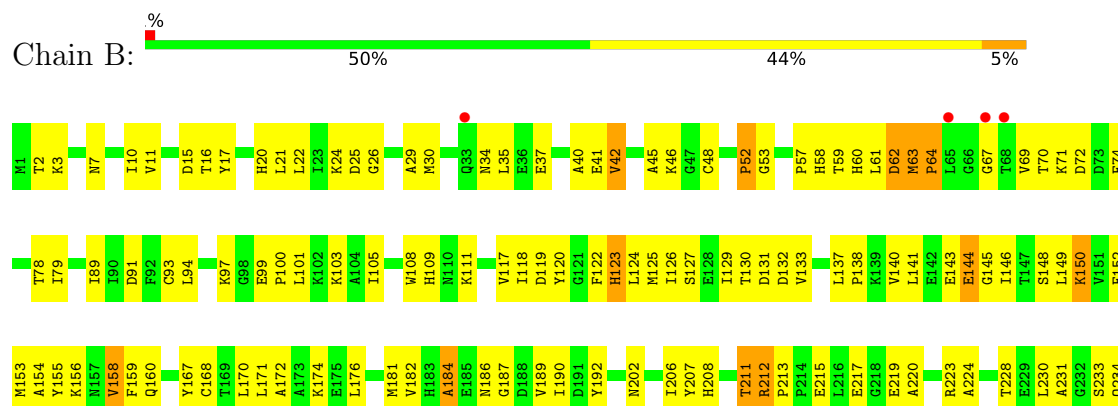
3 Residue-property plots

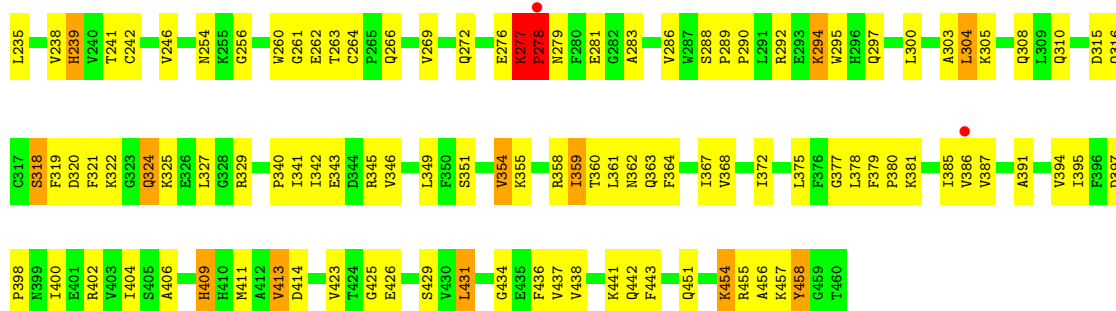
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

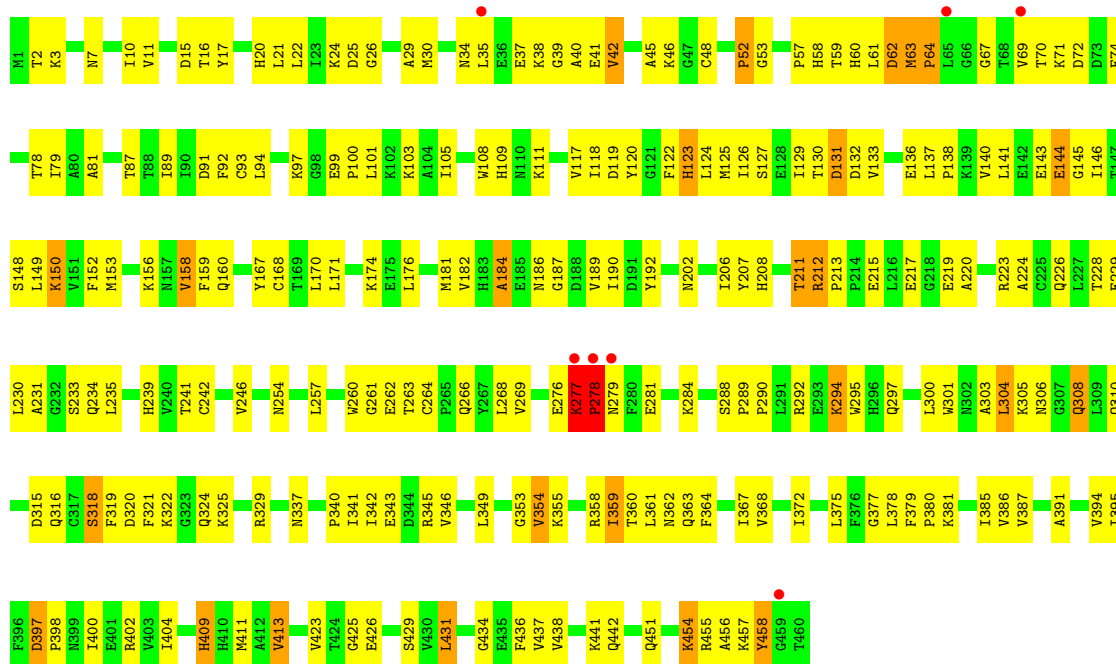


• Molecule 1: D-hydantoinase

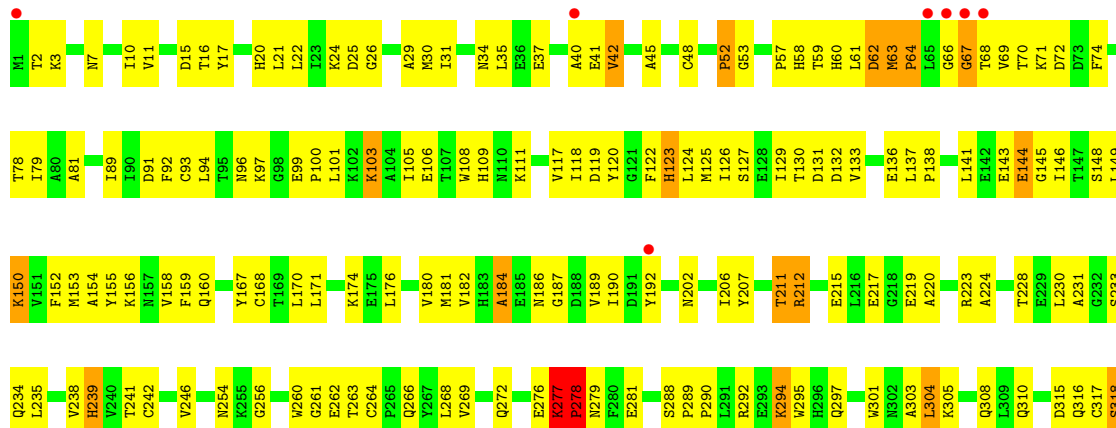


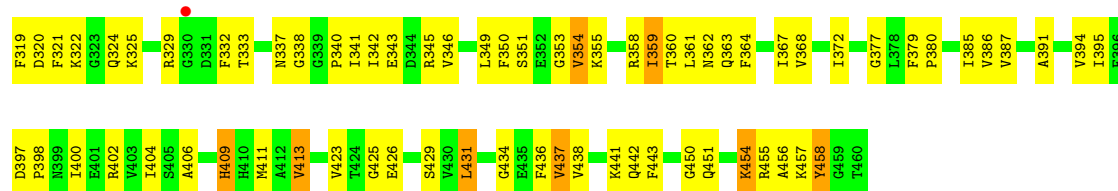


• Molecule 1: D-hydantoinase

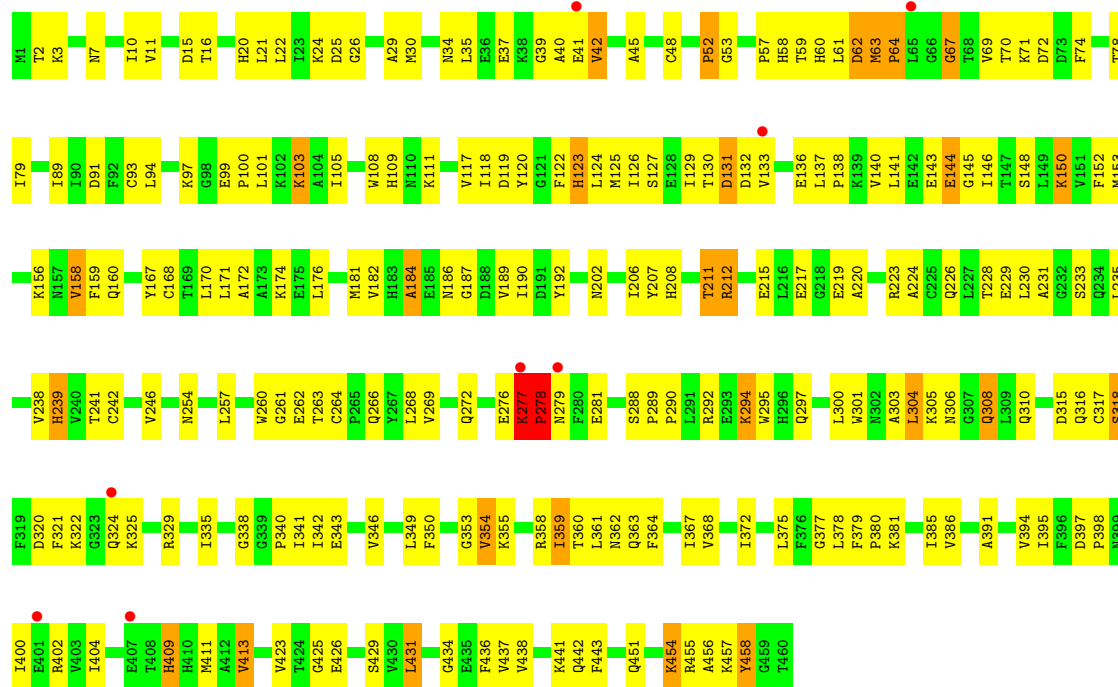


• Molecule 1: D-hydantoinase

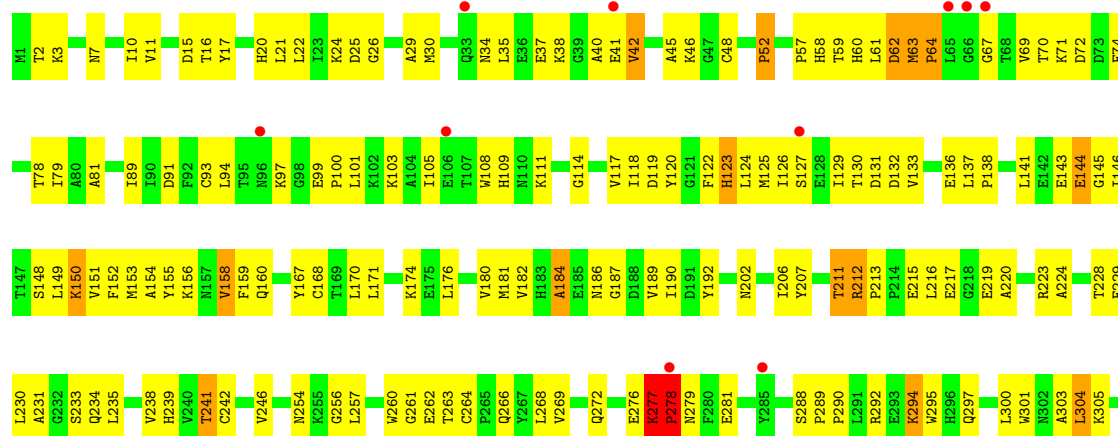


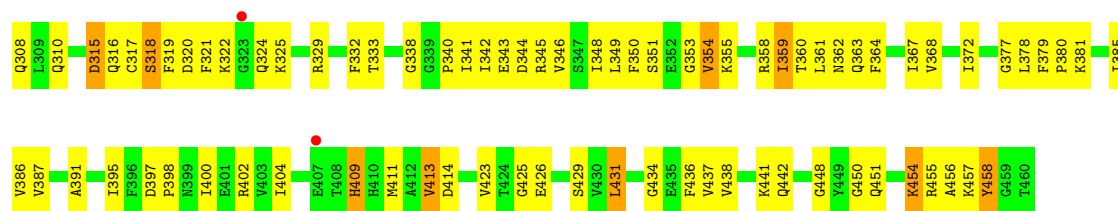


● Molecule 1: D-hydantoinase

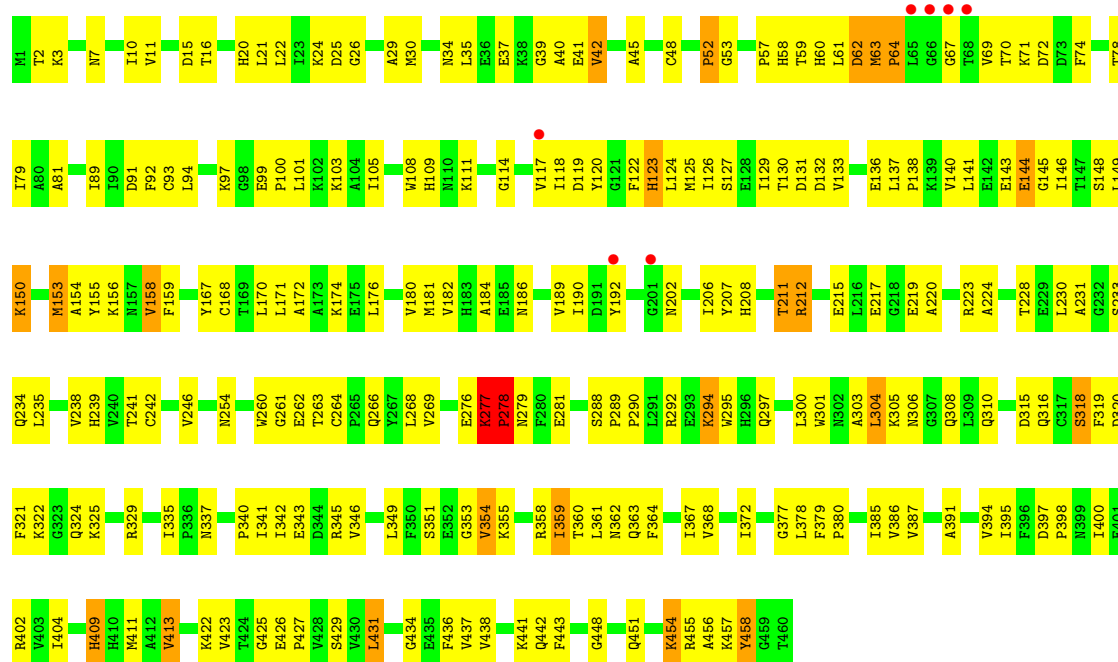


● Molecule 1: D-hydantoinase

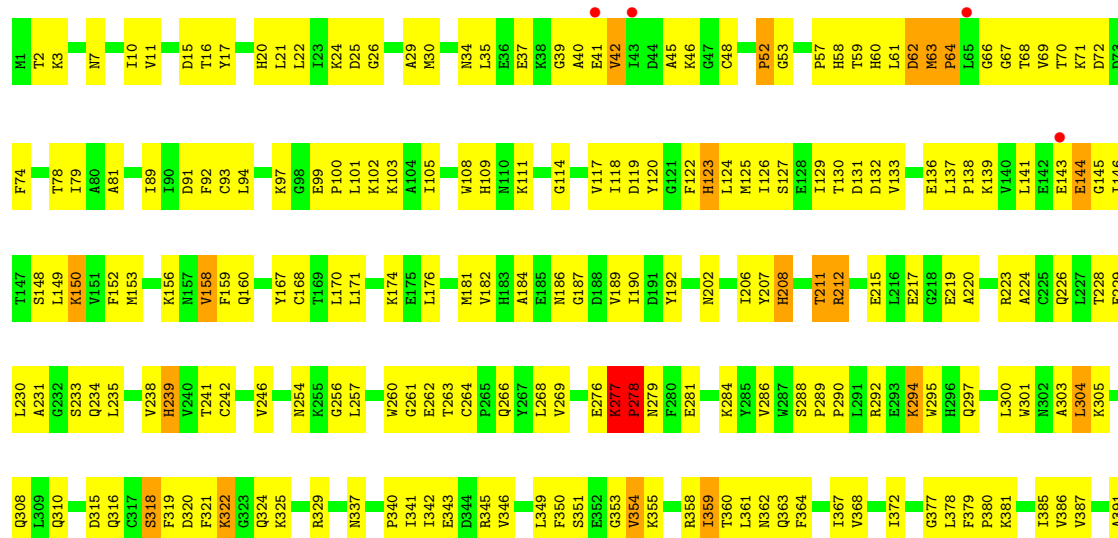


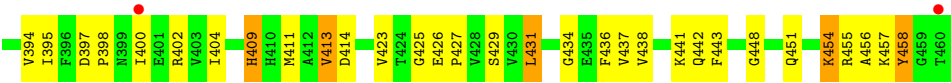


● Molecule 1: D-hydantoinase



● Molecule 1: D-hydantoinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.45Å 182.89Å 156.13Å 90.00° 125.27° 90.00°	Depositor
Resolution (Å)	19.97 – 3.01 19.97 – 3.01	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.97-3.01) 94.6 (19.97-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.04Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.263 , 0.280 0.250 , 0.265	Depositor DCC
R_{free} test set	9599 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	28496	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.56% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	1/3619 (0.0%)	1.08	21/4898 (0.4%)
1	B	0.54	1/3619 (0.0%)	1.08	22/4898 (0.4%)
1	C	0.54	1/3619 (0.0%)	1.07	21/4898 (0.4%)
1	D	0.51	1/3619 (0.0%)	1.08	21/4898 (0.4%)
1	E	0.53	1/3619 (0.0%)	1.07	21/4898 (0.4%)
1	F	0.51	1/3619 (0.0%)	1.07	19/4898 (0.4%)
1	G	0.53	1/3619 (0.0%)	1.08	20/4898 (0.4%)
1	H	0.51	1/3619 (0.0%)	1.08	19/4898 (0.4%)
All	All	0.52	8/28952 (0.0%)	1.08	164/39184 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	SER	C-N	-9.20	1.20	1.33
1	D	148	SER	C-N	-7.99	1.22	1.33
1	A	148	SER	C-N	-7.67	1.22	1.33
1	G	148	SER	C-N	-6.95	1.23	1.33
1	E	148	SER	C-N	-6.46	1.24	1.33
1	H	148	SER	C-N	-6.39	1.24	1.33
1	C	148	SER	C-N	-6.03	1.25	1.33
1	F	148	SER	C-N	-5.35	1.25	1.33

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	LYS	C-N-CD	-17.61	81.87	120.60
1	C	277	LYS	C-N-CD	-17.58	81.93	120.60
1	H	277	LYS	C-N-CD	-17.56	81.96	120.60
1	F	277	LYS	C-N-CD	-17.51	82.07	120.60
1	E	277	LYS	C-N-CD	-17.49	82.12	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	277	LYS	C-N-CD	-17.45	82.20	120.60
1	B	277	LYS	C-N-CD	-17.38	82.36	120.60
1	A	277	LYS	C-N-CD	-17.23	82.69	120.60
1	C	277	LYS	CA-C-N	13.37	159.09	127.00
1	C	277	LYS	C-N-CA	13.37	159.09	127.00
1	H	277	LYS	CA-C-N	13.29	158.89	127.00
1	H	277	LYS	C-N-CA	13.29	158.89	127.00
1	D	277	LYS	CA-C-N	13.21	158.69	127.00
1	D	277	LYS	C-N-CA	13.21	158.69	127.00
1	E	277	LYS	CA-C-N	13.16	158.59	127.00
1	E	277	LYS	C-N-CA	13.16	158.59	127.00
1	B	277	LYS	CA-C-N	13.14	158.54	127.00
1	B	277	LYS	C-N-CA	13.14	158.54	127.00
1	A	277	LYS	CA-C-N	13.01	158.21	127.00
1	A	277	LYS	C-N-CA	13.01	158.21	127.00
1	G	277	LYS	CA-C-N	13.00	158.21	127.00
1	G	277	LYS	C-N-CA	13.00	158.21	127.00
1	F	277	LYS	CA-C-N	12.86	157.85	127.00
1	F	277	LYS	C-N-CA	12.86	157.85	127.00
1	A	212	ARG	CA-C-N	10.06	127.01	119.66
1	A	212	ARG	C-N-CA	10.06	127.01	119.66
1	H	212	ARG	CA-C-N	9.86	126.85	119.66
1	H	212	ARG	C-N-CA	9.86	126.85	119.66
1	D	437	VAL	N-CA-C	-9.59	103.37	112.96
1	B	212	ARG	CA-C-N	9.36	126.49	119.66
1	B	212	ARG	C-N-CA	9.36	126.49	119.66
1	G	212	ARG	CA-C-N	9.35	126.48	119.66
1	G	212	ARG	C-N-CA	9.35	126.48	119.66
1	F	212	ARG	CA-C-N	9.10	126.31	119.66
1	F	212	ARG	C-N-CA	9.10	126.31	119.66
1	C	212	ARG	CA-C-N	8.88	126.14	119.66
1	C	212	ARG	C-N-CA	8.88	126.14	119.66
1	E	212	ARG	CA-C-N	8.49	125.86	119.66
1	E	212	ARG	C-N-CA	8.49	125.86	119.66
1	D	212	ARG	CA-C-N	8.29	125.71	119.66
1	D	212	ARG	C-N-CA	8.29	125.71	119.66
1	G	318	SER	N-CA-C	7.13	120.83	110.28
1	F	458	TYR	N-CA-C	-6.93	104.77	113.23
1	H	458	TYR	N-CA-C	-6.90	104.81	113.23
1	D	458	TYR	N-CA-C	-6.88	104.83	113.23
1	B	318	SER	N-CA-C	6.84	120.41	110.28
1	G	148	SER	CA-C-N	6.83	133.99	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	148	SER	C-N-CA	6.83	133.99	121.70
1	C	318	SER	N-CA-C	6.79	120.33	110.28
1	G	184	ALA	N-CA-C	6.78	120.72	108.17
1	F	269	VAL	N-CA-C	6.78	117.39	111.90
1	A	184	ALA	N-CA-C	6.76	120.70	107.98
1	G	67	GLY	N-CA-C	-6.72	105.05	115.73
1	B	148	SER	CA-C-N	6.71	133.79	121.70
1	B	148	SER	C-N-CA	6.71	133.79	121.70
1	G	52	PRO	N-CA-C	-6.68	100.72	110.80
1	H	52	PRO	N-CA-C	-6.67	100.71	111.19
1	C	184	ALA	N-CA-C	6.67	120.51	108.17
1	E	318	SER	N-CA-C	6.66	120.13	110.28
1	H	184	ALA	N-CA-C	6.65	120.47	108.17
1	H	318	SER	N-CA-C	6.65	119.88	110.50
1	H	269	VAL	N-CA-C	6.60	117.25	111.90
1	E	269	VAL	N-CA-C	6.57	117.22	111.90
1	A	269	VAL	N-CA-C	6.55	117.21	111.90
1	E	52	PRO	N-CA-C	-6.54	100.93	110.80
1	D	184	ALA	N-CA-C	6.51	120.21	108.17
1	A	52	PRO	N-CA-C	-6.50	100.99	111.19
1	D	52	PRO	N-CA-C	-6.48	101.02	111.19
1	C	123	HIS	N-CA-C	-6.45	98.89	109.40
1	B	52	PRO	N-CA-C	-6.44	101.07	111.19
1	G	458	TYR	N-CA-C	-6.43	105.39	113.23
1	D	269	VAL	N-CA-C	6.41	117.09	111.90
1	D	318	SER	N-CA-C	6.40	119.75	110.28
1	B	67	GLY	N-CA-C	-6.39	105.57	115.73
1	F	184	ALA	N-CA-C	6.38	119.98	107.98
1	B	269	VAL	N-CA-C	6.38	117.06	111.90
1	C	52	PRO	N-CA-C	-6.37	101.19	110.80
1	E	67	GLY	N-CA-C	-6.34	105.65	115.73
1	C	67	GLY	N-CA-C	-6.31	105.70	115.73
1	G	269	VAL	N-CA-C	6.30	117.00	111.90
1	F	67	GLY	N-CA-C	-6.27	105.77	115.73
1	A	67	GLY	N-CA-C	-6.26	105.78	115.73
1	G	26	GLY	N-CA-C	-6.24	107.06	115.36
1	A	148	SER	CA-C-N	6.24	132.93	121.70
1	A	148	SER	C-N-CA	6.24	132.93	121.70
1	F	318	SER	N-CA-C	6.21	119.47	110.28
1	F	52	PRO	N-CA-C	-6.21	100.70	111.32
1	H	67	GLY	N-CA-C	-6.20	105.87	115.73
1	E	184	ALA	N-CA-C	6.20	119.63	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ALA	N-CA-C	6.16	119.56	107.98
1	A	318	SER	N-CA-C	6.15	119.39	110.28
1	C	269	VAL	N-CA-C	6.15	116.88	111.90
1	E	123	HIS	N-CA-C	-6.15	99.38	109.40
1	B	272	GLN	N-CA-C	6.14	118.77	111.33
1	C	458	TYR	N-CA-C	-6.11	104.42	113.40
1	A	458	TYR	N-CA-C	-6.08	105.81	113.23
1	D	67	GLY	N-CA-C	-6.07	106.09	115.73
1	B	123	HIS	N-CA-C	-5.93	99.73	109.40
1	D	148	SER	CA-C-N	5.93	132.38	121.70
1	D	148	SER	C-N-CA	5.93	132.38	121.70
1	A	26	GLY	N-CA-C	-5.93	107.47	115.36
1	A	123	HIS	N-CA-C	-5.93	99.74	109.40
1	E	458	TYR	N-CA-C	-5.92	104.70	113.40
1	D	272	GLN	N-CA-C	5.91	118.48	111.33
1	F	295	TRP	N-CA-C	5.90	119.58	112.38
1	H	123	HIS	N-CA-C	-5.89	99.79	109.40
1	F	26	GLY	N-CA-C	-5.89	107.53	115.36
1	H	26	GLY	N-CA-C	-5.83	107.20	115.30
1	G	123	HIS	N-CA-C	-5.82	99.92	109.40
1	H	381	LYS	N-CA-C	-5.74	105.03	111.28
1	H	295	TRP	N-CA-C	5.72	119.36	112.38
1	E	272	GLN	N-CA-C	5.70	118.23	111.33
1	F	272	GLN	N-CA-C	5.67	118.19	111.33
1	F	123	HIS	N-CA-C	-5.67	100.16	109.40
1	B	26	GLY	N-CA-C	-5.67	107.83	115.36
1	H	454	LYS	N-CA-C	-5.66	100.76	109.76
1	B	454	LYS	N-CA-C	-5.66	100.76	109.76
1	C	454	LYS	N-CA-C	-5.65	100.78	109.76
1	A	272	GLN	N-CA-C	5.62	118.13	111.33
1	A	295	TRP	N-CA-C	5.61	119.22	112.38
1	C	295	TRP	N-CA-C	5.60	119.21	112.38
1	A	381	LYS	N-CA-C	-5.59	105.18	111.28
1	E	295	TRP	N-CA-C	5.57	119.18	112.38
1	C	208	HIS	N-CA-C	-5.57	105.29	111.36
1	D	123	HIS	N-CA-C	-5.55	100.36	109.40
1	B	208	HIS	N-CA-C	-5.49	105.37	111.36
1	D	295	TRP	N-CA-C	5.48	119.06	112.38
1	D	454	LYS	N-CA-C	-5.47	101.06	109.76
1	F	315	ASP	N-CA-C	-5.43	104.64	111.92
1	B	458	TYR	N-CA-C	-5.42	105.44	113.40
1	D	26	GLY	N-CA-C	-5.40	107.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	GLY	N-CA-C	-5.39	107.80	115.30
1	A	454	LYS	N-CA-C	-5.37	101.22	109.76
1	B	295	TRP	N-CA-C	5.37	118.93	112.38
1	F	454	LYS	N-CA-C	-5.37	101.23	109.76
1	A	103	LYS	N-CA-C	-5.35	105.09	111.03
1	E	454	LYS	N-CA-C	-5.34	100.59	109.46
1	E	208	HIS	N-CA-C	-5.34	105.54	111.36
1	E	335	ILE	N-CA-C	-5.31	104.06	108.63
1	C	397	ASP	CA-C-N	5.29	125.38	119.87
1	C	397	ASP	C-N-CA	5.29	125.38	119.87
1	E	26	GLY	N-CA-C	-5.29	107.94	115.30
1	G	153	MET	N-CA-C	-5.29	106.82	113.28
1	G	454	LYS	N-CA-C	-5.28	101.37	109.76
1	C	381	LYS	N-CA-C	-5.27	105.53	111.28
1	B	148	SER	O-C-N	-5.27	116.17	123.12
1	G	295	TRP	N-CA-C	5.25	118.78	112.38
1	H	208	HIS	N-CA-C	-5.24	105.65	111.36
1	G	335	ILE	N-CA-C	-5.23	104.14	108.63
1	C	182	VAL	N-CA-C	5.20	116.14	108.45
1	B	381	LYS	N-CA-C	-5.20	105.51	111.07
1	C	131	ASP	N-CA-C	-5.18	105.76	111.71
1	D	103	LYS	N-CA-C	-5.17	105.29	111.03
1	G	208	HIS	N-CA-C	-5.13	105.77	111.36
1	E	381	LYS	N-CA-C	-5.12	105.69	111.28
1	A	208	HIS	N-CA-C	-5.08	105.83	111.36
1	D	406	ALA	N-CA-C	-5.07	106.19	112.38
1	F	381	LYS	N-CA-C	-5.07	105.84	111.36
1	E	103	LYS	N-CA-C	-5.06	105.42	111.03
1	E	131	ASP	N-CA-C	-5.05	105.77	111.28
1	H	148	SER	CA-C-N	5.04	130.76	121.70
1	H	148	SER	C-N-CA	5.04	130.76	121.70
1	B	406	ALA	N-CA-C	-5.03	106.25	112.38
1	F	241	THR	N-CA-C	5.01	119.00	112.13

There are no chirality outliers.

There are no planarity outliers.

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	3560	0	3551	256	0
1	B	3560	0	3549	228	0
1	C	3560	0	3550	248	0
1	D	3560	0	3551	266	0
1	E	3560	0	3550	237	0
1	F	3560	0	3551	254	0
1	G	3560	0	3550	236	0
1	H	3560	0	3550	237	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
All	All	28496	0	28402	1859	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 33.

All (1859) 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:78:THR:HG21	1:C:117:VAL:H	1.08	1.17
1:A:78:THR:HG21	1:A:117:VAL:H	1.05	1.15
1:A:280:PHE:HB3	1:D:67:GLY:HA2	1.29	1.15
1:B:78:THR:HG21	1:B:117:VAL:H	1.06	1.14
1:C:223:ARG:HD3	1:F:223:ARG:HD3	1.32	1.12
1:G:78:THR:HG21	1:G:117:VAL:H	1.08	1.09
1:D:78:THR:HG21	1:D:117:VAL:H	1.06	1.09
1:F:78:THR:HG21	1:F:117:VAL:H	1.03	1.08
1:E:78:THR:HG21	1:E:117:VAL:H	1.06	1.07
1:C:192:TYR:CE2	1:F:129:ILE:HD11	1.89	1.06
1:H:78:THR:HG21	1:H:117:VAL:H	1.07	1.06
1:C:192:TYR:HE2	1:F:129:ILE:HD11	1.12	1.06
1:A:279:ASN:HB3	1:D:66:GLY:H	1.22	1.02
1:A:421:MET:HA	1:D:103:LYS:NZ	1.73	1.02
1:F:261:GLY:H	1:F:310:GLN:NE2	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:402:ARG:HE	1:F:426:GLU:HB2	1.26	1.00
1:C:261:GLY:H	1:C:310:GLN:NE2	1.59	1.00
1:D:261:GLY:H	1:D:310:GLN:NE2	1.58	1.00
1:E:254:ASN:HD21	1:F:254:ASN:HD21	1.04	1.00
1:H:261:GLY:H	1:H:310:GLN:NE2	1.59	1.00
1:F:78:THR:HG21	1:F:117:VAL:N	1.76	1.00
1:A:278:PRO:HD2	1:A:281:GLU:HB2	1.43	0.99
1:B:261:GLY:H	1:B:310:GLN:NE2	1.59	0.99
1:C:386:VAL:HG21	1:D:15:ASP:CG	1.88	0.98
1:H:261:GLY:H	1:H:310:GLN:HE21	1.11	0.98
1:C:153:MET:HE3	1:C:220:ALA:HB1	1.45	0.98
1:G:254:ASN:HD21	1:H:254:ASN:ND2	1.60	0.98
1:H:278:PRO:HD2	1:H:281:GLU:HB2	1.46	0.98
1:B:261:GLY:H	1:B:310:GLN:HE21	1.12	0.97
1:A:261:GLY:H	1:A:310:GLN:NE2	1.61	0.97
1:A:78:THR:HG21	1:A:117:VAL:N	1.79	0.97
1:C:78:THR:HG21	1:C:117:VAL:N	1.80	0.97
1:G:261:GLY:H	1:G:310:GLN:NE2	1.61	0.97
1:F:153:MET:HE3	1:F:220:ALA:HB1	1.46	0.97
1:A:254:ASN:HD21	1:B:254:ASN:HD21	1.10	0.96
1:G:78:THR:HG21	1:G:117:VAL:N	1.80	0.96
1:C:129:ILE:HD11	1:F:192:TYR:HE2	1.29	0.96
1:D:78:THR:HG23	1:D:118:ILE:HG12	1.48	0.96
1:D:402:ARG:HE	1:D:426:GLU:HB2	1.28	0.96
1:E:261:GLY:H	1:E:310:GLN:NE2	1.61	0.96
1:H:78:THR:HG21	1:H:117:VAL:N	1.79	0.96
1:G:254:ASN:ND2	1:H:254:ASN:HD21	1.63	0.96
1:G:303:ALA:HA	1:G:308:GLN:HG2	1.48	0.96
1:B:402:ARG:HE	1:B:426:GLU:HB2	1.30	0.96
1:E:78:THR:HG23	1:E:118:ILE:HG12	1.47	0.96
1:B:78:THR:HG21	1:B:117:VAL:N	1.79	0.95
1:C:261:GLY:H	1:C:310:GLN:HE21	1.11	0.95
1:D:78:THR:HG21	1:D:117:VAL:N	1.80	0.95
1:E:78:THR:HG21	1:E:117:VAL:N	1.79	0.95
1:E:303:ALA:HA	1:E:308:GLN:HG2	1.49	0.95
1:A:279:ASN:HB3	1:D:66:GLY:N	1.79	0.95
1:H:78:THR:HG23	1:H:118:ILE:HG12	1.45	0.95
1:C:78:THR:HG23	1:C:118:ILE:HG12	1.48	0.95
1:F:78:THR:HG23	1:F:118:ILE:HG12	1.49	0.95
1:E:207:TYR:O	1:E:211:THR:HB	1.67	0.95
1:G:153:MET:HE3	1:G:220:ALA:HB1	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HE3	1:A:220:ALA:HB1	1.48	0.94
1:B:303:ALA:HA	1:B:308:GLN:HG2	1.48	0.94
1:F:278:PRO:HD2	1:F:281:GLU:HB2	1.45	0.94
1:H:303:ALA:HA	1:H:308:GLN:HG2	1.48	0.94
1:E:153:MET:HE3	1:E:220:ALA:HB1	1.49	0.94
1:A:303:ALA:HA	1:A:308:GLN:HG2	1.49	0.94
1:B:78:THR:HG23	1:B:118:ILE:HG12	1.50	0.94
1:D:153:MET:HE3	1:D:220:ALA:HB1	1.48	0.94
1:B:278:PRO:HD2	1:B:281:GLU:HB2	1.50	0.93
1:C:278:PRO:HD2	1:C:281:GLU:HB2	1.49	0.93
1:D:278:PRO:HD2	1:D:281:GLU:HB2	1.48	0.93
1:C:402:ARG:HE	1:C:426:GLU:HB2	1.32	0.93
1:A:402:ARG:HE	1:A:426:GLU:HB2	1.29	0.93
1:G:278:PRO:HD2	1:G:281:GLU:HB2	1.48	0.93
1:D:223:ARG:HD3	1:E:223:ARG:HD3	1.49	0.93
1:A:78:THR:HG23	1:A:118:ILE:HG12	1.50	0.93
1:E:402:ARG:HE	1:E:426:GLU:HB2	1.34	0.93
1:A:261:GLY:H	1:A:310:GLN:HE21	1.17	0.93
1:G:402:ARG:HE	1:G:426:GLU:HB2	1.30	0.93
1:H:402:ARG:HE	1:H:426:GLU:HB2	1.30	0.92
1:F:303:ALA:HA	1:F:308:GLN:HG2	1.50	0.92
1:F:261:GLY:H	1:F:310:GLN:HE21	1.14	0.92
1:C:303:ALA:HA	1:C:308:GLN:HG2	1.49	0.92
1:D:303:ALA:HA	1:D:308:GLN:HG2	1.49	0.92
1:B:153:MET:HE3	1:B:220:ALA:HB1	1.49	0.92
1:E:278:PRO:HD2	1:E:281:GLU:HB2	1.51	0.92
1:G:78:THR:HG23	1:G:118:ILE:HG12	1.47	0.92
1:G:261:GLY:H	1:G:310:GLN:HE21	1.13	0.92
1:H:153:MET:HE3	1:H:220:ALA:HB1	1.49	0.92
1:D:261:GLY:H	1:D:310:GLN:HE21	1.11	0.91
1:D:192:TYR:HE2	1:E:129:ILE:HD11	1.34	0.91
1:G:207:TYR:O	1:G:211:THR:HB	1.70	0.91
1:D:305:LYS:NZ	1:D:358:ARG:HA	1.86	0.90
1:E:261:GLY:H	1:E:310:GLN:HE21	1.11	0.90
1:B:207:TYR:O	1:B:211:THR:HB	1.71	0.89
1:G:305:LYS:NZ	1:G:358:ARG:HA	1.87	0.89
1:A:305:LYS:NZ	1:A:358:ARG:HA	1.87	0.89
1:G:263:THR:HG22	1:G:264:CYS:H	1.38	0.89
1:A:280:PHE:CB	1:D:67:GLY:HA2	2.02	0.88
1:E:305:LYS:NZ	1:E:358:ARG:HA	1.88	0.88
1:A:207:TYR:O	1:A:211:THR:HB	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:TYR:O	1:D:211:THR:HB	1.73	0.88
1:C:207:TYR:O	1:C:211:THR:HB	1.72	0.88
1:C:305:LYS:NZ	1:C:358:ARG:HA	1.88	0.87
1:B:305:LYS:NZ	1:B:358:ARG:HA	1.90	0.87
1:F:263:THR:HG22	1:F:264:CYS:H	1.39	0.87
1:F:305:LYS:NZ	1:F:358:ARG:HA	1.90	0.86
1:H:207:TYR:O	1:H:211:THR:HB	1.74	0.86
1:F:207:TYR:O	1:F:211:THR:HB	1.75	0.86
1:A:421:MET:HA	1:D:103:LYS:HZ3	1.41	0.86
1:D:263:THR:HG22	1:D:264:CYS:H	1.42	0.85
1:D:129:ILE:HD11	1:E:192:TYR:CE2	2.11	0.85
1:C:263:THR:HG22	1:C:264:CYS:H	1.40	0.85
1:A:263:THR:HG22	1:A:264:CYS:H	1.42	0.84
1:H:305:LYS:NZ	1:H:358:ARG:HA	1.93	0.84
1:B:263:THR:HG22	1:B:264:CYS:H	1.41	0.84
1:H:52:PRO:HG3	1:H:385:ILE:HG13	1.58	0.84
1:F:174:LYS:HB2	1:F:233:SER:HB3	1.60	0.83
1:A:15:ASP:CG	1:B:386:VAL:HG21	2.04	0.83
1:F:11:VAL:HG11	1:F:361:LEU:HG	1.61	0.83
1:E:59:THR:HG22	1:E:91:ASP:OD2	1.79	0.83
1:E:150:KCX:HB3	1:E:181:MET:HE3	1.61	0.82
1:D:129:ILE:HD11	1:E:192:TYR:HE2	1.45	0.82
1:B:174:LYS:HB2	1:B:233:SER:HB3	1.62	0.82
1:A:11:VAL:HG11	1:A:361:LEU:HG	1.61	0.81
1:F:129:ILE:HD13	1:F:168:CYS:CB	2.11	0.81
1:G:129:ILE:HD13	1:G:168:CYS:CB	2.11	0.81
1:A:174:LYS:HB2	1:A:233:SER:HB3	1.61	0.81
1:A:386:VAL:HG21	1:B:15:ASP:CG	2.05	0.80
1:B:11:VAL:HG11	1:B:361:LEU:HG	1.64	0.80
1:D:129:ILE:HD13	1:D:168:CYS:CB	2.12	0.80
1:G:11:VAL:HG11	1:G:361:LEU:HG	1.63	0.80
1:G:174:LYS:HB2	1:G:233:SER:HB3	1.63	0.80
1:A:223:ARG:HD3	1:H:223:ARG:HD3	1.61	0.80
1:C:129:ILE:HD13	1:C:168:CYS:CB	2.11	0.80
1:D:11:VAL:HG11	1:D:361:LEU:HG	1.62	0.80
1:H:11:VAL:HG11	1:H:361:LEU:HG	1.62	0.80
1:D:167:TYR:CE1	1:D:171:LEU:HD11	2.17	0.79
1:B:129:ILE:HD13	1:B:168:CYS:CB	2.11	0.79
1:A:129:ILE:HD13	1:A:168:CYS:CB	2.12	0.79
1:F:52:PRO:HG3	1:F:385:ILE:HG13	1.64	0.79
1:C:52:PRO:HG3	1:C:385:ILE:HG13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LYS:HB2	1:C:233:SER:HB3	1.65	0.79
1:C:59:THR:HG22	1:C:91:ASP:OD2	1.82	0.79
1:B:129:ILE:HD13	1:B:168:CYS:HB2	1.65	0.79
1:H:263:THR:HG22	1:H:264:CYS:H	1.47	0.79
1:F:59:THR:HG22	1:F:91:ASP:OD2	1.82	0.79
1:A:167:TYR:CE1	1:A:171:LEU:HD11	2.18	0.79
1:H:167:TYR:CE1	1:H:171:LEU:HD11	2.19	0.78
1:G:263:THR:HG22	1:G:264:CYS:N	1.99	0.78
1:H:129:ILE:HD13	1:H:168:CYS:CB	2.13	0.78
1:D:129:ILE:HD13	1:D:168:CYS:HB2	1.65	0.78
1:H:174:LYS:HB2	1:H:233:SER:HB3	1.64	0.78
1:E:263:THR:HG22	1:E:264:CYS:H	1.49	0.78
1:B:52:PRO:HG3	1:B:385:ILE:HG13	1.65	0.78
1:G:167:TYR:CE1	1:G:171:LEU:HD11	2.19	0.78
1:D:59:THR:HG22	1:D:91:ASP:OD2	1.84	0.78
1:D:174:LYS:HB2	1:D:233:SER:HB3	1.64	0.78
1:F:167:TYR:CE1	1:F:171:LEU:HD11	2.18	0.78
1:E:217:GLU:OE1	1:E:241:THR:HB	1.84	0.77
1:E:52:PRO:HG3	1:E:385:ILE:HG13	1.64	0.77
1:B:150:KCX:HB3	1:B:181:MET:HE3	1.67	0.77
1:C:11:VAL:HG11	1:C:361:LEU:HG	1.67	0.77
1:A:78:THR:CG2	1:A:117:VAL:H	1.94	0.77
1:B:400:ILE:HD13	1:B:441:LYS:NZ	2.00	0.77
1:C:217:GLU:OE1	1:C:241:THR:HB	1.85	0.77
1:E:123:HIS:CG	1:E:181:MET:HE1	2.20	0.77
1:H:400:ILE:HD13	1:H:441:LYS:NZ	1.99	0.77
1:A:52:PRO:HG3	1:A:385:ILE:HG13	1.66	0.77
1:B:167:TYR:CE1	1:B:171:LEU:HD11	2.20	0.77
1:E:174:LYS:HB2	1:E:233:SER:HB3	1.65	0.76
1:F:217:GLU:OE1	1:F:241:THR:HB	1.85	0.76
1:F:129:ILE:HD13	1:F:168:CYS:HB2	1.68	0.76
1:D:52:PRO:HG3	1:D:385:ILE:HG13	1.65	0.76
1:E:11:VAL:HG11	1:E:361:LEU:HG	1.67	0.76
1:E:129:ILE:HD13	1:E:168:CYS:HB2	1.68	0.76
1:G:3:LYS:HA	1:G:40:ALA:O	1.85	0.76
1:C:168:CYS:HG	1:F:192:TYR:HD2	1.32	0.76
1:D:123:HIS:CG	1:D:181:MET:HE1	2.21	0.76
1:G:400:ILE:HD13	1:G:441:LYS:NZ	2.01	0.76
1:A:59:THR:HG22	1:A:91:ASP:OD2	1.85	0.76
1:C:129:ILE:HD13	1:C:168:CYS:HB2	1.68	0.76
1:E:129:ILE:HD13	1:E:168:CYS:CB	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:THR:CG2	1:F:117:VAL:H	1.93	0.76
1:A:129:ILE:HD13	1:A:168:CYS:HB2	1.66	0.75
1:B:263:THR:HG22	1:B:264:CYS:N	2.00	0.75
1:D:305:LYS:HZ1	1:D:358:ARG:HA	1.50	0.75
1:G:59:THR:HG22	1:G:91:ASP:OD2	1.86	0.75
1:G:129:ILE:HD13	1:G:168:CYS:HB2	1.66	0.75
1:B:3:LYS:HA	1:B:40:ALA:O	1.86	0.75
1:B:223:ARG:HD3	1:G:223:ARG:HD3	1.66	0.75
1:E:400:ILE:HD13	1:E:441:LYS:NZ	2.02	0.75
1:A:280:PHE:HB3	1:D:67:GLY:CA	2.11	0.75
1:H:129:ILE:HD13	1:H:168:CYS:HB2	1.69	0.75
1:C:400:ILE:HD13	1:C:441:LYS:NZ	2.00	0.75
1:G:305:LYS:HZ3	1:G:358:ARG:HA	1.52	0.75
1:H:360:THR:HG22	1:H:362:ASN:H	1.52	0.75
1:F:360:THR:HG22	1:F:362:ASN:H	1.49	0.75
1:G:78:THR:CG2	1:G:117:VAL:H	1.95	0.75
1:D:217:GLU:OE1	1:D:241:THR:HB	1.86	0.74
1:B:78:THR:CG2	1:B:117:VAL:H	1.94	0.74
1:C:78:THR:CG2	1:C:117:VAL:H	1.96	0.74
1:G:123:HIS:CG	1:G:181:MET:HE1	2.21	0.74
1:F:60:HIS:HB3	1:F:63:MET:HG2	1.70	0.74
1:F:263:THR:HG22	1:F:264:CYS:N	2.00	0.74
1:A:421:MET:HA	1:D:103:LYS:HZ2	1.50	0.74
1:A:263:THR:HG22	1:A:264:CYS:N	2.02	0.74
1:G:52:PRO:HG3	1:G:385:ILE:HG13	1.69	0.74
1:G:360:THR:HG22	1:G:362:ASN:H	1.53	0.74
1:A:60:HIS:HB3	1:A:63:MET:HG2	1.69	0.74
1:C:263:THR:HG22	1:C:264:CYS:N	2.03	0.74
1:H:60:HIS:HB3	1:H:63:MET:HG2	1.68	0.74
1:C:123:HIS:CG	1:C:181:MET:HE1	2.23	0.74
1:F:402:ARG:NE	1:F:426:GLU:HB2	2.03	0.74
1:H:59:THR:HG22	1:H:91:ASP:OD2	1.88	0.74
1:B:59:THR:HG22	1:B:91:ASP:OD2	1.87	0.73
1:B:360:THR:H	1:B:363:GLN:HB2	1.52	0.73
1:D:78:THR:CG2	1:D:117:VAL:H	1.95	0.73
1:G:217:GLU:OE1	1:G:241:THR:HB	1.88	0.73
1:B:60:HIS:HB3	1:B:63:MET:HG2	1.69	0.73
1:F:153:MET:HE1	1:F:220:ALA:O	1.89	0.73
1:A:360:THR:HG22	1:A:362:ASN:H	1.53	0.73
1:C:167:TYR:CE1	1:C:171:LEU:HD11	2.23	0.73
1:A:3:LYS:HA	1:A:40:ALA:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:ILE:HD13	1:D:441:LYS:NZ	2.02	0.73
1:C:360:THR:HG22	1:C:362:ASN:H	1.52	0.73
1:A:123:HIS:CG	1:A:181:MET:HE1	2.23	0.73
1:F:3:LYS:HA	1:F:40:ALA:O	1.89	0.73
1:H:3:LYS:HA	1:H:40:ALA:O	1.88	0.73
1:H:78:THR:CG2	1:H:117:VAL:H	1.95	0.73
1:E:24:LYS:HB2	1:E:29:ALA:HB2	1.71	0.73
1:A:305:LYS:HZ3	1:A:358:ARG:HA	1.53	0.72
1:B:71:LYS:HE3	1:B:320:ASP:OD2	1.88	0.72
1:B:217:GLU:OE1	1:B:241:THR:HB	1.88	0.72
1:D:3:LYS:HA	1:D:40:ALA:O	1.89	0.72
1:E:3:LYS:HA	1:E:40:ALA:O	1.89	0.72
1:F:150:KCX:HB3	1:F:181:MET:HE3	1.70	0.72
1:H:78:THR:CG2	1:H:118:ILE:HG12	2.19	0.72
1:A:420:GLY:C	1:D:103:LYS:HD3	2.13	0.72
1:E:60:HIS:HB3	1:E:63:MET:HG2	1.71	0.72
1:E:167:TYR:CE1	1:E:171:LEU:HD11	2.25	0.72
1:E:360:THR:HG22	1:E:362:ASN:H	1.55	0.72
1:F:400:ILE:HD13	1:F:441:LYS:NZ	2.05	0.72
1:G:360:THR:H	1:G:363:GLN:HB2	1.54	0.72
1:E:360:THR:H	1:E:363:GLN:HB2	1.54	0.72
1:H:24:LYS:HB2	1:H:29:ALA:HB2	1.71	0.72
1:A:400:ILE:HD13	1:A:441:LYS:NZ	2.03	0.72
1:B:192:TYR:HE2	1:G:129:ILE:HD11	1.54	0.72
1:D:263:THR:HG22	1:D:264:CYS:N	2.01	0.72
1:G:402:ARG:NE	1:G:426:GLU:HB2	2.05	0.72
1:D:60:HIS:HB3	1:D:63:MET:HG2	1.72	0.71
1:F:24:LYS:HB2	1:F:29:ALA:HB2	1.72	0.71
1:B:360:THR:HG22	1:B:362:ASN:H	1.55	0.71
1:C:305:LYS:HZ3	1:C:358:ARG:HA	1.52	0.71
1:H:217:GLU:OE1	1:H:241:THR:HB	1.90	0.71
1:C:254:ASN:HD21	1:D:254:ASN:HD21	1.37	0.71
1:D:192:TYR:HD2	1:E:168:CYS:HG	1.38	0.71
1:B:24:LYS:HB2	1:B:29:ALA:HB2	1.73	0.71
1:C:206:ILE:HD12	1:C:276:GLU:HG2	1.73	0.71
1:C:223:ARG:CD	1:F:223:ARG:HD3	2.17	0.71
1:H:123:HIS:CG	1:H:181:MET:HE1	2.26	0.71
1:H:360:THR:H	1:H:363:GLN:HB2	1.54	0.71
1:A:217:GLU:OE1	1:A:241:THR:HB	1.90	0.71
1:C:3:LYS:HA	1:C:40:ALA:O	1.89	0.71
1:D:57:PRO:HD3	1:D:372:ILE:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:HIS:HB3	1:G:63:MET:HG2	1.72	0.70
1:A:280:PHE:CB	1:D:67:GLY:CA	2.68	0.70
1:F:305:LYS:HZ1	1:F:358:ARG:HA	1.53	0.70
1:G:24:LYS:HB2	1:G:29:ALA:HB2	1.73	0.70
1:A:24:LYS:HB2	1:A:29:ALA:HB2	1.73	0.70
1:A:402:ARG:NE	1:A:426:GLU:HB2	2.05	0.70
1:C:24:LYS:HB2	1:C:29:ALA:HB2	1.72	0.70
1:D:360:THR:HG22	1:D:362:ASN:H	1.56	0.70
1:D:24:LYS:HB2	1:D:29:ALA:HB2	1.72	0.70
1:D:340:PRO:HB3	1:D:413:VAL:HG21	1.73	0.70
1:E:386:VAL:HG21	1:F:15:ASP:CG	2.15	0.70
1:B:305:LYS:HZ1	1:B:358:ARG:HA	1.55	0.70
1:F:78:THR:HG22	1:F:117:VAL:HB	1.73	0.70
1:B:206:ILE:HD12	1:B:276:GLU:HG2	1.73	0.70
1:B:400:ILE:HD13	1:B:441:LYS:HZ1	1.56	0.70
1:H:150:KCX:HB3	1:H:181:MET:HE3	1.73	0.70
1:C:223:ARG:HD3	1:F:223:ARG:CD	2.17	0.70
1:C:306:ASN:ND2	1:D:256:GLY:HA2	2.06	0.70
1:F:123:HIS:CG	1:F:181:MET:HE1	2.27	0.70
1:F:340:PRO:HB3	1:F:413:VAL:HG21	1.74	0.70
1:C:340:PRO:HB3	1:C:413:VAL:HG21	1.74	0.70
1:D:360:THR:H	1:D:363:GLN:HB2	1.55	0.70
1:A:206:ILE:HD12	1:A:276:GLU:HG2	1.73	0.69
1:E:78:THR:CG2	1:E:118:ILE:HG12	2.21	0.69
1:B:57:PRO:HD3	1:B:372:ILE:HD13	1.74	0.69
1:C:78:THR:CG2	1:C:118:ILE:HG12	2.22	0.69
1:G:340:PRO:HB3	1:G:413:VAL:HG21	1.73	0.69
1:H:305:LYS:HZ1	1:H:358:ARG:HA	1.55	0.69
1:H:359:ILE:HG22	1:H:360:THR:N	2.06	0.69
1:C:60:HIS:HB3	1:C:63:MET:HG2	1.73	0.69
1:F:359:ILE:HG22	1:F:360:THR:N	2.07	0.69
1:H:263:THR:HG22	1:H:264:CYS:N	2.05	0.69
1:D:78:THR:CG2	1:D:118:ILE:HG12	2.22	0.69
1:D:402:ARG:NE	1:D:426:GLU:HB2	2.05	0.69
1:A:360:THR:H	1:A:363:GLN:HB2	1.58	0.69
1:B:123:HIS:CG	1:B:181:MET:HE1	2.27	0.69
1:C:57:PRO:HD3	1:C:372:ILE:HD13	1.73	0.69
1:H:340:PRO:HB3	1:H:413:VAL:HG21	1.75	0.69
1:A:279:ASN:HB3	1:D:66:GLY:CA	2.23	0.69
1:G:78:THR:CG2	1:G:118:ILE:HG12	2.20	0.69
1:A:340:PRO:HB3	1:A:413:VAL:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:ILE:HD13	1:E:441:LYS:HZ1	1.58	0.68
1:H:71:LYS:HE3	1:H:320:ASP:OD2	1.94	0.68
1:H:402:ARG:NE	1:H:426:GLU:HB2	2.05	0.68
1:B:340:PRO:HB3	1:B:413:VAL:HG21	1.75	0.68
1:F:206:ILE:HD12	1:F:276:GLU:HG2	1.76	0.68
1:F:360:THR:H	1:F:363:GLN:HB2	1.57	0.68
1:A:403:VAL:HG21	1:D:106:GLU:OE1	1.93	0.68
1:E:78:THR:CG2	1:E:117:VAL:H	1.95	0.68
1:D:150:KCX:HB3	1:D:181:MET:HE3	1.76	0.68
1:F:57:PRO:HD3	1:F:372:ILE:HD13	1.74	0.68
1:G:71:LYS:HE3	1:G:320:ASP:OD2	1.92	0.68
1:E:263:THR:HG22	1:E:264:CYS:N	2.08	0.68
1:G:144:GLU:H	1:G:454:LYS:NZ	1.92	0.68
1:G:57:PRO:HD3	1:G:372:ILE:HD13	1.75	0.67
1:A:71:LYS:HE3	1:A:320:ASP:OD2	1.93	0.67
1:C:402:ARG:NE	1:C:426:GLU:HB2	2.07	0.67
1:G:391:ALA:HB3	1:G:434:GLY:N	2.10	0.67
1:A:57:PRO:HD3	1:A:372:ILE:HD13	1.76	0.67
1:G:206:ILE:HD12	1:G:276:GLU:HG2	1.76	0.67
1:H:206:ILE:HD12	1:H:276:GLU:HG2	1.76	0.67
1:B:2:THR:HG21	1:B:37:GLU:OE1	1.93	0.67
1:B:129:ILE:HD11	1:G:192:TYR:HE2	1.59	0.67
1:A:92:PHE:HE2	1:A:150:KCX:HD2	1.59	0.67
1:E:305:LYS:HZ3	1:E:358:ARG:HA	1.57	0.67
1:E:130:THR:HB	1:E:133:VAL:HG23	1.76	0.67
1:E:206:ILE:HD12	1:E:276:GLU:HG2	1.76	0.67
1:E:254:ASN:HD21	1:F:254:ASN:ND2	1.87	0.67
1:H:241:THR:CG2	1:H:292:ARG:HE	2.07	0.67
1:D:2:THR:HG21	1:D:37:GLU:OE1	1.95	0.67
1:D:359:ILE:HG22	1:D:360:THR:N	2.10	0.67
1:E:57:PRO:HD3	1:E:372:ILE:HD13	1.77	0.67
1:E:306:ASN:ND2	1:F:256:GLY:HA2	2.10	0.67
1:H:20:HIS:HD2	1:H:35:LEU:H	1.43	0.67
1:A:78:THR:CG2	1:A:118:ILE:HG12	2.24	0.66
1:A:130:THR:HB	1:A:133:VAL:HG23	1.77	0.66
1:A:279:ASN:CB	1:D:66:GLY:H	2.03	0.66
1:B:402:ARG:NE	1:B:426:GLU:HB2	2.06	0.66
1:C:397:ASP:CG	1:C:400:ILE:HG13	2.19	0.66
1:H:130:THR:HB	1:H:133:VAL:HG23	1.78	0.66
1:A:241:THR:CG2	1:A:292:ARG:HE	2.08	0.66
1:B:78:THR:CG2	1:B:118:ILE:HG12	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLU:O	1:C:144:GLU:HB2	1.95	0.66
1:A:20:HIS:HD2	1:A:35:LEU:H	1.44	0.66
1:G:386:VAL:HG21	1:H:15:ASP:CG	2.20	0.66
1:C:359:ILE:HG22	1:C:360:THR:N	2.10	0.66
1:F:391:ALA:HB3	1:F:434:GLY:N	2.11	0.66
1:G:277:LYS:O	1:G:277:LYS:HG2	1.96	0.66
1:H:57:PRO:HD3	1:H:372:ILE:HD13	1.76	0.66
1:E:2:THR:HG21	1:E:37:GLU:OE1	1.95	0.66
1:G:260:TRP:HE3	1:G:310:GLN:HG3	1.60	0.66
1:H:277:LYS:HG2	1:H:277:LYS:O	1.96	0.66
1:A:239:HIS:CE1	1:A:289:PRO:HD3	2.31	0.66
1:A:359:ILE:HG22	1:A:360:THR:N	2.10	0.66
1:D:391:ALA:HB3	1:D:434:GLY:N	2.10	0.66
1:G:141:LEU:HD11	1:G:176:LEU:HB3	1.78	0.66
1:B:260:TRP:HE3	1:B:310:GLN:HG3	1.61	0.66
1:C:215:GLU:HB2	1:F:230:LEU:HD13	1.78	0.66
1:B:277:LYS:HG2	1:B:277:LYS:O	1.96	0.66
1:C:129:ILE:HD11	1:F:192:TYR:CE2	2.21	0.65
1:C:2:THR:HG21	1:C:37:GLU:OE1	1.96	0.65
1:C:360:THR:H	1:C:363:GLN:HB2	1.59	0.65
1:G:359:ILE:HG22	1:G:360:THR:N	2.12	0.65
1:G:130:THR:HB	1:G:133:VAL:HG23	1.77	0.65
1:H:2:THR:HG21	1:H:37:GLU:OE1	1.97	0.65
1:D:71:LYS:HE3	1:D:320:ASP:OD2	1.96	0.65
1:F:20:HIS:HD2	1:F:35:LEU:H	1.44	0.65
1:F:71:LYS:HE3	1:F:320:ASP:OD2	1.96	0.65
1:F:143:GLU:O	1:F:144:GLU:HB2	1.95	0.65
1:F:397:ASP:CG	1:F:400:ILE:HG13	2.21	0.65
1:D:143:GLU:O	1:D:144:GLU:HB2	1.94	0.65
1:E:340:PRO:HB3	1:E:413:VAL:HG21	1.77	0.65
1:B:130:THR:HB	1:B:133:VAL:HG23	1.77	0.65
1:F:2:THR:HG21	1:F:37:GLU:OE1	1.97	0.65
1:F:359:ILE:HG22	1:F:360:THR:H	1.62	0.65
1:C:130:THR:HB	1:C:133:VAL:HG23	1.79	0.65
1:B:141:LEU:HD11	1:B:176:LEU:HB3	1.79	0.64
1:B:144:GLU:H	1:B:454:LYS:NZ	1.95	0.64
1:D:192:TYR:CE2	1:E:129:ILE:HD11	2.25	0.64
1:F:239:HIS:CE1	1:F:289:PRO:HD3	2.32	0.64
1:F:260:TRP:HE3	1:F:310:GLN:HG3	1.62	0.64
1:H:141:LEU:HD11	1:H:176:LEU:HB3	1.78	0.64
1:H:391:ALA:HB3	1:H:434:GLY:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:HIS:CE1	1:C:289:PRO:HD3	2.33	0.64
1:E:20:HIS:HD2	1:E:35:LEU:H	1.45	0.64
1:E:241:THR:CG2	1:E:292:ARG:HE	2.11	0.64
1:F:78:THR:CG2	1:F:118:ILE:HG12	2.26	0.64
1:B:391:ALA:HB3	1:B:434:GLY:N	2.13	0.64
1:D:241:THR:CG2	1:D:292:ARG:HE	2.11	0.64
1:E:343:GLU:HB3	1:E:411:MET:HE2	1.80	0.64
1:G:20:HIS:HD2	1:G:35:LEU:H	1.45	0.64
1:C:141:LEU:HD11	1:C:176:LEU:HB3	1.79	0.64
1:D:206:ILE:HD12	1:D:276:GLU:HG2	1.78	0.64
1:A:63:MET:HE2	1:A:94:LEU:HD11	1.78	0.64
1:A:143:GLU:O	1:A:144:GLU:HB2	1.98	0.64
1:B:78:THR:HG22	1:B:117:VAL:HB	1.79	0.64
1:D:20:HIS:HD2	1:D:35:LEU:H	1.46	0.64
1:B:20:HIS:HD2	1:B:35:LEU:H	1.45	0.64
1:D:230:LEU:HD13	1:E:215:GLU:HB2	1.80	0.64
1:E:359:ILE:HG22	1:E:360:THR:N	2.10	0.64
1:G:2:THR:HG21	1:G:37:GLU:OE1	1.97	0.64
1:H:397:ASP:CG	1:H:400:ILE:HG13	2.23	0.64
1:B:206:ILE:HD12	1:B:276:GLU:CG	2.28	0.64
1:G:241:THR:CG2	1:G:292:ARG:HE	2.11	0.64
1:A:2:THR:HG21	1:A:37:GLU:OE1	1.97	0.64
1:B:359:ILE:HG22	1:B:360:THR:N	2.12	0.64
1:E:260:TRP:HE3	1:E:310:GLN:HG3	1.63	0.64
1:E:402:ARG:NE	1:E:426:GLU:HB2	2.09	0.64
1:F:130:THR:HB	1:F:133:VAL:HG23	1.79	0.64
1:A:277:LYS:HD2	1:D:96:ASN:CG	2.23	0.64
1:A:391:ALA:HB3	1:A:434:GLY:N	2.13	0.64
1:B:143:GLU:O	1:B:144:GLU:HB2	1.98	0.64
1:C:7:ASN:H	1:C:20:HIS:CE1	2.16	0.64
1:C:71:LYS:HE3	1:C:320:ASP:OD2	1.97	0.64
1:E:143:GLU:O	1:E:144:GLU:HB2	1.98	0.64
1:F:144:GLU:H	1:F:454:LYS:NZ	1.96	0.64
1:H:400:ILE:HD13	1:H:441:LYS:HZ1	1.60	0.64
1:E:305:LYS:HZ1	1:E:358:ARG:HA	1.64	0.63
1:A:141:LEU:HD11	1:A:176:LEU:HB3	1.80	0.63
1:C:391:ALA:HB3	1:C:434:GLY:N	2.13	0.63
1:C:78:THR:HG22	1:C:117:VAL:HB	1.80	0.63
1:C:343:GLU:HB3	1:C:411:MET:HE2	1.81	0.63
1:D:294:LYS:HD2	1:D:297:GLN:NE2	2.13	0.63
1:E:391:ALA:HB3	1:E:434:GLY:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:GLU:H	1:H:454:LYS:NZ	1.95	0.63
1:B:241:THR:CG2	1:B:292:ARG:HE	2.11	0.63
1:D:260:TRP:HE3	1:D:310:GLN:HG3	1.64	0.63
1:F:20:HIS:HB2	1:F:35:LEU:HG	1.79	0.63
1:F:294:LYS:HD2	1:F:297:GLN:NE2	2.14	0.63
1:H:7:ASN:H	1:H:20:HIS:CE1	2.16	0.63
1:H:239:HIS:CE1	1:H:289:PRO:HD3	2.33	0.63
1:B:239:HIS:CE1	1:B:289:PRO:HD3	2.34	0.63
1:E:78:THR:HG22	1:E:117:VAL:HB	1.79	0.63
1:G:78:THR:HG22	1:G:117:VAL:HB	1.81	0.63
1:G:206:ILE:HD12	1:G:276:GLU:CG	2.29	0.63
1:H:143:GLU:O	1:H:144:GLU:HB2	1.98	0.63
1:D:78:THR:HG22	1:D:117:VAL:HB	1.80	0.63
1:G:400:ILE:HD13	1:G:441:LYS:HZ1	1.64	0.63
1:G:150:KCX:HB3	1:G:181:MET:HE3	1.80	0.63
1:A:144:GLU:H	1:A:454:LYS:NZ	1.97	0.63
1:A:260:TRP:HE3	1:A:310:GLN:HG3	1.63	0.63
1:A:277:LYS:O	1:A:277:LYS:HG2	1.99	0.63
1:A:78:THR:HG22	1:A:117:VAL:HB	1.81	0.62
1:E:144:GLU:H	1:E:454:LYS:NZ	1.96	0.62
1:C:206:ILE:HD12	1:C:276:GLU:CG	2.29	0.62
1:F:277:LYS:O	1:F:277:LYS:HG2	1.99	0.62
1:G:391:ALA:HB3	1:G:434:GLY:H	1.64	0.62
1:A:294:LYS:HD2	1:A:297:GLN:NE2	2.15	0.62
1:D:130:THR:HB	1:D:133:VAL:HG23	1.81	0.62
1:D:277:LYS:O	1:D:277:LYS:HG2	1.99	0.62
1:G:20:HIS:HB2	1:G:35:LEU:HG	1.81	0.62
1:G:153:MET:HE1	1:G:220:ALA:O	1.99	0.62
1:D:141:LEU:HD11	1:D:176:LEU:HB3	1.80	0.62
1:D:343:GLU:HB3	1:D:411:MET:HE2	1.80	0.62
1:E:71:LYS:HE3	1:E:320:ASP:OD2	2.00	0.62
1:E:397:ASP:CG	1:E:400:ILE:HG13	2.24	0.62
1:A:206:ILE:HD12	1:A:276:GLU:CG	2.30	0.62
1:A:420:GLY:O	1:D:103:LYS:HD3	1.98	0.62
1:C:168:CYS:SG	1:F:192:TYR:HD2	2.23	0.62
1:C:241:THR:CG2	1:C:292:ARG:HE	2.11	0.62
1:C:400:ILE:HD13	1:C:441:LYS:HZ1	1.64	0.62
1:D:397:ASP:CG	1:D:400:ILE:HG13	2.25	0.62
1:E:69:VAL:CG2	1:G:422:LYS:HD2	2.30	0.62
1:H:431:LEU:HB3	1:H:436:PHE:HA	1.82	0.62
1:C:20:HIS:HD2	1:C:35:LEU:H	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:MET:HE2	1:C:35:LEU:HD22	1.80	0.62
1:E:59:THR:HG21	1:E:89:ILE:HD12	1.80	0.62
1:G:15:ASP:CG	1:H:386:VAL:HG21	2.25	0.62
1:A:386:VAL:HG11	1:B:17:TYR:CE1	2.34	0.62
1:C:386:VAL:HG21	1:D:15:ASP:OD1	1.99	0.61
1:A:7:ASN:H	1:A:20:HIS:CE1	2.17	0.61
1:B:7:ASN:H	1:B:20:HIS:CE1	2.18	0.61
1:D:239:HIS:CE1	1:D:289:PRO:HD3	2.35	0.61
1:F:141:LEU:HD11	1:F:176:LEU:HB3	1.82	0.61
1:G:397:ASP:CG	1:G:400:ILE:HG13	2.25	0.61
1:H:20:HIS:HB2	1:H:35:LEU:HG	1.82	0.61
1:A:153:MET:HE1	1:A:220:ALA:O	2.00	0.61
1:C:260:TRP:HE3	1:C:310:GLN:HG3	1.65	0.61
1:A:92:PHE:CE2	1:A:150:KCX:HD2	2.36	0.61
1:A:79:ILE:HG12	1:A:117:VAL:HG21	1.82	0.61
1:A:343:GLU:HB3	1:A:411:MET:HE2	1.81	0.61
1:D:59:THR:HG21	1:D:89:ILE:HD12	1.81	0.61
1:E:7:ASN:H	1:E:20:HIS:CE1	2.19	0.61
1:D:7:ASN:H	1:D:20:HIS:CE1	2.17	0.61
1:E:239:HIS:CE1	1:E:289:PRO:HD3	2.35	0.61
1:G:239:HIS:CE1	1:G:289:PRO:HD3	2.35	0.61
1:F:400:ILE:HD13	1:F:441:LYS:HZ3	1.65	0.61
1:G:7:ASN:H	1:G:20:HIS:CE1	2.18	0.61
1:B:79:ILE:HG12	1:B:117:VAL:HG21	1.83	0.61
1:G:294:LYS:HD2	1:G:297:GLN:NE2	2.16	0.61
1:H:206:ILE:HD12	1:H:276:GLU:CG	2.31	0.61
1:D:167:TYR:CE2	1:D:230:LEU:HD23	2.36	0.60
1:B:20:HIS:HB2	1:B:35:LEU:HG	1.83	0.60
1:G:143:GLU:O	1:G:144:GLU:HB2	1.99	0.60
1:D:153:MET:HE1	1:D:220:ALA:O	2.01	0.60
1:D:305:LYS:HZ3	1:D:358:ARG:HA	1.67	0.60
1:F:206:ILE:HD12	1:F:276:GLU:CG	2.31	0.60
1:F:343:GLU:HB3	1:F:411:MET:HE2	1.84	0.60
1:G:263:THR:CG2	1:G:264:CYS:H	2.11	0.60
1:D:20:HIS:HB2	1:D:35:LEU:HG	1.82	0.60
1:E:30:MET:HE2	1:E:35:LEU:HD22	1.83	0.60
1:E:141:LEU:HD11	1:E:176:LEU:HB3	1.81	0.60
1:E:277:LYS:HG2	1:E:277:LYS:O	2.01	0.60
1:A:30:MET:HE2	1:A:35:LEU:HD22	1.83	0.60
1:B:63:MET:HE2	1:B:94:LEU:HD11	1.82	0.60
1:F:241:THR:CG2	1:F:292:ARG:HE	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:ASN:H	1:F:20:HIS:CE1	2.20	0.60
1:A:20:HIS:HB2	1:A:35:LEU:HG	1.83	0.60
1:B:145:GLY:HA3	1:B:454:LYS:HA	1.84	0.60
1:D:30:MET:HE2	1:D:35:LEU:HD22	1.83	0.60
1:D:391:ALA:HB3	1:D:434:GLY:H	1.66	0.60
1:C:59:THR:HG21	1:C:89:ILE:HD12	1.84	0.60
1:C:261:GLY:N	1:C:310:GLN:HE21	1.93	0.60
1:D:400:ILE:HD13	1:D:441:LYS:HZ1	1.65	0.60
1:H:78:THR:HG22	1:H:117:VAL:HB	1.82	0.60
1:H:343:GLU:HB3	1:H:411:MET:HE2	1.83	0.60
1:H:260:TRP:HE3	1:H:310:GLN:HG3	1.65	0.60
1:B:397:ASP:CG	1:B:400:ILE:HG13	2.27	0.59
1:C:144:GLU:H	1:C:454:LYS:NZ	1.99	0.59
1:F:431:LEU:HB3	1:F:436:PHE:HA	1.83	0.59
1:H:59:THR:HG21	1:H:89:ILE:HD12	1.84	0.59
1:H:359:ILE:HG22	1:H:360:THR:H	1.66	0.59
1:A:167:TYR:CE2	1:A:230:LEU:HD23	2.36	0.59
1:A:397:ASP:CG	1:A:400:ILE:HG13	2.27	0.59
1:C:360:THR:HG22	1:C:361:LEU:N	2.17	0.59
1:E:153:MET:HE1	1:E:220:ALA:O	2.02	0.59
1:F:219:GLU:OE1	1:F:223:ARG:NH1	2.36	0.59
1:B:263:THR:CG2	1:B:264:CYS:H	2.14	0.59
1:C:192:TYR:HD2	1:F:168:CYS:HG	1.48	0.59
1:E:206:ILE:HD12	1:E:276:GLU:CG	2.31	0.59
1:C:153:MET:HE1	1:C:220:ALA:O	2.02	0.59
1:D:153:MET:CE	1:D:220:ALA:HB1	2.30	0.59
1:F:263:THR:CG2	1:F:264:CYS:H	2.13	0.59
1:G:277:LYS:O	1:G:277:LYS:CG	2.51	0.59
1:H:391:ALA:HB3	1:H:434:GLY:H	1.68	0.59
1:D:130:THR:HG22	1:D:132:ASP:H	1.67	0.59
1:F:261:GLY:N	1:F:310:GLN:HE21	1.95	0.59
1:F:391:ALA:HB3	1:F:434:GLY:H	1.68	0.59
1:H:63:MET:HE2	1:H:94:LEU:HD11	1.85	0.59
1:A:40:ALA:C	1:A:42:VAL:H	2.11	0.59
1:A:130:THR:HG22	1:A:132:ASP:H	1.67	0.59
1:A:359:ILE:HG22	1:A:360:THR:H	1.67	0.59
1:D:266:GLN:CD	1:D:341:ILE:HD13	2.27	0.59
1:E:20:HIS:HB2	1:E:35:LEU:HG	1.84	0.59
1:E:63:MET:HE2	1:E:94:LEU:HD11	1.85	0.59
1:H:277:LYS:O	1:H:277:LYS:CG	2.51	0.59
1:B:294:LYS:HD2	1:B:297:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLU:H	1:D:454:LYS:NZ	2.00	0.59
1:H:59:THR:CG2	1:H:61:LEU:HG	2.33	0.59
1:B:431:LEU:HB3	1:B:436:PHE:HA	1.84	0.58
1:F:30:MET:HE2	1:F:35:LEU:HD22	1.85	0.58
1:F:63:MET:HE2	1:F:94:LEU:HD11	1.85	0.58
1:G:288:SER:HA	1:G:289:PRO:C	2.28	0.58
1:D:40:ALA:C	1:D:42:VAL:H	2.11	0.58
1:D:206:ILE:HD12	1:D:276:GLU:CG	2.33	0.58
1:G:431:LEU:HB3	1:G:436:PHE:HA	1.85	0.58
1:A:278:PRO:CD	1:A:281:GLU:HB2	2.28	0.58
1:A:305:LYS:HZ1	1:A:358:ARG:HA	1.68	0.58
1:B:277:LYS:O	1:B:277:LYS:CG	2.50	0.58
1:E:40:ALA:C	1:E:42:VAL:H	2.12	0.58
1:G:360:THR:HG22	1:G:361:LEU:N	2.18	0.58
1:H:30:MET:HE2	1:H:35:LEU:HD22	1.85	0.58
1:A:59:THR:HG21	1:A:89:ILE:HD12	1.85	0.58
1:B:343:GLU:HB3	1:B:411:MET:HE2	1.86	0.58
1:C:17:TYR:CE1	1:D:386:VAL:HG11	2.39	0.58
1:C:130:THR:HG22	1:C:132:ASP:H	1.67	0.58
1:A:153:MET:CE	1:A:220:ALA:HB1	2.28	0.58
1:E:167:TYR:CE2	1:E:230:LEU:HD23	2.39	0.58
1:G:63:MET:HE2	1:G:94:LEU:HD11	1.84	0.58
1:A:192:TYR:CE2	1:H:129:ILE:HD11	2.39	0.58
1:B:30:MET:HE2	1:B:35:LEU:HD22	1.84	0.58
1:C:277:LYS:HG2	1:C:277:LYS:O	2.02	0.58
1:D:457:LYS:O	1:D:458:TYR:HB3	2.04	0.58
1:E:202:ASN:HB3	1:E:207:TYR:CD2	2.39	0.58
1:G:130:THR:HG22	1:G:132:ASP:H	1.68	0.58
1:H:202:ASN:HB3	1:H:207:TYR:CD2	2.38	0.58
1:C:192:TYR:HE2	1:F:129:ILE:CD1	2.02	0.58
1:D:219:GLU:OE1	1:D:223:ARG:NH1	2.37	0.58
1:F:79:ILE:HG12	1:F:117:VAL:HG21	1.85	0.58
1:F:395:ILE:HD12	1:F:429:SER:HB2	1.85	0.58
1:G:343:GLU:HB3	1:G:411:MET:HE2	1.85	0.58
1:B:130:THR:HG22	1:B:132:ASP:H	1.69	0.58
1:C:391:ALA:HB3	1:C:434:GLY:H	1.69	0.58
1:G:59:THR:CG2	1:G:61:LEU:HG	2.33	0.58
1:H:153:MET:HE1	1:H:220:ALA:O	2.04	0.58
1:A:224:ALA:HB1	1:A:235:LEU:HD21	1.86	0.58
1:B:59:THR:HG21	1:B:89:ILE:HD12	1.86	0.58
1:G:61:LEU:HD13	1:G:74:PHE:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ILE:HG12	1:G:117:VAL:HG21	1.85	0.58
1:A:363:GLN:O	1:A:367:ILE:HG13	2.04	0.57
1:C:186:ASN:OD1	1:C:189:VAL:HG23	2.04	0.57
1:E:363:GLN:O	1:E:367:ILE:HG13	2.04	0.57
1:F:40:ALA:C	1:F:42:VAL:H	2.12	0.57
1:A:431:LEU:HB3	1:A:436:PHE:HA	1.85	0.57
1:G:30:MET:HE2	1:G:35:LEU:HD22	1.85	0.57
1:G:145:GLY:HA3	1:G:454:LYS:HA	1.86	0.57
1:G:260:TRP:CE3	1:G:310:GLN:HG3	2.39	0.57
1:H:145:GLY:HA3	1:H:454:LYS:HA	1.86	0.57
1:H:363:GLN:O	1:H:367:ILE:HG13	2.04	0.57
1:A:145:GLY:HA3	1:A:454:LYS:HA	1.86	0.57
1:A:202:ASN:HB3	1:A:207:TYR:CD2	2.40	0.57
1:C:59:THR:CG2	1:C:61:LEU:HG	2.34	0.57
1:B:202:ASN:HB3	1:B:207:TYR:CD2	2.39	0.57
1:B:224:ALA:HB1	1:B:235:LEU:HD21	1.85	0.57
1:D:263:THR:CG2	1:D:264:CYS:H	2.14	0.57
1:E:241:THR:HG21	1:E:292:ARG:HE	1.68	0.57
1:E:294:LYS:HD2	1:E:297:GLN:NE2	2.19	0.57
1:F:61:LEU:HD13	1:F:74:PHE:HA	1.85	0.57
1:F:260:TRP:CE3	1:F:310:GLN:HG3	2.40	0.57
1:D:59:THR:CG2	1:D:61:LEU:HG	2.34	0.57
1:F:266:GLN:CD	1:F:341:ILE:HD13	2.30	0.57
1:B:129:ILE:HD11	1:G:192:TYR:CE2	2.39	0.57
1:D:431:LEU:HB3	1:D:436:PHE:HA	1.85	0.57
1:B:346:VAL:HG22	1:B:368:VAL:HG11	1.86	0.57
1:G:219:GLU:OE1	1:G:223:ARG:NH1	2.38	0.57
1:G:254:ASN:HD21	1:H:254:ASN:HD21	0.78	0.57
1:G:359:ILE:HG22	1:G:360:THR:H	1.70	0.57
1:G:400:ILE:HD13	1:G:441:LYS:HZ3	1.70	0.57
1:A:277:LYS:O	1:A:277:LYS:CG	2.53	0.57
1:D:359:ILE:HG22	1:D:360:THR:H	1.69	0.57
1:F:59:THR:HG21	1:F:89:ILE:HD12	1.86	0.57
1:A:400:ILE:HD13	1:A:441:LYS:HZ3	1.68	0.57
1:B:79:ILE:CG1	1:B:117:VAL:HG21	2.35	0.57
1:G:395:ILE:HD12	1:G:429:SER:HB2	1.85	0.56
1:H:224:ALA:HB1	1:H:235:LEU:HD21	1.86	0.56
1:H:294:LYS:HD2	1:H:297:GLN:NE2	2.20	0.56
1:C:40:ALA:C	1:C:42:VAL:H	2.13	0.56
1:E:145:GLY:HA3	1:E:454:LYS:HA	1.87	0.56
1:E:224:ALA:HB1	1:E:235:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:LYS:O	1:E:458:TYR:HB3	2.05	0.56
1:G:79:ILE:CG1	1:G:117:VAL:HG21	2.35	0.56
1:B:153:MET:HE1	1:B:220:ALA:O	2.06	0.56
1:C:20:HIS:HB2	1:C:35:LEU:HG	1.86	0.56
1:D:360:THR:HG22	1:D:361:LEU:N	2.18	0.56
1:D:363:GLN:O	1:D:367:ILE:HG13	2.05	0.56
1:F:156:LYS:O	1:F:158:VAL:HG23	2.06	0.56
1:F:363:GLN:O	1:F:367:ILE:HG13	2.05	0.56
1:G:40:ALA:C	1:G:42:VAL:H	2.14	0.56
1:G:167:TYR:CE2	1:G:230:LEU:HD23	2.39	0.56
1:G:305:LYS:HZ1	1:G:358:ARG:HA	1.66	0.56
1:B:40:ALA:C	1:B:42:VAL:H	2.13	0.56
1:B:59:THR:CG2	1:B:61:LEU:HG	2.36	0.56
1:D:156:LYS:O	1:D:158:VAL:HG23	2.06	0.56
1:E:431:LEU:HB3	1:E:436:PHE:HA	1.86	0.56
1:A:400:ILE:HD13	1:A:441:LYS:HZ1	1.69	0.56
1:D:61:LEU:HD13	1:D:74:PHE:HA	1.86	0.56
1:F:153:MET:CE	1:F:220:ALA:HB1	2.29	0.56
1:H:130:THR:HG22	1:H:132:ASP:H	1.70	0.56
1:A:241:THR:HG21	1:A:292:ARG:HE	1.71	0.56
1:B:261:GLY:N	1:B:310:GLN:NE2	2.43	0.56
1:C:241:THR:HG21	1:C:292:ARG:HE	1.71	0.56
1:H:40:ALA:C	1:H:42:VAL:H	2.14	0.56
1:A:59:THR:CG2	1:A:61:LEU:HG	2.36	0.56
1:C:363:GLN:O	1:C:367:ILE:HG13	2.05	0.56
1:D:145:GLY:HA3	1:D:454:LYS:HA	1.87	0.56
1:D:318:SER:HB2	1:D:413:VAL:HG13	1.87	0.56
1:A:261:GLY:N	1:A:310:GLN:HE21	1.97	0.56
1:B:192:TYR:CE2	1:G:129:ILE:HD11	2.37	0.56
1:G:156:LYS:O	1:G:158:VAL:HG23	2.06	0.56
1:H:397:ASP:O	1:H:425:GLY:HA2	2.05	0.56
1:A:260:TRP:CE3	1:A:310:GLN:HG3	2.41	0.56
1:C:130:THR:HG22	1:C:131:ASP:N	2.21	0.56
1:C:288:SER:HA	1:C:289:PRO:C	2.31	0.56
1:D:260:TRP:CE3	1:D:310:GLN:HG3	2.41	0.56
1:E:266:GLN:CD	1:E:341:ILE:HD13	2.30	0.56
1:F:130:THR:HG22	1:F:132:ASP:H	1.70	0.56
1:F:360:THR:HG22	1:F:361:LEU:N	2.20	0.56
1:A:79:ILE:CG1	1:A:117:VAL:HG21	2.34	0.56
1:B:397:ASP:O	1:B:425:GLY:HA2	2.05	0.56
1:C:397:ASP:O	1:C:425:GLY:HA2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ILE:HG12	1:D:117:VAL:HG21	1.86	0.56
1:D:404:ILE:HD11	1:D:423:VAL:HG21	1.87	0.56
1:E:59:THR:CG2	1:E:61:LEU:HG	2.36	0.56
1:H:153:MET:CE	1:H:220:ALA:HB1	2.30	0.56
1:A:263:THR:CG2	1:A:264:CYS:H	2.16	0.55
1:B:167:TYR:CE2	1:B:230:LEU:HD23	2.41	0.55
1:B:260:TRP:CE3	1:B:310:GLN:HG3	2.40	0.55
1:C:359:ILE:HG22	1:C:360:THR:H	1.70	0.55
1:E:79:ILE:HG12	1:E:117:VAL:HG21	1.87	0.55
1:E:130:THR:HG22	1:E:132:ASP:H	1.70	0.55
1:F:10:ILE:CD1	1:F:21:LEU:HD21	2.36	0.55
1:G:261:GLY:N	1:G:310:GLN:HE21	1.95	0.55
1:C:263:THR:CG2	1:C:264:CYS:H	2.15	0.55
1:C:431:LEU:HB3	1:C:436:PHE:HA	1.88	0.55
1:E:391:ALA:HB3	1:E:434:GLY:H	1.70	0.55
1:F:79:ILE:CG1	1:F:117:VAL:HG21	2.35	0.55
1:G:22:LEU:HD23	1:G:30:MET:HG2	1.87	0.55
1:A:22:LEU:HD23	1:A:30:MET:HG2	1.88	0.55
1:A:219:GLU:OE1	1:A:223:ARG:NH1	2.39	0.55
1:B:215:GLU:OE1	1:B:215:GLU:N	2.40	0.55
1:F:160:GLN:OE1	1:F:187:GLY:HA3	2.07	0.55
1:G:397:ASP:O	1:G:425:GLY:HA2	2.07	0.55
1:C:202:ASN:HB3	1:C:207:TYR:CD2	2.42	0.55
1:E:261:GLY:N	1:E:310:GLN:HE21	1.92	0.55
1:F:397:ASP:O	1:F:425:GLY:HA2	2.07	0.55
1:H:261:GLY:N	1:H:310:GLN:HE21	1.94	0.55
1:D:261:GLY:N	1:D:310:GLN:HE21	1.93	0.55
1:F:145:GLY:HA3	1:F:454:LYS:HA	1.86	0.55
1:B:457:LYS:O	1:B:458:TYR:HB3	2.06	0.55
1:C:294:LYS:HD2	1:C:297:GLN:NE2	2.22	0.55
1:C:457:LYS:O	1:C:458:TYR:HB3	2.05	0.55
1:D:400:ILE:HD13	1:D:441:LYS:HZ3	1.70	0.55
1:F:263:THR:CG2	1:F:264:CYS:N	2.70	0.55
1:H:318:SER:HB2	1:H:413:VAL:HG13	1.88	0.55
1:F:167:TYR:CE2	1:F:230:LEU:HD23	2.42	0.55
1:F:278:PRO:CD	1:F:281:GLU:HB2	2.29	0.55
1:H:186:ASN:OD1	1:H:189:VAL:HG23	2.06	0.55
1:D:288:SER:HA	1:D:289:PRO:C	2.31	0.55
1:E:219:GLU:OE1	1:E:223:ARG:NH1	2.40	0.55
1:F:59:THR:CG2	1:F:61:LEU:HG	2.35	0.55
1:H:130:THR:HG22	1:H:131:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:CD1	1:A:21:LEU:HD21	2.37	0.55
1:A:391:ALA:HB3	1:A:434:GLY:H	1.71	0.55
1:C:277:LYS:HG3	1:C:278:PRO:HD3	1.89	0.55
1:H:79:ILE:HG12	1:H:117:VAL:HG21	1.88	0.55
1:H:360:THR:HG22	1:H:361:LEU:N	2.21	0.55
1:C:386:VAL:HG21	1:D:15:ASP:OD2	2.07	0.55
1:F:202:ASN:HB3	1:F:207:TYR:CD2	2.42	0.55
1:B:93:CYS:HA	1:B:108:TRP:CE2	2.42	0.54
1:B:261:GLY:N	1:B:310:GLN:HE21	1.94	0.54
1:B:395:ILE:HD12	1:B:429:SER:HB2	1.89	0.54
1:B:400:ILE:CD1	1:B:441:LYS:HZ1	2.19	0.54
1:C:305:LYS:HZ1	1:C:358:ARG:HA	1.70	0.54
1:D:397:ASP:O	1:D:425:GLY:HA2	2.07	0.54
1:G:224:ALA:HB1	1:G:235:LEU:HD21	1.90	0.54
1:H:241:THR:HG21	1:H:292:ARG:HE	1.70	0.54
1:D:346:VAL:HG22	1:D:368:VAL:HG11	1.89	0.54
1:E:22:LEU:HD23	1:E:30:MET:HG2	1.89	0.54
1:E:260:TRP:CE3	1:E:310:GLN:HG3	2.42	0.54
1:H:79:ILE:CG1	1:H:117:VAL:HG21	2.37	0.54
1:H:202:ASN:HB3	1:H:207:TYR:CE2	2.43	0.54
1:H:266:GLN:CD	1:H:341:ILE:HD13	2.32	0.54
1:C:167:TYR:CE2	1:C:230:LEU:HD23	2.41	0.54
1:D:63:MET:HE2	1:D:94:LEU:HD11	1.88	0.54
1:D:277:LYS:HG3	1:D:278:PRO:HD3	1.90	0.54
1:E:93:CYS:HA	1:E:108:TRP:CE2	2.42	0.54
1:G:457:LYS:O	1:G:458:TYR:HB3	2.07	0.54
1:B:202:ASN:HB3	1:B:207:TYR:CE2	2.42	0.54
1:B:363:GLN:O	1:B:367:ILE:HG13	2.07	0.54
1:C:22:LEU:HD23	1:C:30:MET:HG2	1.90	0.54
1:C:260:TRP:CE3	1:C:310:GLN:HG3	2.43	0.54
1:E:277:LYS:O	1:E:277:LYS:CG	2.55	0.54
1:C:15:ASP:CG	1:D:386:VAL:HG21	2.32	0.54
1:E:277:LYS:HG3	1:E:278:PRO:HD3	1.90	0.54
1:F:22:LEU:HD23	1:F:30:MET:HG2	1.89	0.54
1:F:318:SER:HB2	1:F:413:VAL:HG13	1.88	0.54
1:G:202:ASN:HB3	1:G:207:TYR:CD2	2.42	0.54
1:A:241:THR:HG22	1:A:292:ARG:HE	1.72	0.54
1:B:266:GLN:CD	1:B:341:ILE:HD13	2.32	0.54
1:B:391:ALA:HB3	1:B:434:GLY:H	1.70	0.54
1:C:395:ILE:HD12	1:C:429:SER:HB2	1.88	0.54
1:D:224:ALA:HB1	1:D:235:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:LYS:O	1:D:277:LYS:CG	2.56	0.54
1:E:202:ASN:HB3	1:E:207:TYR:CE2	2.43	0.54
1:H:457:LYS:O	1:H:458:TYR:HB3	2.08	0.54
1:A:457:LYS:O	1:A:458:TYR:HB3	2.07	0.54
1:B:62:ASP:HB3	1:B:111:LYS:NZ	2.23	0.54
1:D:130:THR:HG22	1:D:131:ASP:N	2.22	0.54
1:E:130:THR:HG22	1:E:131:ASP:N	2.23	0.54
1:F:261:GLY:N	1:F:310:GLN:NE2	2.42	0.54
1:G:241:THR:HG21	1:G:292:ARG:HE	1.72	0.54
1:H:260:TRP:CE3	1:H:310:GLN:HG3	2.43	0.54
1:A:63:MET:CE	1:A:94:LEU:HD11	2.38	0.54
1:D:93:CYS:HA	1:D:108:TRP:CE2	2.43	0.54
1:E:61:LEU:HD13	1:E:74:PHE:HA	1.89	0.54
1:F:171:LEU:HD23	1:F:231:ALA:HB1	1.90	0.54
1:H:241:THR:CG2	1:H:292:ARG:HG2	2.38	0.54
1:A:266:GLN:CD	1:A:341:ILE:HD13	2.33	0.54
1:A:278:PRO:CD	1:A:278:PRO:O	2.55	0.54
1:B:219:GLU:OE1	1:B:223:ARG:NH1	2.41	0.54
1:C:93:CYS:HA	1:C:108:TRP:CE2	2.43	0.54
1:D:143:GLU:O	1:D:144:GLU:CB	2.56	0.54
1:E:254:ASN:ND2	1:F:254:ASN:HD21	1.89	0.54
1:A:61:LEU:HD13	1:A:74:PHE:HA	1.90	0.53
1:C:150:KCX:HB3	1:C:181:MET:HE3	1.89	0.53
1:F:457:LYS:O	1:F:458:TYR:HB3	2.08	0.53
1:G:59:THR:HG21	1:G:89:ILE:HD12	1.89	0.53
1:G:266:GLN:CD	1:G:341:ILE:HD13	2.32	0.53
1:H:261:GLY:N	1:H:310:GLN:NE2	2.44	0.53
1:H:400:ILE:CD1	1:H:441:LYS:HZ1	2.22	0.53
1:A:130:THR:HG22	1:A:131:ASP:N	2.23	0.53
1:B:153:MET:CE	1:B:220:ALA:HB1	2.30	0.53
1:B:359:ILE:HG22	1:B:360:THR:H	1.73	0.53
1:E:288:SER:HA	1:E:289:PRO:C	2.32	0.53
1:F:45:ALA:O	1:F:48:CYS:HB2	2.08	0.53
1:A:404:ILE:HD11	1:A:423:VAL:HG21	1.91	0.53
1:C:61:LEU:HD13	1:C:74:PHE:HA	1.90	0.53
1:C:277:LYS:O	1:C:277:LYS:CG	2.56	0.53
1:D:395:ILE:HD12	1:D:429:SER:HB2	1.90	0.53
1:E:397:ASP:O	1:E:425:GLY:HA2	2.07	0.53
1:F:277:LYS:O	1:F:277:LYS:CG	2.56	0.53
1:C:224:ALA:HB1	1:C:235:LEU:HD21	1.90	0.53
1:D:10:ILE:CD1	1:D:21:LEU:HD21	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ILE:CG1	1:D:117:VAL:HG21	2.39	0.53
1:H:288:SER:HA	1:H:289:PRO:C	2.33	0.53
1:B:61:LEU:HD13	1:B:74:PHE:HA	1.89	0.53
1:B:288:SER:HA	1:B:289:PRO:C	2.34	0.53
1:C:79:ILE:HG12	1:C:117:VAL:HG21	1.90	0.53
1:E:395:ILE:HD12	1:E:429:SER:HB2	1.90	0.53
1:F:404:ILE:HD11	1:F:423:VAL:HG21	1.89	0.53
1:G:141:LEU:CD1	1:G:176:LEU:HB3	2.38	0.53
1:B:145:GLY:HA3	1:B:454:LYS:CA	2.37	0.53
1:C:63:MET:HE2	1:C:94:LEU:HD11	1.89	0.53
1:C:202:ASN:HB3	1:C:207:TYR:CE2	2.44	0.53
1:D:241:THR:HG21	1:D:292:ARG:HE	1.72	0.53
1:D:340:PRO:CB	1:D:413:VAL:HG21	2.39	0.53
1:E:241:THR:CG2	1:E:292:ARG:HG2	2.39	0.53
1:F:62:ASP:HB3	1:F:111:LYS:NZ	2.23	0.53
1:H:141:LEU:CD1	1:H:176:LEU:HB3	2.38	0.53
1:A:288:SER:HA	1:A:289:PRO:C	2.33	0.53
1:C:141:LEU:CD1	1:C:176:LEU:HB3	2.39	0.53
1:H:102:LYS:HZ1	1:H:139:LYS:CD	2.21	0.53
1:F:224:ALA:HB1	1:F:235:LEU:HD21	1.91	0.53
1:F:340:PRO:CB	1:F:413:VAL:HG21	2.39	0.53
1:H:277:LYS:HG3	1:H:278:PRO:HD3	1.91	0.53
1:B:141:LEU:CD1	1:B:176:LEU:HB3	2.38	0.53
1:B:145:GLY:HA3	1:B:455:ARG:H	1.74	0.53
1:C:79:ILE:CG1	1:C:117:VAL:HG21	2.38	0.53
1:C:261:GLY:N	1:C:310:GLN:NE2	2.43	0.53
1:E:318:SER:HB2	1:E:413:VAL:HG13	1.90	0.53
1:F:93:CYS:HA	1:F:108:TRP:CE2	2.44	0.53
1:F:241:THR:HG21	1:F:292:ARG:HE	1.74	0.53
1:H:117:VAL:HG12	1:H:437:VAL:HG13	1.90	0.53
1:C:145:GLY:HA3	1:C:454:LYS:HA	1.90	0.53
1:C:153:MET:CE	1:C:220:ALA:HB1	2.27	0.53
1:H:145:GLY:HA3	1:H:454:LYS:CA	2.39	0.53
1:H:400:ILE:HD13	1:H:441:LYS:HZ3	1.71	0.53
1:A:45:ALA:O	1:A:48:CYS:HB2	2.09	0.52
1:B:241:THR:HG21	1:B:292:ARG:HE	1.74	0.52
1:B:404:ILE:HD11	1:B:423:VAL:HG21	1.91	0.52
1:E:261:GLY:N	1:E:310:GLN:NE2	2.44	0.52
1:E:360:THR:HG22	1:E:361:LEU:N	2.23	0.52
1:F:61:LEU:O	1:F:70:THR:HB	2.08	0.52
1:G:318:SER:HB2	1:G:413:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:VAL:CG2	1:D:106:GLU:OE1	2.57	0.52
1:B:277:LYS:HG3	1:B:278:PRO:HD3	1.91	0.52
1:C:400:ILE:HD13	1:C:441:LYS:HZ3	1.71	0.52
1:D:202:ASN:HB3	1:D:207:TYR:CD2	2.45	0.52
1:G:93:CYS:HA	1:G:108:TRP:CE2	2.44	0.52
1:H:78:THR:HG21	1:H:118:ILE:H	1.74	0.52
1:H:219:GLU:OE1	1:H:223:ARG:NH1	2.42	0.52
1:A:129:ILE:HD11	1:H:192:TYR:CE2	2.44	0.52
1:B:130:THR:HG22	1:B:131:ASP:N	2.24	0.52
1:C:278:PRO:O	1:C:279:ASN:HB2	2.10	0.52
1:D:117:VAL:HG12	1:D:437:VAL:HG13	1.92	0.52
1:E:79:ILE:CG1	1:E:117:VAL:HG21	2.39	0.52
1:E:171:LEU:HD23	1:E:231:ALA:HB1	1.91	0.52
1:G:130:THR:HG22	1:G:131:ASP:N	2.25	0.52
1:G:241:THR:CG2	1:G:292:ARG:HG2	2.39	0.52
1:H:167:TYR:CE2	1:H:230:LEU:HD23	2.43	0.52
1:A:202:ASN:HB3	1:A:207:TYR:CE2	2.44	0.52
1:B:241:THR:CG2	1:B:292:ARG:HG2	2.39	0.52
1:C:404:ILE:HD11	1:C:423:VAL:HG21	1.91	0.52
1:E:359:ILE:HG22	1:E:360:THR:H	1.74	0.52
1:H:145:GLY:HA3	1:H:455:ARG:H	1.74	0.52
1:H:241:THR:HG22	1:H:292:ARG:HE	1.71	0.52
1:B:241:THR:HG22	1:B:292:ARG:HE	1.74	0.52
1:E:141:LEU:HD23	1:E:146:ILE:O	2.10	0.52
1:G:215:GLU:OE1	1:G:215:GLU:N	2.41	0.52
1:G:277:LYS:HG3	1:G:278:PRO:HD3	1.90	0.52
1:H:404:ILE:HD11	1:H:423:VAL:HG21	1.89	0.52
1:A:397:ASP:O	1:A:425:GLY:HA2	2.09	0.52
1:B:22:LEU:HD23	1:B:30:MET:HG2	1.91	0.52
1:C:266:GLN:CD	1:C:341:ILE:HD13	2.35	0.52
1:H:22:LEU:HD23	1:H:30:MET:HG2	1.91	0.52
1:H:102:LYS:HZ1	1:H:139:LYS:HD2	1.75	0.52
1:A:360:THR:HG22	1:A:361:LEU:N	2.25	0.52
1:B:360:THR:HG22	1:B:361:LEU:N	2.24	0.52
1:C:219:GLU:OE1	1:C:223:ARG:NH1	2.42	0.52
1:C:241:THR:CG2	1:C:292:ARG:HG2	2.39	0.52
1:H:263:THR:CG2	1:H:264:CYS:H	2.19	0.52
1:B:11:VAL:HG22	1:B:16:THR:HG23	1.92	0.52
1:C:143:GLU:O	1:C:144:GLU:CB	2.56	0.52
1:F:277:LYS:HG3	1:F:278:PRO:HD3	1.91	0.52
1:F:288:SER:HA	1:F:289:PRO:C	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:VAL:HG22	1:H:368:VAL:HG11	1.92	0.52
1:A:143:GLU:O	1:A:144:GLU:CB	2.58	0.52
1:B:101:LEU:HD11	1:B:133:VAL:HG13	1.92	0.52
1:D:45:ALA:O	1:D:48:CYS:HB2	2.09	0.52
1:F:143:GLU:O	1:F:144:GLU:CB	2.57	0.52
1:A:11:VAL:HG22	1:A:16:THR:HG23	1.92	0.52
1:B:305:LYS:HZ3	1:B:358:ARG:HA	1.70	0.52
1:F:141:LEU:CD1	1:F:176:LEU:HB3	2.40	0.52
1:G:304:LEU:HG	1:G:367:ILE:HD13	1.92	0.52
1:B:318:SER:HB2	1:B:413:VAL:HG13	1.91	0.51
1:G:377:GLY:HA3	1:G:456:ALA:HB3	1.92	0.51
1:H:93:CYS:HA	1:H:108:TRP:CE2	2.45	0.51
1:A:141:LEU:CD1	1:A:176:LEU:HB3	2.40	0.51
1:A:241:THR:CG2	1:A:292:ARG:HG2	2.40	0.51
1:D:101:LEU:HD11	1:D:133:VAL:HG13	1.92	0.51
1:F:241:THR:CG2	1:F:292:ARG:HG2	2.40	0.51
1:A:145:GLY:HA3	1:A:454:LYS:CA	2.40	0.51
1:A:318:SER:HB2	1:A:413:VAL:HG13	1.90	0.51
1:B:278:PRO:O	1:B:279:ASN:HB2	2.10	0.51
1:F:64:PRO:HB3	1:F:69:VAL:HG22	1.92	0.51
1:F:202:ASN:HB3	1:F:207:TYR:CE2	2.44	0.51
1:G:78:THR:HG21	1:G:118:ILE:H	1.75	0.51
1:G:101:LEU:HD11	1:G:133:VAL:HG13	1.93	0.51
1:B:143:GLU:O	1:B:144:GLU:CB	2.59	0.51
1:D:61:LEU:O	1:D:70:THR:HB	2.11	0.51
1:E:170:LEU:HD13	1:E:228:THR:HA	1.93	0.51
1:G:386:VAL:HG21	1:H:15:ASP:OD1	2.11	0.51
1:H:92:PHE:HE2	1:H:150:KCX:HD2	1.75	0.51
1:H:278:PRO:O	1:H:279:ASN:HB2	2.11	0.51
1:A:61:LEU:O	1:A:70:THR:HB	2.11	0.51
1:A:277:LYS:HG3	1:A:278:PRO:HD3	1.92	0.51
1:D:22:LEU:HD23	1:D:30:MET:HG2	1.92	0.51
1:D:171:LEU:HD23	1:D:231:ALA:HB1	1.91	0.51
1:G:10:ILE:CD1	1:G:21:LEU:HD21	2.40	0.51
1:G:363:GLN:O	1:G:367:ILE:HG13	2.10	0.51
1:C:117:VAL:HG12	1:C:437:VAL:HG13	1.93	0.51
1:E:143:GLU:O	1:E:144:GLU:CB	2.58	0.51
1:E:145:GLY:HA3	1:E:455:ARG:H	1.74	0.51
1:E:409:HIS:C	1:E:409:HIS:CD2	2.89	0.51
1:F:170:LEU:HD13	1:F:228:THR:HA	1.93	0.51
1:G:117:VAL:HG12	1:G:437:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:LYS:HZ3	1:F:358:ARG:HA	1.71	0.51
1:A:156:LYS:O	1:A:158:VAL:HG23	2.11	0.51
1:D:170:LEU:HD13	1:D:228:THR:HA	1.93	0.51
1:E:141:LEU:CD1	1:E:176:LEU:HB3	2.40	0.51
1:E:145:GLY:HA3	1:E:454:LYS:CA	2.40	0.51
1:F:409:HIS:C	1:F:409:HIS:CD2	2.89	0.51
1:A:145:GLY:HA3	1:A:455:ARG:H	1.75	0.51
1:B:304:LEU:HG	1:B:367:ILE:HD13	1.93	0.51
1:C:11:VAL:HG22	1:C:16:THR:HG23	1.92	0.51
1:C:78:THR:HG21	1:C:118:ILE:H	1.76	0.51
1:D:64:PRO:HB3	1:D:69:VAL:HG22	1.92	0.51
1:E:404:ILE:HD11	1:E:423:VAL:HG21	1.91	0.51
1:F:11:VAL:HG22	1:F:16:THR:HG23	1.93	0.51
1:H:278:PRO:CD	1:H:281:GLU:HB2	2.32	0.51
1:A:101:LEU:HD11	1:A:133:VAL:HG13	1.93	0.51
1:A:340:PRO:CB	1:A:413:VAL:HG21	2.40	0.51
1:C:346:VAL:HG22	1:C:368:VAL:HG11	1.93	0.51
1:D:241:THR:CG2	1:D:292:ARG:HG2	2.41	0.51
1:F:145:GLY:HA3	1:F:454:LYS:CA	2.41	0.51
1:G:45:ALA:O	1:G:48:CYS:HB2	2.10	0.51
1:G:241:THR:HG22	1:G:292:ARG:HE	1.76	0.51
1:H:10:ILE:CD1	1:H:21:LEU:HD21	2.41	0.51
1:H:45:ALA:O	1:H:48:CYS:HB2	2.10	0.50
1:H:61:LEU:HD13	1:H:74:PHE:HA	1.93	0.50
1:H:143:GLU:O	1:H:144:GLU:CB	2.59	0.50
1:A:62:ASP:HB3	1:A:111:LYS:NZ	2.26	0.50
1:B:278:PRO:O	1:B:278:PRO:CD	2.58	0.50
1:D:278:PRO:O	1:D:279:ASN:HB2	2.11	0.50
1:F:117:VAL:HG12	1:F:437:VAL:HG13	1.93	0.50
1:E:278:PRO:O	1:E:279:ASN:HB2	2.11	0.50
1:F:278:PRO:CD	1:F:278:PRO:O	2.58	0.50
1:G:143:GLU:O	1:G:144:GLU:CB	2.59	0.50
1:G:145:GLY:HA3	1:G:454:LYS:CA	2.41	0.50
1:D:261:GLY:N	1:D:310:GLN:NE2	2.43	0.50
1:E:156:LYS:O	1:E:158:VAL:HG23	2.11	0.50
1:G:62:ASP:HB3	1:G:111:LYS:NZ	2.26	0.50
1:A:62:ASP:HB3	1:A:111:LYS:HD3	1.93	0.50
1:F:130:THR:HG22	1:F:131:ASP:N	2.26	0.50
1:F:145:GLY:HA3	1:F:455:ARG:H	1.76	0.50
1:G:61:LEU:O	1:G:70:THR:HB	2.11	0.50
1:G:64:PRO:HB3	1:G:69:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:VAL:HG22	1:H:16:THR:HG23	1.92	0.50
1:B:45:ALA:O	1:B:48:CYS:HB2	2.12	0.50
1:B:377:GLY:HA3	1:B:456:ALA:HB3	1.94	0.50
1:D:11:VAL:HG22	1:D:16:THR:HG23	1.94	0.50
1:D:62:ASP:HB3	1:D:111:LYS:NZ	2.26	0.50
1:D:141:LEU:CD1	1:D:176:LEU:HB3	2.40	0.50
1:E:263:THR:HG21	1:E:300:LEU:HD13	1.92	0.50
1:F:62:ASP:HB3	1:F:111:LYS:HD3	1.94	0.50
1:G:202:ASN:HB3	1:G:207:TYR:CE2	2.46	0.50
1:A:215:GLU:OE1	1:A:215:GLU:N	2.39	0.50
1:A:278:PRO:O	1:A:279:ASN:HB2	2.11	0.50
1:C:318:SER:HB2	1:C:413:VAL:HG13	1.93	0.50
1:D:241:THR:HG22	1:D:292:ARG:HE	1.76	0.50
1:H:64:PRO:HB3	1:H:69:VAL:HG22	1.93	0.50
1:H:359:ILE:CG2	1:H:360:THR:N	2.74	0.50
1:B:61:LEU:O	1:B:70:THR:HB	2.11	0.50
1:A:93:CYS:HA	1:A:108:TRP:CE2	2.46	0.50
1:B:63:MET:CE	1:B:94:LEU:HD11	2.42	0.50
1:B:186:ASN:O	1:B:190:ILE:HG13	2.11	0.50
1:C:101:LEU:HD11	1:C:133:VAL:HG13	1.94	0.50
1:D:145:GLY:HA3	1:D:454:LYS:CA	2.42	0.50
1:G:278:PRO:O	1:G:279:ASN:HB2	2.12	0.50
1:D:125:MET:HE2	1:D:127:SER:HB3	1.94	0.49
1:F:242:CYS:O	1:F:246:VAL:HG23	2.12	0.49
1:F:400:ILE:HD13	1:F:441:LYS:HZ1	1.76	0.49
1:A:117:VAL:HG12	1:A:437:VAL:HG13	1.94	0.49
1:A:409:HIS:C	1:A:409:HIS:CD2	2.90	0.49
1:B:156:LYS:O	1:B:158:VAL:HG23	2.11	0.49
1:E:117:VAL:HG12	1:E:437:VAL:HG13	1.94	0.49
1:F:78:THR:CG2	1:F:117:VAL:HB	2.41	0.49
1:H:263:THR:CG2	1:H:264:CYS:N	2.75	0.49
1:B:10:ILE:CD1	1:B:21:LEU:HD21	2.42	0.49
1:B:117:VAL:HG12	1:B:437:VAL:HG13	1.93	0.49
1:B:170:LEU:HD13	1:B:228:THR:HA	1.93	0.49
1:C:303:ALA:HA	1:C:308:GLN:CG	2.33	0.49
1:C:409:HIS:C	1:C:409:HIS:CD2	2.90	0.49
1:D:386:VAL:HG12	1:D:387:VAL:N	2.27	0.49
1:G:186:ASN:OD1	1:G:189:VAL:HG23	2.13	0.49
1:G:409:HIS:CD2	1:G:409:HIS:C	2.91	0.49
1:H:241:THR:CG2	1:H:292:ARG:CG	2.89	0.49
1:C:10:ILE:CD1	1:C:21:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ASN:HB3	1:D:207:TYR:CE2	2.48	0.49
1:D:409:HIS:C	1:D:409:HIS:CD2	2.89	0.49
1:E:241:THR:CG2	1:E:292:ARG:CG	2.90	0.49
1:A:141:LEU:HD23	1:A:146:ILE:O	2.11	0.49
1:C:45:ALA:O	1:C:48:CYS:HB2	2.12	0.49
1:C:213:PRO:HG3	1:F:230:LEU:HD11	1.93	0.49
1:C:457:LYS:O	1:C:458:TYR:CB	2.60	0.49
1:E:61:LEU:O	1:E:70:THR:HB	2.13	0.49
1:E:101:LEU:HD11	1:E:133:VAL:HG13	1.94	0.49
1:E:278:PRO:O	1:E:278:PRO:CD	2.58	0.49
1:E:457:LYS:O	1:E:458:TYR:CB	2.60	0.49
1:F:141:LEU:HD23	1:F:146:ILE:O	2.12	0.49
1:F:359:ILE:CG2	1:F:360:THR:N	2.75	0.49
1:G:167:TYR:HE1	1:G:171:LEU:HD11	1.74	0.49
1:G:404:ILE:HD11	1:G:423:VAL:HG21	1.94	0.49
1:H:215:GLU:OE1	1:H:215:GLU:N	2.42	0.49
1:C:62:ASP:HB3	1:C:111:LYS:NZ	2.27	0.49
1:E:10:ILE:CD1	1:E:21:LEU:HD21	2.42	0.49
1:E:400:ILE:CD1	1:E:441:LYS:HZ1	2.22	0.49
1:F:10:ILE:HD13	1:F:21:LEU:HD21	1.95	0.49
1:G:11:VAL:HG22	1:G:16:THR:HG23	1.95	0.49
1:G:145:GLY:HA3	1:G:455:ARG:H	1.77	0.49
1:H:61:LEU:O	1:H:70:THR:HB	2.12	0.49
1:H:170:LEU:HD13	1:H:228:THR:HA	1.94	0.49
1:A:395:ILE:HD12	1:A:429:SER:HB2	1.93	0.49
1:C:171:LEU:HD23	1:C:231:ALA:HB1	1.95	0.49
1:D:78:THR:HG21	1:D:118:ILE:H	1.78	0.49
1:E:69:VAL:HG23	1:G:422:LYS:HD2	1.94	0.49
1:E:186:ASN:OD1	1:E:189:VAL:HG23	2.11	0.49
1:C:156:LYS:O	1:C:158:VAL:HG23	2.12	0.49
1:D:58:HIS:CD2	1:D:315:ASP:HA	2.48	0.49
1:D:117:VAL:CG1	1:D:437:VAL:HG13	2.43	0.49
1:D:192:TYR:HD2	1:E:168:CYS:SG	2.35	0.49
1:E:263:THR:CG2	1:E:264:CYS:H	2.24	0.49
1:G:303:ALA:HA	1:G:308:GLN:CG	2.33	0.49
1:H:345:ARG:NH1	1:H:368:VAL:HG13	2.28	0.49
1:A:457:LYS:O	1:A:458:TYR:CB	2.61	0.49
1:C:105:ILE:HG21	1:C:144:GLU:HG2	1.95	0.49
1:E:431:LEU:N	1:E:431:LEU:HD23	2.28	0.49
1:F:278:PRO:O	1:F:279:ASN:HB2	2.13	0.49
1:G:278:PRO:O	1:G:278:PRO:CD	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLY:HA3	1:A:456:ALA:HB3	1.95	0.49
1:D:278:PRO:CD	1:D:281:GLU:HB2	2.33	0.49
1:E:63:MET:CE	1:E:94:LEU:HD11	2.43	0.49
1:F:386:VAL:HG12	1:F:387:VAL:N	2.28	0.49
1:H:319:PHE:HB2	1:H:325:LYS:HE2	1.95	0.49
1:B:105:ILE:HG21	1:B:144:GLU:HG2	1.95	0.48
1:G:153:MET:CE	1:G:220:ALA:HB1	2.32	0.48
1:G:457:LYS:O	1:G:458:TYR:CB	2.61	0.48
1:B:70:THR:HG22	1:B:72:ASP:H	1.78	0.48
1:C:62:ASP:HB3	1:C:111:LYS:HD3	1.96	0.48
1:C:340:PRO:CB	1:C:413:VAL:HG21	2.42	0.48
1:D:377:GLY:HA3	1:D:456:ALA:HB3	1.94	0.48
1:E:11:VAL:HG22	1:E:16:THR:HG23	1.93	0.48
1:E:109:HIS:NE2	1:E:144:GLU:OE2	2.46	0.48
1:E:153:MET:CE	1:E:220:ALA:HB1	2.31	0.48
1:E:202:ASN:HB3	1:E:207:TYR:CG	2.48	0.48
1:G:340:PRO:CB	1:G:413:VAL:HG21	2.39	0.48
1:H:20:HIS:CD2	1:H:34:ASN:N	2.81	0.48
1:A:379:PHE:CE1	1:A:380:PRO:HB3	2.49	0.48
1:F:359:ILE:CG2	1:F:360:THR:H	2.27	0.48
1:H:377:GLY:HA3	1:H:456:ALA:HB3	1.96	0.48
1:D:457:LYS:O	1:D:458:TYR:CB	2.58	0.48
1:E:400:ILE:HD13	1:E:441:LYS:HZ3	1.79	0.48
1:F:241:THR:CG2	1:F:292:ARG:CG	2.91	0.48
1:F:278:PRO:HD2	1:F:281:GLU:CB	2.30	0.48
1:H:20:HIS:CD2	1:H:34:ASN:H	2.30	0.48
1:H:101:LEU:HD11	1:H:133:VAL:HG13	1.94	0.48
1:H:202:ASN:HB3	1:H:207:TYR:CG	2.48	0.48
1:A:160:GLN:OE1	1:A:187:GLY:HA3	2.13	0.48
1:B:64:PRO:HB3	1:B:69:VAL:HG22	1.96	0.48
1:B:117:VAL:CG1	1:B:437:VAL:HG13	2.44	0.48
1:B:171:LEU:HD23	1:B:231:ALA:HB1	1.94	0.48
1:B:457:LYS:O	1:B:458:TYR:CB	2.60	0.48
1:C:145:GLY:HA3	1:C:455:ARG:H	1.78	0.48
1:D:145:GLY:HA3	1:D:455:ARG:H	1.78	0.48
1:E:70:THR:HG22	1:E:72:ASP:H	1.79	0.48
1:E:305:LYS:HE3	1:E:305:LYS:HB2	1.72	0.48
1:F:137:LEU:N	1:F:138:PRO:HD2	2.29	0.48
1:A:429:SER:HA	1:A:438:VAL:O	2.13	0.48
1:E:182:VAL:O	1:E:238:VAL:HG22	2.13	0.48
1:A:386:VAL:HG11	1:B:17:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:HB3	1:B:111:LYS:HD3	1.96	0.48
1:C:360:THR:CG2	1:C:361:LEU:N	2.76	0.48
1:E:429:SER:HA	1:E:438:VAL:O	2.13	0.48
1:F:101:LEU:HD11	1:F:133:VAL:HG13	1.96	0.48
1:G:105:ILE:HG21	1:G:144:GLU:HG2	1.96	0.48
1:G:346:VAL:HG22	1:G:368:VAL:HG11	1.95	0.48
1:H:278:PRO:O	1:H:278:PRO:CD	2.61	0.48
1:A:20:HIS:CD2	1:A:34:ASN:N	2.81	0.48
1:A:137:LEU:N	1:A:138:PRO:HD2	2.28	0.48
1:C:61:LEU:O	1:C:70:THR:HB	2.14	0.48
1:C:145:GLY:HA3	1:C:454:LYS:CA	2.44	0.48
1:E:186:ASN:O	1:E:190:ILE:HG13	2.14	0.48
1:E:379:PHE:CE1	1:E:380:PRO:HB3	2.49	0.48
1:G:58:HIS:CD2	1:G:315:ASP:HA	2.48	0.48
1:H:167:TYR:HE1	1:H:171:LEU:HD11	1.76	0.48
1:H:340:PRO:CB	1:H:413:VAL:HG21	2.43	0.48
1:H:429:SER:HA	1:H:438:VAL:O	2.13	0.48
1:A:171:LEU:HD23	1:A:231:ALA:HB1	1.95	0.48
1:A:346:VAL:HG22	1:A:368:VAL:HG11	1.96	0.48
1:B:58:HIS:CD2	1:B:315:ASP:HA	2.48	0.48
1:C:30:MET:HE1	1:D:30:MET:SD	2.53	0.48
1:E:67:GLY:O	1:G:422:LYS:N	2.41	0.48
1:E:346:VAL:HG22	1:E:368:VAL:HG11	1.95	0.48
1:H:378:LEU:HD21	1:H:455:ARG:HG2	1.96	0.48
1:A:20:HIS:CD2	1:A:34:ASN:H	2.31	0.47
1:A:368:VAL:O	1:A:368:VAL:HG12	2.13	0.47
1:A:386:VAL:HG12	1:A:387:VAL:N	2.29	0.47
1:B:431:LEU:N	1:B:431:LEU:HD23	2.29	0.47
1:C:70:THR:HG22	1:C:72:ASP:H	1.79	0.47
1:F:143:GLU:OE2	1:F:143:GLU:HA	2.15	0.47
1:G:92:PHE:HE2	1:G:150:KCX:HD2	1.79	0.47
1:G:186:ASN:O	1:G:190:ILE:HG13	2.14	0.47
1:H:305:LYS:HZ3	1:H:358:ARG:HA	1.76	0.47
1:H:409:HIS:C	1:H:409:HIS:CD2	2.91	0.47
1:C:92:PHE:HE2	1:C:150:KCX:HD2	1.78	0.47
1:C:266:GLN:OE1	1:C:266:GLN:N	2.39	0.47
1:F:109:HIS:NE2	1:F:144:GLU:OE2	2.47	0.47
1:F:431:LEU:HD23	1:F:431:LEU:N	2.29	0.47
1:G:63:MET:CE	1:G:94:LEU:HD11	2.44	0.47
1:H:62:ASP:HB3	1:H:111:LYS:HD3	1.95	0.47
1:H:141:LEU:HD23	1:H:146:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:THR:OG1	1:B:235:LEU:HD22	2.13	0.47
1:C:30:MET:HB2	1:D:31:ILE:O	2.14	0.47
1:D:141:LEU:HD23	1:D:146:ILE:O	2.14	0.47
1:D:429:SER:HA	1:D:438:VAL:O	2.14	0.47
1:F:20:HIS:CD2	1:F:34:ASN:N	2.82	0.47
1:F:20:HIS:CD2	1:F:34:ASN:H	2.33	0.47
1:H:58:HIS:CD2	1:H:315:ASP:HA	2.48	0.47
1:H:117:VAL:CG1	1:H:437:VAL:HG13	2.44	0.47
1:H:304:LEU:HG	1:H:367:ILE:HD13	1.97	0.47
1:H:395:ILE:HD12	1:H:429:SER:HB2	1.95	0.47
1:A:266:GLN:OE1	1:A:266:GLN:N	2.40	0.47
1:C:359:ILE:CG2	1:C:360:THR:N	2.77	0.47
1:C:431:LEU:HD23	1:C:431:LEU:N	2.29	0.47
1:D:70:THR:HG22	1:D:72:ASP:H	1.79	0.47
1:D:359:ILE:CG2	1:D:360:THR:N	2.77	0.47
1:E:78:THR:HG21	1:E:118:ILE:H	1.79	0.47
1:H:171:LEU:HD23	1:H:231:ALA:HB1	1.95	0.47
1:B:141:LEU:HD23	1:B:146:ILE:O	2.13	0.47
1:B:266:GLN:OE1	1:B:266:GLN:N	2.40	0.47
1:C:202:ASN:HB3	1:C:207:TYR:CG	2.50	0.47
1:D:41:GLU:O	1:D:42:VAL:C	2.57	0.47
1:D:74:PHE:O	1:D:78:THR:OG1	2.27	0.47
1:E:377:GLY:HA3	1:E:456:ALA:HB3	1.96	0.47
1:F:360:THR:CG2	1:F:361:LEU:N	2.78	0.47
1:H:62:ASP:HB3	1:H:111:LYS:NZ	2.28	0.47
1:A:186:ASN:OD1	1:A:189:VAL:HG23	2.14	0.47
1:A:329:ARG:CZ	1:D:67:GLY:HA3	2.45	0.47
1:C:141:LEU:HD23	1:C:146:ILE:O	2.14	0.47
1:C:263:THR:HG21	1:C:300:LEU:HD13	1.97	0.47
1:D:63:MET:CE	1:D:94:LEU:HD11	2.44	0.47
1:E:241:THR:HG22	1:E:292:ARG:HE	1.79	0.47
1:F:319:PHE:HB2	1:F:325:LYS:HE2	1.95	0.47
1:F:457:LYS:O	1:F:458:TYR:CB	2.63	0.47
1:G:109:HIS:NE2	1:G:144:GLU:OE2	2.48	0.47
1:G:360:THR:CG2	1:G:361:LEU:N	2.78	0.47
1:A:241:THR:CG2	1:A:292:ARG:CG	2.92	0.47
1:A:263:THR:CG2	1:A:264:CYS:N	2.72	0.47
1:B:41:GLU:O	1:B:42:VAL:C	2.58	0.47
1:C:117:VAL:CG1	1:C:437:VAL:HG13	2.44	0.47
1:D:167:TYR:HE1	1:D:171:LEU:HD11	1.73	0.47
1:D:242:CYS:O	1:D:246:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:PRO:CB	1:E:413:VAL:HG21	2.44	0.47
1:F:215:GLU:OE1	1:F:215:GLU:N	2.42	0.47
1:F:304:LEU:HG	1:F:367:ILE:HD13	1.96	0.47
1:G:70:THR:HG22	1:G:72:ASP:H	1.80	0.47
1:H:63:MET:CE	1:H:94:LEU:HD11	2.43	0.47
1:H:78:THR:CG2	1:H:118:ILE:H	2.28	0.47
1:H:156:LYS:O	1:H:158:VAL:HG23	2.15	0.47
1:A:70:THR:HG22	1:A:72:ASP:H	1.80	0.47
1:A:105:ILE:HG21	1:A:144:GLU:HG2	1.97	0.47
1:A:278:PRO:HD2	1:A:281:GLU:CB	2.29	0.47
1:C:160:GLN:OE1	1:C:187:GLY:HA3	2.15	0.47
1:D:360:THR:CG2	1:D:361:LEU:N	2.78	0.47
1:E:67:GLY:O	1:G:422:LYS:HB3	2.15	0.47
1:F:317:CYS:HB3	1:F:338:GLY:HA3	1.96	0.47
1:A:202:ASN:HB3	1:A:207:TYR:CG	2.49	0.47
1:B:409:HIS:C	1:B:409:HIS:CD2	2.92	0.47
1:D:105:ILE:HG21	1:D:144:GLU:HG2	1.97	0.47
1:D:125:MET:HG2	1:D:126:ILE:N	2.30	0.47
1:E:125:MET:HE2	1:E:127:SER:HB3	1.97	0.47
1:E:263:THR:CG2	1:E:264:CYS:N	2.78	0.47
1:F:125:MET:HE2	1:F:127:SER:HB3	1.96	0.47
1:F:346:VAL:HG22	1:F:368:VAL:HG11	1.96	0.47
1:H:431:LEU:N	1:H:431:LEU:HD23	2.30	0.47
1:B:241:THR:CG2	1:B:292:ARG:CG	2.93	0.47
1:C:64:PRO:HB3	1:C:69:VAL:HG22	1.97	0.47
1:E:160:GLN:OE1	1:E:187:GLY:HA3	2.15	0.47
1:G:429:SER:HA	1:G:438:VAL:O	2.15	0.47
1:H:212:ARG:HG3	1:H:290:PRO:HG3	1.96	0.47
1:A:261:GLY:N	1:A:310:GLN:NE2	2.46	0.46
1:B:125:MET:HE2	1:B:127:SER:HB3	1.97	0.46
1:C:170:LEU:HD13	1:C:228:THR:HA	1.97	0.46
1:C:241:THR:CG2	1:C:292:ARG:CG	2.92	0.46
1:E:304:LEU:HG	1:E:367:ILE:HD13	1.96	0.46
1:F:117:VAL:CG1	1:F:437:VAL:HG13	2.45	0.46
1:G:241:THR:CG2	1:G:292:ARG:CG	2.93	0.46
1:B:359:ILE:CG2	1:B:360:THR:N	2.78	0.46
1:C:20:HIS:CD2	1:C:34:ASN:H	2.33	0.46
1:C:168:CYS:SG	1:F:192:TYR:CD2	3.03	0.46
1:E:62:ASP:HB3	1:E:111:LYS:NZ	2.30	0.46
1:F:70:THR:HG22	1:F:72:ASP:H	1.80	0.46
1:G:119:ASP:OD1	1:G:451:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:CG1	1:A:437:VAL:HG13	2.45	0.46
1:B:78:THR:HG21	1:B:118:ILE:H	1.80	0.46
1:B:202:ASN:HB3	1:B:207:TYR:CG	2.51	0.46
1:C:120:TYR:N	1:C:120:TYR:CD1	2.83	0.46
1:D:431:LEU:N	1:D:431:LEU:HD23	2.31	0.46
1:E:117:VAL:CG1	1:E:437:VAL:HG13	2.46	0.46
1:G:78:THR:CG2	1:G:118:ILE:H	2.29	0.46
1:G:261:GLY:N	1:G:310:GLN:NE2	2.46	0.46
1:H:109:HIS:NE2	1:H:144:GLU:OE2	2.49	0.46
1:H:158:VAL:HG12	1:H:159:PHE:CE1	2.50	0.46
1:H:359:ILE:CG2	1:H:360:THR:H	2.29	0.46
1:H:400:ILE:CD1	1:H:441:LYS:NZ	2.75	0.46
1:A:78:THR:HG21	1:A:118:ILE:H	1.81	0.46
1:B:137:LEU:N	1:B:138:PRO:HD2	2.31	0.46
1:C:278:PRO:O	1:C:278:PRO:CD	2.61	0.46
1:D:10:ILE:HD13	1:D:21:LEU:HD21	1.98	0.46
1:D:129:ILE:HD13	1:D:168:CYS:HB3	1.97	0.46
1:D:137:LEU:N	1:D:138:PRO:HD2	2.30	0.46
1:D:318:SER:HB2	1:D:413:VAL:CG1	2.46	0.46
1:E:378:LEU:HD21	1:E:455:ARG:HG2	1.98	0.46
1:F:241:THR:HG22	1:F:292:ARG:HE	1.78	0.46
1:G:117:VAL:CG1	1:G:437:VAL:HG13	2.45	0.46
1:G:242:CYS:O	1:G:246:VAL:HG23	2.16	0.46
1:H:353:GLY:HA3	1:H:359:ILE:HD12	1.98	0.46
1:A:10:ILE:HD13	1:A:21:LEU:HD21	1.97	0.46
1:A:58:HIS:CD2	1:A:315:ASP:HA	2.51	0.46
1:A:305:LYS:HB2	1:A:305:LYS:HE3	1.75	0.46
1:C:377:GLY:HA3	1:C:456:ALA:HB3	1.98	0.46
1:D:379:PHE:CE1	1:D:380:PRO:HB3	2.51	0.46
1:F:105:ILE:HG21	1:F:144:GLU:HG2	1.97	0.46
1:G:53:GLY:HA2	1:G:394:VAL:HG23	1.98	0.46
1:G:349:LEU:HD11	1:G:359:ILE:HD11	1.97	0.46
1:A:41:GLU:O	1:A:42:VAL:C	2.58	0.46
1:A:279:ASN:ND2	1:D:64:PRO:O	2.48	0.46
1:C:10:ILE:O	1:C:16:THR:HA	2.16	0.46
1:C:78:THR:CG2	1:C:118:ILE:H	2.29	0.46
1:C:122:PHE:HB2	1:C:146:ILE:HD12	1.97	0.46
1:C:137:LEU:N	1:C:138:PRO:HD2	2.30	0.46
1:D:20:HIS:CD2	1:D:34:ASN:H	2.33	0.46
1:E:15:ASP:CG	1:F:386:VAL:HG21	2.40	0.46
1:F:78:THR:HG21	1:F:118:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:ASN:OD1	1:F:189:VAL:HG23	2.16	0.46
1:F:202:ASN:HB3	1:F:207:TYR:CG	2.50	0.46
1:G:359:ILE:CG2	1:G:360:THR:N	2.79	0.46
1:G:368:VAL:O	1:G:368:VAL:HG12	2.16	0.46
1:H:119:ASP:OD1	1:H:451:GLN:HG2	2.16	0.46
1:A:316:GLN:HB2	1:A:342:ILE:HB	1.98	0.46
1:B:316:GLN:HB2	1:B:342:ILE:HB	1.98	0.46
1:B:340:PRO:CB	1:B:413:VAL:HG21	2.42	0.46
1:C:400:ILE:CD1	1:C:441:LYS:HZ1	2.27	0.46
1:D:20:HIS:CD2	1:D:34:ASN:N	2.84	0.46
1:D:160:GLN:OE1	1:D:187:GLY:HA3	2.16	0.46
1:D:186:ASN:OD1	1:D:189:VAL:HG23	2.15	0.46
1:D:304:LEU:HG	1:D:367:ILE:HD13	1.97	0.46
1:F:122:PHE:HB2	1:F:146:ILE:HD12	1.97	0.46
1:F:355:LYS:HE3	1:F:398:PRO:O	2.16	0.46
1:F:368:VAL:O	1:F:368:VAL:HG12	2.15	0.46
1:F:377:GLY:HA3	1:F:456:ALA:HB3	1.98	0.46
1:H:63:MET:HA	1:H:64:PRO:HD3	1.66	0.46
1:B:63:MET:HA	1:B:64:PRO:HD3	1.66	0.46
1:C:242:CYS:O	1:C:246:VAL:HG23	2.16	0.46
1:G:52:PRO:O	1:G:53:GLY:C	2.58	0.46
1:H:70:THR:HG22	1:H:72:ASP:H	1.80	0.46
1:H:241:THR:HG23	1:H:292:ARG:HG2	1.98	0.46
1:A:170:LEU:HD13	1:A:228:THR:HA	1.97	0.46
1:C:230:LEU:HD22	1:F:216:LEU:HD21	1.98	0.46
1:D:345:ARG:NH1	1:D:368:VAL:HG13	2.31	0.46
1:H:125:MET:HG2	1:H:126:ILE:N	2.30	0.46
1:A:64:PRO:HB3	1:A:69:VAL:HG22	1.99	0.45
1:D:62:ASP:HB3	1:D:111:LYS:HD3	1.98	0.45
1:G:202:ASN:HB3	1:G:207:TYR:CG	2.51	0.45
1:H:137:LEU:N	1:H:138:PRO:HD2	2.31	0.45
1:H:457:LYS:O	1:H:458:TYR:CB	2.62	0.45
1:A:150:KCX:HB3	1:A:181:MET:HE3	1.99	0.45
1:A:186:ASN:O	1:A:190:ILE:HG13	2.16	0.45
1:A:192:TYR:HE2	1:H:129:ILE:HD11	1.80	0.45
1:A:304:LEU:HG	1:A:367:ILE:HD13	1.98	0.45
1:B:160:GLN:OE1	1:B:187:GLY:HA3	2.16	0.45
1:F:429:SER:HA	1:F:438:VAL:O	2.15	0.45
1:G:10:ILE:O	1:G:16:THR:HA	2.16	0.45
1:G:129:ILE:HD13	1:G:168:CYS:HB3	1.97	0.45
1:G:129:ILE:HG13	1:G:129:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:LEU:HD23	1:G:231:ALA:HB1	1.98	0.45
1:H:92:PHE:CE2	1:H:150:KCX:HD2	2.51	0.45
1:A:109:HIS:NE2	1:A:144:GLU:OE2	2.48	0.45
1:B:119:ASP:OD1	1:B:451:GLN:HG2	2.15	0.45
1:B:186:ASN:OD1	1:B:189:VAL:HG23	2.16	0.45
1:B:278:PRO:CD	1:B:281:GLU:HB2	2.35	0.45
1:D:143:GLU:HA	1:D:143:GLU:OE2	2.16	0.45
1:E:137:LEU:N	1:E:138:PRO:HD2	2.32	0.45
1:E:152:PHE:CD1	1:E:159:PHE:HB3	2.52	0.45
1:F:63:MET:CE	1:F:94:LEU:HD11	2.46	0.45
1:G:10:ILE:HD11	1:G:21:LEU:HD21	1.99	0.45
1:H:186:ASN:O	1:H:190:ILE:HG13	2.16	0.45
1:A:167:TYR:HE1	1:A:171:LEU:HD11	1.74	0.45
1:A:212:ARG:HG3	1:A:290:PRO:HG3	1.99	0.45
1:D:10:ILE:HD11	1:D:21:LEU:HD21	1.99	0.45
1:D:262:GLU:HG2	1:D:263:THR:N	2.31	0.45
1:E:58:HIS:CD2	1:E:315:ASP:HA	2.52	0.45
1:E:359:ILE:CG2	1:E:360:THR:N	2.77	0.45
1:G:100:PRO:HG2	1:G:103:LYS:HB2	1.99	0.45
1:G:141:LEU:HD23	1:G:146:ILE:O	2.16	0.45
1:G:321:PHE:HA	1:G:325:LYS:HB2	1.99	0.45
1:A:17:TYR:CE1	1:B:386:VAL:HG11	2.51	0.45
1:A:129:ILE:HD11	1:H:192:TYR:HE2	1.80	0.45
1:A:150:KCX:HG2	1:A:151:VAL:N	2.30	0.45
1:B:100:PRO:HG2	1:B:103:LYS:HB2	1.99	0.45
1:B:378:LEU:HD21	1:B:455:ARG:HG2	1.98	0.45
1:C:20:HIS:CD2	1:C:34:ASN:N	2.85	0.45
1:C:303:ALA:CA	1:C:308:GLN:HG2	2.35	0.45
1:C:304:LEU:HG	1:C:367:ILE:HD13	1.98	0.45
1:D:241:THR:CG2	1:D:292:ARG:CG	2.94	0.45
1:E:316:GLN:HB2	1:E:342:ILE:HB	1.99	0.45
1:F:262:GLU:HG2	1:F:263:THR:N	2.31	0.45
1:H:304:LEU:HD12	1:H:304:LEU:HA	1.80	0.45
1:H:316:GLN:HB2	1:H:342:ILE:HB	1.97	0.45
1:B:97:LYS:C	1:B:99:GLU:H	2.24	0.45
1:E:10:ILE:O	1:E:16:THR:HA	2.17	0.45
1:E:78:THR:CG2	1:E:117:VAL:HB	2.46	0.45
1:E:105:ILE:HG21	1:E:144:GLU:HG2	1.98	0.45
1:E:212:ARG:HG3	1:E:290:PRO:HG3	1.99	0.45
1:F:167:TYR:HE1	1:F:171:LEU:HD11	1.74	0.45
1:F:353:GLY:HA3	1:F:359:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LEU:HD13	1:G:228:THR:HA	1.98	0.45
1:G:278:PRO:HD2	1:G:281:GLU:CB	2.33	0.45
1:H:105:ILE:HG21	1:H:144:GLU:HG2	1.99	0.45
1:H:145:GLY:HA3	1:H:455:ARG:N	2.32	0.45
1:A:125:MET:HE2	1:A:127:SER:HB3	1.99	0.45
1:A:262:GLU:HG2	1:A:263:THR:N	2.30	0.45
1:B:145:GLY:HA3	1:B:455:ARG:N	2.31	0.45
1:D:278:PRO:O	1:D:278:PRO:CD	2.62	0.45
1:F:120:TYR:CD1	1:F:120:TYR:N	2.84	0.45
1:F:152:PHE:CD1	1:F:159:PHE:HB3	2.51	0.45
1:H:41:GLU:O	1:H:42:VAL:C	2.60	0.45
1:H:129:ILE:O	1:H:129:ILE:HG13	2.17	0.45
1:H:266:GLN:OE1	1:H:266:GLN:N	2.42	0.45
1:A:125:MET:HG2	1:A:126:ILE:N	2.31	0.45
1:A:278:PRO:HD2	1:A:278:PRO:O	2.16	0.45
1:B:20:HIS:CD2	1:B:34:ASN:N	2.85	0.45
1:B:321:PHE:HA	1:B:325:LYS:HB2	1.99	0.45
1:C:52:PRO:O	1:C:53:GLY:C	2.60	0.45
1:C:230:LEU:HD11	1:F:213:PRO:HG3	1.98	0.45
1:D:129:ILE:HG13	1:D:129:ILE:O	2.17	0.45
1:F:212:ARG:HG3	1:F:290:PRO:HG3	1.99	0.45
1:F:304:LEU:HD12	1:F:304:LEU:HA	1.77	0.45
1:F:318:SER:HB2	1:F:413:VAL:CG1	2.47	0.45
1:G:144:GLU:H	1:G:454:LYS:HZ1	1.60	0.45
1:G:278:PRO:CD	1:G:281:GLU:HB2	2.33	0.45
1:H:124:LEU:HB2	1:H:146:ILE:HG21	1.99	0.45
1:C:202:ASN:HB3	1:C:207:TYR:CZ	2.51	0.45
1:C:386:VAL:HG11	1:D:17:TYR:CE1	2.51	0.45
1:D:212:ARG:HG3	1:D:290:PRO:HG3	1.99	0.45
1:E:60:HIS:ND1	1:E:63:MET:HE3	2.32	0.45
1:H:360:THR:CG2	1:H:361:LEU:N	2.80	0.45
1:A:10:ILE:HD11	1:A:21:LEU:HD21	1.99	0.45
1:A:345:ARG:NH1	1:A:368:VAL:HG13	2.31	0.45
1:B:124:LEU:HB2	1:B:146:ILE:HG21	1.99	0.45
1:B:320:ASP:HB3	1:B:414:ASP:OD2	2.17	0.45
1:C:212:ARG:HG3	1:C:290:PRO:HG3	1.99	0.45
1:D:230:LEU:HD13	1:E:215:GLU:CB	2.45	0.45
1:D:353:GLY:HA3	1:D:359:ILE:HD12	1.99	0.45
1:E:215:GLU:OE1	1:E:215:GLU:N	2.45	0.45
1:E:278:PRO:CD	1:E:281:GLU:HB2	2.35	0.45
1:E:349:LEU:HD11	1:E:359:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:THR:CG2	1:F:118:ILE:H	2.30	0.45
1:F:176:LEU:O	1:F:457:LYS:HE2	2.17	0.45
1:F:305:LYS:HB2	1:F:305:LYS:HE3	1.75	0.45
1:G:212:ARG:HG3	1:G:290:PRO:HG3	1.99	0.45
1:G:262:GLU:HG2	1:G:263:THR:N	2.32	0.45
1:A:129:ILE:O	1:A:129:ILE:HG13	2.17	0.44
1:A:320:ASP:HB3	1:A:414:ASP:OD2	2.17	0.44
1:C:58:HIS:CD2	1:C:315:ASP:HA	2.52	0.44
1:C:63:MET:CE	1:C:94:LEU:HD11	2.47	0.44
1:C:241:THR:HG22	1:C:292:ARG:HE	1.78	0.44
1:D:170:LEU:HD23	1:D:180:VAL:HG21	1.99	0.44
1:D:278:PRO:HD2	1:D:281:GLU:CB	2.33	0.44
1:F:129:ILE:HD13	1:F:168:CYS:HB3	1.93	0.44
1:F:186:ASN:O	1:F:190:ILE:HG13	2.16	0.44
1:F:379:PHE:CE1	1:F:380:PRO:HB3	2.51	0.44
1:H:120:TYR:CD1	1:H:120:TYR:N	2.85	0.44
1:H:379:PHE:CE1	1:H:380:PRO:HB3	2.52	0.44
1:D:202:ASN:HB3	1:D:207:TYR:CG	2.52	0.44
1:E:129:ILE:HG13	1:E:129:ILE:O	2.17	0.44
1:E:409:HIS:HD2	1:E:409:HIS:O	1.99	0.44
1:G:304:LEU:HD12	1:G:304:LEU:HA	1.75	0.44
1:A:431:LEU:N	1:A:431:LEU:HD23	2.32	0.44
1:B:429:SER:HA	1:B:438:VAL:O	2.16	0.44
1:C:129:ILE:HD13	1:C:168:CYS:HB3	1.97	0.44
1:C:215:GLU:OE1	1:C:215:GLU:N	2.45	0.44
1:D:368:VAL:O	1:D:368:VAL:HG12	2.18	0.44
1:E:125:MET:HG2	1:E:126:ILE:N	2.33	0.44
1:G:63:MET:HA	1:G:64:PRO:HD3	1.67	0.44
1:G:431:LEU:N	1:G:431:LEU:HD23	2.32	0.44
1:B:354:VAL:CG2	1:B:364:PHE:HB2	2.47	0.44
1:D:100:PRO:HG2	1:D:103:LYS:HB2	1.99	0.44
1:F:124:LEU:HB2	1:F:146:ILE:HG21	1.98	0.44
1:F:150:KCX:HD3	1:F:151:VAL:H	1.81	0.44
1:G:117:VAL:HG11	1:G:443:PHE:HE1	1.83	0.44
1:H:263:THR:HG21	1:H:300:LEU:HD13	1.98	0.44
1:B:129:ILE:HG13	1:B:129:ILE:O	2.17	0.44
1:B:182:VAL:O	1:B:238:VAL:HG22	2.17	0.44
1:E:145:GLY:HA3	1:E:455:ARG:N	2.32	0.44
1:F:409:HIS:O	1:F:409:HIS:HD2	2.01	0.44
1:H:125:MET:HE2	1:H:127:SER:HB3	1.99	0.44
1:H:242:CYS:O	1:H:246:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:OD1	1:B:386:VAL:HG21	2.16	0.44
1:C:97:LYS:C	1:C:99:GLU:H	2.26	0.44
1:C:429:SER:HA	1:C:438:VAL:O	2.17	0.44
1:F:41:GLU:O	1:F:42:VAL:C	2.60	0.44
1:G:97:LYS:C	1:G:99:GLU:H	2.25	0.44
1:A:97:LYS:C	1:A:99:GLU:H	2.25	0.44
1:C:379:PHE:CE1	1:C:380:PRO:HB3	2.53	0.44
1:D:153:MET:HE2	1:D:184:ALA:HA	2.00	0.44
1:D:158:VAL:HG12	1:D:159:PHE:CE1	2.51	0.44
1:E:143:GLU:HA	1:E:143:GLU:OE2	2.17	0.44
1:F:101:LEU:HD13	1:F:124:LEU:HD21	2.00	0.44
1:G:176:LEU:O	1:G:457:LYS:HE2	2.18	0.44
1:H:10:ILE:HD13	1:H:21:LEU:HD21	2.00	0.44
1:H:160:GLN:OE1	1:H:187:GLY:HA3	2.17	0.44
1:A:145:GLY:HA3	1:A:455:ARG:N	2.33	0.44
1:B:10:ILE:O	1:B:16:THR:HA	2.18	0.44
1:B:260:TRP:CE2	1:B:375:LEU:HD21	2.53	0.44
1:B:278:PRO:HD2	1:B:281:GLU:CB	2.35	0.44
1:B:345:ARG:NH1	1:B:368:VAL:HG13	2.33	0.44
1:C:101:LEU:HD13	1:C:124:LEU:HD21	2.00	0.44
1:C:316:GLN:HB2	1:C:342:ILE:HB	1.99	0.44
1:C:386:VAL:HG12	1:C:387:VAL:N	2.33	0.44
1:D:223:ARG:HD3	1:E:223:ARG:CD	2.34	0.44
1:D:319:PHE:HB2	1:D:325:LYS:HE2	1.99	0.44
1:E:41:GLU:O	1:E:42:VAL:C	2.61	0.44
1:E:318:SER:HB2	1:E:413:VAL:CG1	2.48	0.44
1:F:97:LYS:C	1:F:99:GLU:H	2.26	0.44
1:G:62:ASP:HB3	1:G:111:LYS:HD3	1.99	0.44
1:G:306:ASN:ND2	1:H:256:GLY:HA2	2.33	0.44
1:A:319:PHE:HB2	1:A:325:LYS:HE2	1.99	0.44
1:B:72:ASP:H	1:B:318:SER:HG	1.66	0.44
1:C:30:MET:CE	1:C:35:LEU:HD22	2.46	0.44
1:D:78:THR:CG2	1:D:118:ILE:H	2.30	0.44
1:D:400:ILE:CD1	1:D:441:LYS:HZ1	2.29	0.44
1:E:158:VAL:HG12	1:E:159:PHE:CE1	2.53	0.44
1:E:176:LEU:O	1:E:457:LYS:HE2	2.17	0.44
1:F:321:PHE:HA	1:F:325:LYS:HB2	2.00	0.44
1:G:41:GLU:O	1:G:42:VAL:C	2.59	0.44
1:G:409:HIS:HD2	1:G:409:HIS:O	2.01	0.44
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.75	0.43
1:C:226:GLN:OE1	1:F:219:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:LYS:HE3	1:C:398:PRO:O	2.17	0.43
1:D:219:GLU:HA	1:E:226:GLN:OE1	2.18	0.43
1:D:355:LYS:HE3	1:D:398:PRO:O	2.18	0.43
1:E:45:ALA:O	1:E:48:CYS:HB2	2.18	0.43
1:F:153:MET:HE1	1:F:220:ALA:C	2.41	0.43
1:F:158:VAL:HG12	1:F:159:PHE:CE1	2.53	0.43
1:F:359:ILE:HG22	1:F:360:THR:O	2.17	0.43
1:G:137:LEU:N	1:G:138:PRO:HD2	2.32	0.43
1:H:117:VAL:HG11	1:H:443:PHE:HE1	1.83	0.43
1:A:10:ILE:O	1:A:16:THR:HA	2.19	0.43
1:A:53:GLY:HA2	1:A:394:VAL:HG23	1.99	0.43
1:A:192:TYR:CD2	1:H:129:ILE:HD11	2.54	0.43
1:B:10:ILE:HD13	1:B:21:LEU:HD21	2.00	0.43
1:B:109:HIS:NE2	1:B:144:GLU:OE2	2.51	0.43
1:B:368:VAL:O	1:B:368:VAL:HG12	2.18	0.43
1:B:379:PHE:CE1	1:B:380:PRO:HB3	2.53	0.43
1:C:152:PHE:O	1:C:160:GLN:HA	2.18	0.43
1:D:317:CYS:HB3	1:D:338:GLY:HA3	2.00	0.43
1:D:349:LEU:HD11	1:D:359:ILE:HD11	2.00	0.43
1:E:101:LEU:HD13	1:E:124:LEU:HD21	2.00	0.43
1:E:136:GLU:O	1:E:137:LEU:C	2.61	0.43
1:A:40:ALA:C	1:A:42:VAL:N	2.76	0.43
1:A:122:PHE:HB2	1:A:146:ILE:HD12	1.99	0.43
1:A:242:CYS:O	1:A:246:VAL:HG23	2.18	0.43
1:A:332:PHE:CE2	1:A:333:THR:HG22	2.53	0.43
1:E:242:CYS:O	1:E:246:VAL:HG23	2.18	0.43
1:F:10:ILE:HD11	1:F:21:LEU:HD21	1.99	0.43
1:G:20:HIS:CD2	1:G:34:ASN:H	2.36	0.43
1:H:122:PHE:HB2	1:H:146:ILE:HD12	1.99	0.43
1:H:355:LYS:HE3	1:H:398:PRO:O	2.19	0.43
1:B:20:HIS:CD2	1:B:34:ASN:H	2.36	0.43
1:D:122:PHE:HB2	1:D:146:ILE:HD12	2.00	0.43
1:D:126:ILE:HD12	1:D:149:LEU:HB3	2.00	0.43
1:F:58:HIS:CD2	1:F:315:ASP:HA	2.53	0.43
1:F:202:ASN:HB3	1:F:207:TYR:CZ	2.53	0.43
1:G:20:HIS:CD2	1:G:34:ASN:N	2.86	0.43
1:G:316:GLN:HB2	1:G:342:ILE:HB	2.01	0.43
1:H:176:LEU:O	1:H:457:LYS:HE2	2.18	0.43
1:B:171:LEU:O	1:B:172:ALA:C	2.61	0.43
1:B:202:ASN:HB3	1:B:207:TYR:CZ	2.54	0.43
1:B:242:CYS:O	1:B:246:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:VAL:HG12	1:B:387:VAL:N	2.32	0.43
1:C:78:THR:CG2	1:C:117:VAL:HB	2.47	0.43
1:C:125:MET:HE2	1:C:127:SER:HB3	1.99	0.43
1:C:368:VAL:O	1:C:368:VAL:HG12	2.18	0.43
1:D:78:THR:CG2	1:D:117:VAL:HB	2.47	0.43
1:D:316:GLN:HB2	1:D:342:ILE:HB	2.00	0.43
1:H:60:HIS:ND1	1:H:63:MET:HE3	2.33	0.43
1:H:78:THR:CG2	1:H:117:VAL:HB	2.48	0.43
1:H:268:LEU:HG	1:H:301:TRP:CE2	2.53	0.43
1:A:359:ILE:CG2	1:A:360:THR:N	2.77	0.43
1:B:212:ARG:HG3	1:B:290:PRO:HG3	2.01	0.43
1:C:10:ILE:HD13	1:C:21:LEU:HD21	2.00	0.43
1:D:120:TYR:CD1	1:D:120:TYR:N	2.86	0.43
1:E:120:TYR:N	1:E:120:TYR:CD1	2.86	0.43
1:G:351:SER:HB2	1:G:423:VAL:HG13	2.01	0.43
1:H:126:ILE:HD12	1:H:149:LEU:HB3	2.01	0.43
1:H:318:SER:HB2	1:H:413:VAL:CG1	2.48	0.43
1:H:354:VAL:CG2	1:H:364:PHE:HB2	2.49	0.43
1:A:152:PHE:CD1	1:A:159:PHE:HB3	2.54	0.43
1:A:294:LYS:HD2	1:A:297:GLN:HE22	1.84	0.43
1:B:71:LYS:CE	1:B:320:ASP:OD2	2.63	0.43
1:C:41:GLU:O	1:C:42:VAL:C	2.61	0.43
1:C:192:TYR:HD2	1:F:168:CYS:SG	2.40	0.43
1:C:349:LEU:HD11	1:C:359:ILE:HD11	2.01	0.43
1:D:97:LYS:C	1:D:99:GLU:H	2.26	0.43
1:D:215:GLU:OE1	1:D:215:GLU:N	2.45	0.43
1:E:78:THR:CG2	1:E:118:ILE:H	2.32	0.43
1:E:355:LYS:HE3	1:E:398:PRO:O	2.18	0.43
1:F:126:ILE:HD12	1:F:149:LEU:HB3	2.00	0.43
1:F:350:PHE:O	1:F:354:VAL:HB	2.19	0.43
1:G:145:GLY:HA3	1:G:455:ARG:N	2.34	0.43
1:G:263:THR:HG21	1:G:300:LEU:HD13	2.01	0.43
1:G:386:VAL:HG12	1:G:387:VAL:N	2.34	0.43
1:H:281:GLU:OE2	1:H:284:LYS:HE3	2.19	0.43
1:A:119:ASP:OD1	1:A:451:GLN:HG2	2.18	0.43
1:A:120:TYR:N	1:A:120:TYR:CD1	2.86	0.43
1:A:143:GLU:HA	1:A:143:GLU:OE2	2.19	0.43
1:B:122:PHE:HB2	1:B:146:ILE:HD12	2.00	0.43
1:B:262:GLU:HG2	1:B:263:THR:N	2.32	0.43
1:B:304:LEU:HA	1:B:304:LEU:HD12	1.81	0.43
1:C:58:HIS:HE1	1:C:239:HIS:CD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ALA:HB2	1:D:342:ILE:CD1	2.49	0.43
1:D:321:PHE:HA	1:D:325:LYS:HB2	2.00	0.43
1:D:359:ILE:HG22	1:D:360:THR:O	2.18	0.43
1:E:53:GLY:HA2	1:E:394:VAL:HG23	2.00	0.43
1:E:64:PRO:HB3	1:E:69:VAL:HG22	1.99	0.43
1:F:89:ILE:O	1:F:120:TYR:HA	2.19	0.43
1:F:316:GLN:HB2	1:F:342:ILE:HB	2.00	0.43
1:G:114:GLY:HA2	1:G:448:GLY:HA2	2.01	0.43
1:A:351:SER:HB2	1:A:423:VAL:HG13	2.01	0.43
1:A:353:GLY:HA3	1:A:359:ILE:HD12	1.99	0.43
1:C:125:MET:HG2	1:C:126:ILE:N	2.32	0.43
1:E:10:ILE:HD13	1:E:21:LEU:HD21	2.01	0.43
1:E:62:ASP:HB3	1:E:111:LYS:HD3	2.00	0.43
1:E:67:GLY:O	1:G:422:LYS:CB	2.67	0.43
1:E:262:GLU:HG2	1:E:263:THR:N	2.34	0.43
1:E:321:PHE:HA	1:E:325:LYS:HB2	2.00	0.43
1:G:182:VAL:O	1:G:238:VAL:HG22	2.19	0.43
1:B:117:VAL:HG11	1:B:443:PHE:HE1	1.84	0.43
1:C:109:HIS:NE2	1:C:144:GLU:OE2	2.52	0.43
1:C:136:GLU:O	1:C:137:LEU:C	2.62	0.43
1:C:345:ARG:NH1	1:C:368:VAL:HG13	2.33	0.43
1:C:378:LEU:HD21	1:C:455:ARG:HG2	2.01	0.43
1:D:60:HIS:ND1	1:D:63:MET:HE3	2.34	0.43
1:E:202:ASN:HB3	1:E:207:TYR:CZ	2.53	0.43
1:E:358:ARG:O	1:E:359:ILE:O	2.37	0.43
1:E:360:THR:CG2	1:E:361:LEU:N	2.82	0.43
1:F:136:GLU:O	1:F:137:LEU:C	2.62	0.43
1:G:378:LEU:HD21	1:G:455:ARG:HG2	2.01	0.43
1:H:351:SER:HB2	1:H:423:VAL:HG13	2.00	0.43
1:A:52:PRO:O	1:A:53:GLY:C	2.61	0.42
1:A:78:THR:CG2	1:A:118:ILE:H	2.32	0.42
1:A:359:ILE:CG2	1:A:360:THR:H	2.30	0.42
1:C:119:ASP:OD1	1:C:451:GLN:HG2	2.19	0.42
1:D:129:ILE:HD11	1:E:192:TYR:CD2	2.53	0.42
1:F:100:PRO:HG2	1:F:103:LYS:HB2	2.01	0.42
1:F:118:ILE:O	1:F:450:GLY:HA3	2.19	0.42
1:F:170:LEU:HA	1:F:180:VAL:HG21	2.01	0.42
1:H:143:GLU:HA	1:H:143:GLU:OE2	2.19	0.42
1:H:337:ASN:N	1:H:337:ASN:HD22	2.16	0.42
1:H:349:LEU:HD11	1:H:359:ILE:HD11	2.00	0.42
1:H:386:VAL:HG12	1:H:387:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:HD11	1:A:359:ILE:HD11	2.02	0.42
1:B:60:HIS:ND1	1:B:63:MET:HE3	2.34	0.42
1:C:409:HIS:HD2	1:C:409:HIS:O	2.02	0.42
1:E:20:HIS:CD2	1:E:34:ASN:H	2.37	0.42
1:E:124:LEU:HB2	1:E:146:ILE:HG21	2.01	0.42
1:E:317:CYS:HB3	1:E:338:GLY:HA3	2.01	0.42
1:F:152:PHE:O	1:F:160:GLN:HA	2.19	0.42
1:G:124:LEU:HB2	1:G:146:ILE:HG21	2.00	0.42
1:G:143:GLU:HA	1:G:143:GLU:OE2	2.19	0.42
1:G:319:PHE:HB2	1:G:325:LYS:HE2	2.00	0.42
1:G:354:VAL:CG2	1:G:364:PHE:HB2	2.48	0.42
1:H:10:ILE:O	1:H:16:THR:HA	2.19	0.42
1:H:202:ASN:HB3	1:H:207:TYR:CZ	2.54	0.42
1:H:241:THR:HG22	1:H:242:CYS:N	2.33	0.42
1:A:354:VAL:CG2	1:A:364:PHE:HB2	2.49	0.42
1:B:263:THR:HG21	1:B:300:LEU:HD13	2.01	0.42
1:D:337:ASN:N	1:D:337:ASN:HD22	2.17	0.42
1:F:268:LEU:HG	1:F:301:TRP:CE2	2.54	0.42
1:F:278:PRO:HD2	1:F:278:PRO:O	2.19	0.42
1:F:344:ASP:O	1:F:348:ILE:HG13	2.20	0.42
1:G:355:LYS:HE3	1:G:398:PRO:O	2.19	0.42
1:H:241:THR:HG21	1:H:292:ARG:NE	2.33	0.42
1:H:278:PRO:HD2	1:H:281:GLU:CB	2.32	0.42
1:B:400:ILE:HD13	1:B:441:LYS:HZ3	1.77	0.42
1:C:152:PHE:CD1	1:C:159:PHE:HB3	2.54	0.42
1:C:268:LEU:HG	1:C:301:TRP:CE2	2.55	0.42
1:D:152:PHE:CD1	1:D:159:PHE:HB3	2.54	0.42
1:G:125:MET:HG2	1:G:126:ILE:N	2.34	0.42
1:H:66:GLY:C	1:H:68:THR:H	2.27	0.42
1:A:101:LEU:HD13	1:A:124:LEU:HD21	2.01	0.42
1:B:125:MET:HG2	1:B:126:ILE:N	2.33	0.42
1:C:40:ALA:C	1:C:42:VAL:N	2.78	0.42
1:D:66:GLY:C	1:D:68:THR:H	2.28	0.42
1:D:124:LEU:HB2	1:D:146:ILE:HG21	2.01	0.42
1:D:359:ILE:CG2	1:D:360:THR:H	2.32	0.42
1:E:20:HIS:CD2	1:E:34:ASN:N	2.87	0.42
1:E:122:PHE:HB2	1:E:146:ILE:HD12	2.01	0.42
1:E:353:GLY:HA3	1:E:359:ILE:HD12	2.01	0.42
1:F:145:GLY:HA3	1:F:455:ARG:N	2.34	0.42
1:F:378:LEU:HD21	1:F:455:ARG:HG2	2.02	0.42
1:G:60:HIS:ND1	1:G:63:MET:HE3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:LEU:HD13	1:H:124:LEU:HD21	2.01	0.42
1:A:321:PHE:HA	1:A:325:LYS:HB2	2.02	0.42
1:B:120:TYR:N	1:B:120:TYR:CD1	2.86	0.42
1:B:349:LEU:HD11	1:B:359:ILE:HD11	2.01	0.42
1:C:45:ALA:O	1:C:46:LYS:C	2.62	0.42
1:C:321:PHE:HA	1:C:325:LYS:HB2	2.01	0.42
1:H:229:GLU:HG3	1:H:257:LEU:HD21	2.01	0.42
1:A:124:LEU:HB2	1:A:146:ILE:HG21	2.00	0.42
1:C:124:LEU:HB2	1:C:146:ILE:HG21	2.01	0.42
1:C:359:ILE:CG2	1:C:360:THR:H	2.32	0.42
1:F:129:ILE:O	1:F:129:ILE:HG13	2.19	0.42
1:G:120:TYR:CD1	1:G:120:TYR:N	2.87	0.42
1:G:154:ALA:O	1:G:155:TYR:HB2	2.19	0.42
1:H:97:LYS:C	1:H:99:GLU:H	2.27	0.42
1:A:30:MET:SD	1:B:30:MET:HE1	2.60	0.42
1:B:176:LEU:O	1:B:457:LYS:HE2	2.19	0.42
1:B:319:PHE:HB2	1:B:325:LYS:HE2	2.02	0.42
1:C:143:GLU:HA	1:C:143:GLU:OE2	2.20	0.42
1:C:186:ASN:O	1:C:190:ILE:HG13	2.19	0.42
1:C:262:GLU:HG2	1:C:263:THR:N	2.34	0.42
1:C:400:ILE:CD1	1:C:441:LYS:NZ	2.76	0.42
1:D:154:ALA:O	1:D:155:TYR:HB2	2.19	0.42
1:E:119:ASP:OD1	1:E:451:GLN:HG2	2.19	0.42
1:F:58:HIS:HE1	1:F:239:HIS:CD2	2.38	0.42
1:F:332:PHE:CE2	1:F:333:THR:HG22	2.54	0.42
1:G:153:MET:HE1	1:G:220:ALA:C	2.45	0.42
1:B:78:THR:CG2	1:B:118:ILE:H	2.33	0.42
1:B:355:LYS:HE3	1:B:398:PRO:O	2.20	0.42
1:D:145:GLY:HA3	1:D:455:ARG:N	2.35	0.42
1:D:182:VAL:O	1:D:238:VAL:HG22	2.20	0.42
1:D:354:VAL:CG2	1:D:364:PHE:HB2	2.49	0.42
1:F:119:ASP:OD1	1:F:451:GLN:HG2	2.20	0.42
1:H:262:GLU:HG2	1:H:263:THR:N	2.34	0.42
1:H:321:PHE:HA	1:H:325:LYS:HB2	2.01	0.42
1:A:30:MET:CE	1:A:35:LEU:HD22	2.50	0.42
1:A:59:THR:HG23	1:A:61:LEU:HG	2.02	0.42
1:A:317:CYS:HB3	1:A:338:GLY:HA3	2.02	0.42
1:A:409:HIS:O	1:A:409:HIS:HD2	2.03	0.42
1:B:310:GLN:CD	1:B:310:GLN:N	2.78	0.42
1:C:145:GLY:HA3	1:C:455:ARG:N	2.35	0.42
1:C:226:GLN:O	1:C:229:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:HA	1:C:304:LEU:HD12	1.75	0.42
1:C:359:ILE:HG22	1:C:360:THR:O	2.19	0.42
1:E:97:LYS:C	1:E:99:GLU:H	2.27	0.42
1:E:229:GLU:HG3	1:E:257:LEU:HD21	2.02	0.42
1:E:368:VAL:O	1:E:368:VAL:HG12	2.20	0.42
1:F:263:THR:HG21	1:F:300:LEU:HD13	2.02	0.42
1:G:122:PHE:HB2	1:G:146:ILE:HD12	2.01	0.42
1:G:140:VAL:HG12	1:G:146:ILE:HB	2.02	0.42
1:H:426:GLU:HA	1:H:427:PRO:HD3	1.92	0.42
1:A:126:ILE:HD12	1:A:149:LEU:HB3	2.01	0.41
1:A:318:SER:HB2	1:A:413:VAL:CG1	2.48	0.41
1:B:324:GLN:O	1:B:327:LEU:HG	2.19	0.41
1:C:100:PRO:HG2	1:C:103:LYS:HB2	2.02	0.41
1:C:278:PRO:HD2	1:C:281:GLU:CB	2.34	0.41
1:C:353:GLY:HA3	1:C:359:ILE:HD12	2.02	0.41
1:D:10:ILE:O	1:D:16:THR:HA	2.19	0.41
1:E:72:ASP:HB2	1:E:318:SER:OG	2.20	0.41
1:E:123:HIS:HB3	1:E:181:MET:HE1	2.02	0.41
1:E:278:PRO:HD2	1:E:281:GLU:CB	2.36	0.41
1:F:229:GLU:HG3	1:F:257:LEU:HD21	2.02	0.41
1:G:266:GLN:OE1	1:G:266:GLN:N	2.42	0.41
1:G:400:ILE:CD1	1:G:441:LYS:HZ1	2.30	0.41
1:H:17:TYR:N	1:H:17:TYR:CD1	2.88	0.41
1:A:268:LEU:HG	1:A:301:TRP:CE2	2.55	0.41
1:A:306:ASN:ND2	1:B:256:GLY:HA2	2.35	0.41
1:B:40:ALA:C	1:B:42:VAL:N	2.78	0.41
1:D:52:PRO:O	1:D:53:GLY:C	2.62	0.41
1:D:53:GLY:HA2	1:D:394:VAL:HG23	2.02	0.41
1:D:241:THR:HG22	1:D:242:CYS:N	2.34	0.41
1:E:268:LEU:HG	1:E:301:TRP:CE2	2.55	0.41
1:F:182:VAL:O	1:F:238:VAL:HG22	2.19	0.41
1:F:345:ARG:NH1	1:F:368:VAL:HG13	2.36	0.41
1:G:158:VAL:HG12	1:G:159:PHE:CE1	2.55	0.41
1:G:345:ARG:NH1	1:G:368:VAL:HG13	2.35	0.41
1:G:379:PHE:CE1	1:G:380:PRO:HB3	2.55	0.41
1:H:45:ALA:O	1:H:46:LYS:C	2.63	0.41
1:H:100:PRO:HG2	1:H:103:LYS:HB2	2.02	0.41
1:A:355:LYS:HE3	1:A:398:PRO:O	2.19	0.41
1:B:45:ALA:O	1:B:46:LYS:C	2.63	0.41
1:B:153:MET:CE	1:B:184:ALA:HA	2.50	0.41
1:D:176:LEU:O	1:D:457:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LYS:HB2	1:D:305:LYS:HE3	1.75	0.41
1:D:351:SER:HB2	1:D:423:VAL:HG13	2.01	0.41
1:E:63:MET:HA	1:E:64:PRO:HD3	1.68	0.41
1:E:228:THR:OG1	1:E:235:LEU:HD22	2.20	0.41
1:E:386:VAL:HG21	1:F:15:ASP:OD1	2.19	0.41
1:G:268:LEU:HG	1:G:301:TRP:CE2	2.55	0.41
1:A:140:VAL:HG12	1:A:146:ILE:HB	2.03	0.41
1:A:182:VAL:O	1:A:238:VAL:HG22	2.20	0.41
1:B:360:THR:CG2	1:B:361:LEU:N	2.83	0.41
1:C:140:VAL:O	1:C:144:GLU:O	2.39	0.41
1:C:202:ASN:HB3	1:C:207:TYR:CD1	2.56	0.41
1:C:319:PHE:HB2	1:C:325:LYS:HE2	2.02	0.41
1:D:170:LEU:HA	1:D:180:VAL:HG21	2.01	0.41
1:D:268:LEU:HG	1:D:301:TRP:CE2	2.56	0.41
1:D:294:LYS:HD2	1:D:297:GLN:HE22	1.85	0.41
1:E:117:VAL:HG11	1:E:443:PHE:HE1	1.85	0.41
1:E:241:THR:HG22	1:E:242:CYS:N	2.35	0.41
1:E:350:PHE:O	1:E:354:VAL:HB	2.21	0.41
1:E:378:LEU:CD2	1:E:455:ARG:HG2	2.50	0.41
1:F:154:ALA:O	1:F:155:TYR:HB2	2.20	0.41
1:F:354:VAL:CG2	1:F:364:PHE:HB2	2.51	0.41
1:G:126:ILE:HD12	1:G:149:LEU:HB3	2.02	0.41
1:G:337:ASN:N	1:G:337:ASN:HD22	2.17	0.41
1:A:89:ILE:O	1:A:120:TYR:HA	2.20	0.41
1:A:277:LYS:HB2	1:D:96:ASN:OD1	2.21	0.41
1:A:451:GLN:HE21	1:A:451:GLN:HB3	1.68	0.41
1:B:152:PHE:CD1	1:B:159:PHE:HB3	2.56	0.41
1:B:153:MET:HE2	1:B:184:ALA:HA	2.02	0.41
1:B:318:SER:HB2	1:B:413:VAL:CG1	2.50	0.41
1:C:81:ALA:HB2	1:C:342:ILE:HG12	2.02	0.41
1:C:213:PRO:CG	1:F:230:LEU:HD11	2.51	0.41
1:E:140:VAL:HG12	1:E:146:ILE:HB	2.02	0.41
1:F:125:MET:HG2	1:F:126:ILE:N	2.34	0.41
1:F:266:GLN:OE1	1:F:266:GLN:N	2.43	0.41
1:G:136:GLU:O	1:G:137:LEU:C	2.63	0.41
1:G:202:ASN:HB3	1:G:207:TYR:CZ	2.55	0.41
1:A:100:PRO:HG2	1:A:103:LYS:HB2	2.02	0.41
1:B:153:MET:HE1	1:B:220:ALA:C	2.45	0.41
1:D:136:GLU:O	1:D:137:LEU:C	2.64	0.41
1:E:153:MET:HE2	1:E:184:ALA:HA	2.02	0.41
1:E:354:VAL:CG2	1:E:364:PHE:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:THR:HG22	1:F:242:CYS:N	2.35	0.41
1:G:81:ALA:HB2	1:G:342:ILE:HG12	2.03	0.41
1:G:318:SER:HB2	1:G:413:VAL:CG1	2.50	0.41
1:G:353:GLY:HA3	1:G:359:ILE:HD12	2.03	0.41
1:H:53:GLY:HA2	1:H:394:VAL:HG23	2.01	0.41
1:H:226:GLN:O	1:H:229:GLU:HB3	2.19	0.41
1:A:158:VAL:HG12	1:A:159:PHE:CE1	2.56	0.41
1:A:202:ASN:HB3	1:A:207:TYR:CZ	2.55	0.41
1:A:263:THR:HG21	1:A:300:LEU:HD13	2.02	0.41
1:A:280:PHE:CD2	1:D:67:GLY:HA2	2.56	0.41
1:A:350:PHE:O	1:A:354:VAL:HB	2.21	0.41
1:B:143:GLU:HA	1:B:143:GLU:OE2	2.21	0.41
1:C:53:GLY:HA2	1:C:394:VAL:HG23	2.03	0.41
1:C:223:ARG:O	1:C:224:ALA:C	2.63	0.41
1:D:92:PHE:HE2	1:D:150:KCX:HD2	1.85	0.41
1:D:186:ASN:O	1:D:190:ILE:HG13	2.21	0.41
1:D:303:ALA:HA	1:D:308:GLN:CG	2.35	0.41
1:D:304:LEU:HA	1:D:304:LEU:HD12	1.75	0.41
1:E:52:PRO:O	1:E:53:GLY:C	2.63	0.41
1:E:59:THR:HG23	1:E:61:LEU:HG	2.03	0.41
1:F:72:ASP:H	1:F:318:SER:HG	1.68	0.41
1:G:10:ILE:HD13	1:G:21:LEU:HD21	2.02	0.41
1:H:81:ALA:HB2	1:H:342:ILE:CD1	2.51	0.41
1:A:226:GLN:O	1:A:229:GLU:HB3	2.21	0.41
1:A:241:THR:HG21	1:A:292:ARG:NE	2.36	0.41
1:A:358:ARG:O	1:A:359:ILE:O	2.39	0.41
1:A:420:GLY:C	1:D:103:LYS:CD	2.88	0.41
1:C:153:MET:HE2	1:C:184:ALA:HA	2.01	0.41
1:C:176:LEU:O	1:C:457:LYS:HE2	2.21	0.41
1:D:81:ALA:HB2	1:D:342:ILE:HG12	2.03	0.41
1:D:409:HIS:O	1:D:409:HIS:HD2	2.02	0.41
1:E:123:HIS:CB	1:E:181:MET:HE1	2.51	0.41
1:E:140:VAL:O	1:E:144:GLU:O	2.39	0.41
1:F:40:ALA:C	1:F:42:VAL:N	2.77	0.41
1:H:114:GLY:HA2	1:H:448:GLY:HA2	2.02	0.41
1:H:228:THR:OG1	1:H:235:LEU:HD22	2.21	0.41
1:A:45:ALA:O	1:A:46:LYS:C	2.64	0.41
1:A:280:PHE:CG	1:D:67:GLY:HA2	2.56	0.41
1:A:329:ARG:NE	1:D:67:GLY:HA3	2.36	0.41
1:B:53:GLY:HA2	1:B:394:VAL:HG23	2.02	0.41
1:B:101:LEU:HD13	1:B:124:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ILE:HG22	1:B:360:THR:O	2.21	0.41
1:B:378:LEU:CD2	1:B:455:ARG:HG2	2.51	0.41
1:C:60:HIS:ND1	1:C:63:MET:HE3	2.35	0.41
1:C:87:THR:O	1:C:118:ILE:HB	2.21	0.41
1:C:281:GLU:OE2	1:C:284:LYS:HE3	2.20	0.41
1:D:30:MET:CE	1:D:35:LEU:HD22	2.50	0.41
1:D:40:ALA:O	1:D:42:VAL:N	2.54	0.41
1:D:118:ILE:O	1:D:450:GLY:HA3	2.21	0.41
1:E:260:TRP:CE2	1:E:375:LEU:HD21	2.55	0.41
1:E:278:PRO:HD2	1:E:278:PRO:O	2.21	0.41
1:F:10:ILE:O	1:F:16:THR:HA	2.21	0.41
1:F:81:ALA:HB2	1:F:342:ILE:CD1	2.51	0.41
1:F:153:MET:HE2	1:F:184:ALA:HA	2.03	0.41
1:G:72:ASP:HB2	1:G:318:SER:OG	2.20	0.41
1:G:125:MET:HE2	1:G:127:SER:HB3	2.02	0.41
1:H:182:VAL:O	1:H:238:VAL:HG22	2.21	0.41
1:A:123:HIS:HB3	1:A:181:MET:HE1	2.03	0.41
1:A:360:THR:CG2	1:A:361:LEU:N	2.83	0.41
1:D:109:HIS:NE2	1:D:144:GLU:OE2	2.54	0.41
1:D:119:ASP:OD1	1:D:451:GLN:HG2	2.21	0.41
1:G:170:LEU:HD23	1:G:180:VAL:HG21	2.03	0.41
1:G:171:LEU:O	1:G:172:ALA:C	2.63	0.41
1:G:223:ARG:O	1:G:224:ALA:C	2.64	0.41
1:H:81:ALA:HB2	1:H:342:ILE:HG12	2.02	0.41
1:H:359:ILE:HG22	1:H:360:THR:O	2.21	0.41
1:C:129:ILE:O	1:C:129:ILE:HG13	2.20	0.40
1:C:451:GLN:HE21	1:C:451:GLN:HB3	1.65	0.40
1:D:117:VAL:HG11	1:D:443:PHE:HE1	1.86	0.40
1:D:332:PHE:CE2	1:D:333:THR:HG22	2.56	0.40
1:E:100:PRO:HG2	1:E:103:LYS:HB2	2.02	0.40
1:E:359:ILE:CG2	1:E:360:THR:H	2.34	0.40
1:F:45:ALA:O	1:F:46:LYS:C	2.63	0.40
1:F:60:HIS:ND1	1:F:63:MET:HE3	2.36	0.40
1:F:114:GLY:HA2	1:F:448:GLY:HA2	2.04	0.40
1:F:239:HIS:ND1	1:F:289:PRO:HD3	2.35	0.40
1:F:351:SER:HB2	1:F:423:VAL:HG13	2.02	0.40
1:G:238:VAL:HG23	1:G:239:HIS:CE1	2.56	0.40
1:A:78:THR:CG2	1:A:117:VAL:HB	2.48	0.40
1:B:123:HIS:HB3	1:B:181:MET:HE1	2.03	0.40
1:B:212:ARG:HA	1:B:213:PRO:HD2	1.87	0.40
1:B:278:PRO:HD2	1:B:278:PRO:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:VAL:CG2	1:C:364:PHE:HB2	2.50	0.40
1:D:202:ASN:HB3	1:D:207:TYR:CZ	2.56	0.40
1:D:223:ARG:O	1:D:224:ALA:C	2.63	0.40
1:D:238:VAL:HG23	1:D:239:HIS:CE1	2.56	0.40
1:E:63:MET:HE2	1:E:63:MET:HB2	1.94	0.40
1:F:72:ASP:HB2	1:F:318:SER:OG	2.22	0.40
1:F:349:LEU:HD11	1:F:359:ILE:HD11	2.03	0.40
1:G:426:GLU:HA	1:G:427:PRO:HD3	1.93	0.40
1:H:136:GLU:O	1:H:137:LEU:C	2.64	0.40
1:H:208:HIS:CD2	1:H:286:VAL:HG13	2.56	0.40
1:H:350:PHE:O	1:H:354:VAL:HB	2.21	0.40
1:B:283:ALA:HA	1:B:286:VAL:HG23	2.04	0.40
1:C:229:GLU:HG3	1:C:257:LEU:HD21	2.03	0.40
1:C:241:THR:HG22	1:C:242:CYS:N	2.34	0.40
1:E:171:LEU:O	1:E:172:ALA:C	2.65	0.40
1:F:59:THR:HG23	1:F:61:LEU:HG	2.03	0.40
1:F:320:ASP:HB3	1:F:414:ASP:OD2	2.21	0.40
1:G:170:LEU:HA	1:G:180:VAL:HG21	2.02	0.40
1:G:351:SER:CB	1:G:423:VAL:HG13	2.51	0.40
1:H:322:LYS:HG3	1:H:414:ASP:OD2	2.22	0.40
1:B:140:VAL:O	1:B:144:GLU:O	2.40	0.40
1:B:154:ALA:O	1:B:155:TYR:HB2	2.21	0.40
1:C:158:VAL:HG12	1:C:159:PHE:CE1	2.56	0.40
1:C:337:ASN:N	1:C:337:ASN:HD22	2.19	0.40
1:F:17:TYR:CD1	1:F:17:TYR:N	2.89	0.40
1:G:228:THR:OG1	1:G:235:LEU:HD22	2.22	0.40
1:A:17:TYR:CD1	1:A:17:TYR:N	2.89	0.40
1:B:140:VAL:HG12	1:B:146:ILE:HB	2.04	0.40
1:B:303:ALA:HA	1:B:308:GLN:CG	2.34	0.40
1:B:351:SER:HB2	1:B:423:VAL:HG13	2.03	0.40
1:C:37:GLU:O	1:C:38:LYS:C	2.65	0.40
1:C:212:ARG:HA	1:C:213:PRO:HD2	1.88	0.40
1:C:260:TRP:CE2	1:C:375:LEU:HD21	2.57	0.40
1:D:350:PHE:O	1:D:354:VAL:HB	2.21	0.40
1:F:37:GLU:O	1:F:38:LYS:C	2.65	0.40
1:G:103:LYS:HB2	1:G:103:LYS:HE2	1.93	0.40
1:G:189:VAL:O	1:G:190:ILE:C	2.64	0.40
1:G:206:ILE:O	1:G:206:ILE:HG12	2.21	0.40
1:H:152:PHE:CD1	1:H:159:PHE:HB3	2.57	0.40
1:H:368:VAL:O	1:H:368:VAL:HG12	2.20	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	457/460 (99%)	397 (87%)	51 (11%)	9 (2%)	6	26
1	B	457/460 (99%)	399 (87%)	48 (10%)	10 (2%)	5	24
1	C	457/460 (99%)	399 (87%)	48 (10%)	10 (2%)	5	24
1	D	457/460 (99%)	399 (87%)	49 (11%)	9 (2%)	6	26
1	E	457/460 (99%)	398 (87%)	48 (10%)	11 (2%)	4	23
1	F	457/460 (99%)	400 (88%)	48 (10%)	9 (2%)	6	26
1	G	457/460 (99%)	399 (87%)	48 (10%)	10 (2%)	5	24
1	H	457/460 (99%)	396 (87%)	50 (11%)	11 (2%)	4	23
All	All	3656/3680 (99%)	3187 (87%)	390 (11%)	79 (2%)	5	24

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	278	PRO
1	A	322	LYS
1	A	359	ILE
1	B	42	VAL
1	B	278	PRO
1	B	322	LYS
1	B	359	ILE
1	C	42	VAL
1	C	278	PRO
1	C	322	LYS
1	C	359	ILE
1	D	42	VAL
1	D	278	PRO
1	D	322	LYS
1	D	359	ILE
1	E	42	VAL

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Mol	Chain	Res	Type
1	E	278	PRO
1	E	322	LYS
1	E	359	ILE
1	F	42	VAL
1	F	278	PRO
1	F	322	LYS
1	F	359	ILE
1	G	42	VAL
1	G	278	PRO
1	G	322	LYS
1	G	359	ILE
1	H	42	VAL
1	H	278	PRO
1	H	322	LYS
1	H	359	ILE
1	A	294	LYS
1	B	294	LYS
1	D	294	LYS
1	E	294	LYS
1	A	64	PRO
1	B	64	PRO
1	C	64	PRO
1	C	294	LYS
1	E	239	HIS
1	G	64	PRO
1	G	294	LYS
1	H	64	PRO
1	H	239	HIS
1	A	354	VAL
1	B	239	HIS
1	D	64	PRO
1	D	239	HIS
1	E	64	PRO
1	F	64	PRO
1	F	294	LYS
1	F	354	VAL
1	H	294	LYS
1	B	354	VAL
1	C	354	VAL
1	F	277	LYS
1	H	354	VAL
1	E	354	VAL

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Mol	Chain	Res	Type
1	G	277	LYS
1	H	277	LYS
1	A	158	VAL
1	A	277	LYS
1	B	158	VAL
1	B	277	LYS
1	D	277	LYS
1	E	277	LYS
1	G	354	VAL
1	C	39	GLY
1	C	158	VAL
1	C	277	LYS
1	D	354	VAL
1	E	39	GLY
1	E	158	VAL
1	H	158	VAL
1	F	158	VAL
1	G	39	GLY
1	G	158	VAL
1	H	39	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/379 (100%)	364 (96%)	15 (4%)	28	60
1	B	379/379 (100%)	364 (96%)	15 (4%)	28	60
1	C	379/379 (100%)	363 (96%)	16 (4%)	26	59
1	D	379/379 (100%)	364 (96%)	15 (4%)	28	60
1	E	379/379 (100%)	365 (96%)	14 (4%)	30	63
1	F	379/379 (100%)	365 (96%)	14 (4%)	30	63
1	G	379/379 (100%)	365 (96%)	14 (4%)	30	63
1	H	379/379 (100%)	364 (96%)	15 (4%)	28	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3032/3032 (100%)	2914 (96%)	118 (4%)	28 61

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	62	ASP
1	A	63	MET
1	A	144	GLU
1	A	211	THR
1	A	234	GLN
1	A	262	GLU
1	A	278	PRO
1	A	304	LEU
1	A	324	GLN
1	A	329	ARG
1	A	409	HIS
1	A	413	VAL
1	A	431	LEU
1	A	442	GLN
1	B	25	ASP
1	B	62	ASP
1	B	63	MET
1	B	144	GLU
1	B	149	LEU
1	B	211	THR
1	B	234	GLN
1	B	278	PRO
1	B	304	LEU
1	B	324	GLN
1	B	329	ARG
1	B	409	HIS
1	B	413	VAL
1	B	431	LEU
1	B	442	GLN
1	C	25	ASP
1	C	62	ASP
1	C	63	MET
1	C	144	GLU
1	C	149	LEU
1	C	211	THR
1	C	234	GLN

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Mol	Chain	Res	Type
1	C	278	PRO
1	C	304	LEU
1	C	308	GLN
1	C	324	GLN
1	C	329	ARG
1	C	409	HIS
1	C	413	VAL
1	C	431	LEU
1	C	442	GLN
1	D	25	ASP
1	D	62	ASP
1	D	63	MET
1	D	144	GLU
1	D	211	THR
1	D	234	GLN
1	D	277	LYS
1	D	278	PRO
1	D	304	LEU
1	D	324	GLN
1	D	329	ARG
1	D	409	HIS
1	D	413	VAL
1	D	431	LEU
1	D	442	GLN
1	E	25	ASP
1	E	62	ASP
1	E	63	MET
1	E	144	GLU
1	E	211	THR
1	E	278	PRO
1	E	304	LEU
1	E	308	GLN
1	E	324	GLN
1	E	329	ARG
1	E	409	HIS
1	E	413	VAL
1	E	431	LEU
1	E	442	GLN
1	F	25	ASP
1	F	62	ASP
1	F	63	MET
1	F	144	GLU

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Mol	Chain	Res	Type
1	F	211	THR
1	F	234	GLN
1	F	278	PRO
1	F	304	LEU
1	F	324	GLN
1	F	329	ARG
1	F	409	HIS
1	F	413	VAL
1	F	431	LEU
1	F	442	GLN
1	G	25	ASP
1	G	62	ASP
1	G	63	MET
1	G	144	GLU
1	G	211	THR
1	G	234	GLN
1	G	278	PRO
1	G	304	LEU
1	G	324	GLN
1	G	329	ARG
1	G	409	HIS
1	G	413	VAL
1	G	431	LEU
1	G	442	GLN
1	H	25	ASP
1	H	62	ASP
1	H	63	MET
1	H	144	GLU
1	H	211	THR
1	H	234	GLN
1	H	277	LYS
1	H	278	PRO
1	H	304	LEU
1	H	324	GLN
1	H	329	ARG
1	H	409	HIS
1	H	413	VAL
1	H	431	LEU
1	H	442	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	157	ASN
1	A	226	GLN
1	A	297	GLN
1	A	310	GLN
1	A	337	ASN
1	A	362	ASN
1	A	451	GLN
1	B	20	HIS
1	B	157	ASN
1	B	254	ASN
1	B	279	ASN
1	B	297	GLN
1	B	306	ASN
1	B	310	GLN
1	B	337	ASN
1	B	362	ASN
1	B	451	GLN
1	C	20	HIS
1	C	157	ASN
1	C	254	ASN
1	C	279	ASN
1	C	297	GLN
1	C	306	ASN
1	C	310	GLN
1	C	337	ASN
1	C	362	ASN
1	C	399	ASN
1	C	451	GLN
1	D	20	HIS
1	D	157	ASN
1	D	226	GLN
1	D	279	ASN
1	D	297	GLN
1	D	306	ASN
1	D	310	GLN
1	D	337	ASN
1	D	362	ASN
1	D	451	GLN
1	E	20	HIS
1	E	157	ASN
1	E	254	ASN
1	E	279	ASN

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Mol	Chain	Res	Type
1	E	297	GLN
1	E	306	ASN
1	E	310	GLN
1	E	337	ASN
1	E	362	ASN
1	E	399	ASN
1	E	451	GLN
1	F	20	HIS
1	F	157	ASN
1	F	279	ASN
1	F	297	GLN
1	F	306	ASN
1	F	310	GLN
1	F	337	ASN
1	F	362	ASN
1	F	451	GLN
1	G	20	HIS
1	G	157	ASN
1	G	254	ASN
1	G	279	ASN
1	G	297	GLN
1	G	306	ASN
1	G	310	GLN
1	G	337	ASN
1	G	362	ASN
1	G	451	GLN
1	H	20	HIS
1	H	226	GLN
1	H	279	ASN
1	H	297	GLN
1	H	310	GLN
1	H	337	ASN
1	H	362	ASN
1	H	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	E	150	1,2	10,11,12	1.17	1 (10%)	6,12,14	1.25	1 (16%)
1	KCX	G	150	1,2	10,11,12	1.05	1 (10%)	6,12,14	1.75	1 (16%)
1	KCX	F	150	1,2	10,11,12	1.22	1 (10%)	6,12,14	1.18	1 (16%)
1	KCX	A	150	1,2	10,11,12	1.93	2 (20%)	6,12,14	2.40	1 (16%)
1	KCX	B	150	1,2	10,11,12	1.37	2 (20%)	6,12,14	2.09	2 (33%)
1	KCX	D	150	1,2	10,11,12	1.15	1 (10%)	6,12,14	1.68	1 (16%)
1	KCX	H	150	1,2	10,11,12	1.34	2 (20%)	6,12,14	1.89	1 (16%)
1	KCX	C	150	1,2	10,11,12	1.58	2 (20%)	6,12,14	1.27	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	E	150	1,2	-	1/9/10/12	-
1	KCX	G	150	1,2	-	3/9/10/12	-
1	KCX	F	150	1,2	-	1/9/10/12	-
1	KCX	A	150	1,2	-	3/9/10/12	-
1	KCX	B	150	1,2	-	5/9/10/12	-
1	KCX	D	150	1,2	-	3/9/10/12	-
1	KCX	H	150	1,2	-	3/9/10/12	-
1	KCX	C	150	1,2	-	2/9/10/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	KCX	CX-NZ	-4.81	1.26	1.35
1	C	150	KCX	CX-NZ	-3.63	1.28	1.35
1	B	150	KCX	CX-NZ	2.88	1.40	1.35
1	F	150	KCX	OQ1-CX	2.81	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	KCX	OQ1-CX	2.58	1.26	1.21
1	C	150	KCX	OQ1-CX	2.56	1.26	1.21
1	H	150	KCX	CX-NZ	-2.54	1.30	1.35
1	D	150	KCX	OQ1-CX	2.44	1.26	1.21
1	E	150	KCX	OQ1-CX	2.37	1.26	1.21
1	H	150	KCX	OQ1-CX	2.26	1.25	1.21
1	G	150	KCX	OQ1-CX	2.14	1.25	1.21
1	B	150	KCX	OQ1-CX	2.02	1.25	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	KCX	OQ1-CX-NZ	-5.54	116.51	124.92
1	H	150	KCX	OQ1-CX-NZ	-4.26	118.45	124.92
1	G	150	KCX	OQ1-CX-NZ	-4.02	118.81	124.92
1	D	150	KCX	OQ1-CX-NZ	-3.77	119.20	124.92
1	B	150	KCX	CE-NZ-CX	-3.65	115.79	121.98
1	B	150	KCX	OQ1-CX-NZ	-3.18	120.09	124.92
1	E	150	KCX	OQ1-CX-NZ	-2.47	121.17	124.92
1	F	150	KCX	OQ1-CX-NZ	-2.33	121.39	124.92
1	C	150	KCX	CE-NZ-CX	2.03	125.43	121.98
1	C	150	KCX	OQ1-CX-NZ	-2.01	121.87	124.92

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	150	KCX	OQ1-CX-NZ-CE
1	B	150	KCX	C-CA-CB-CG
1	B	150	KCX	O-C-CA-CB
1	C	150	KCX	O-C-CA-CB
1	D	150	KCX	C-CA-CB-CG
1	E	150	KCX	C-CA-CB-CG
1	F	150	KCX	C-CA-CB-CG
1	G	150	KCX	C-CA-CB-CG
1	H	150	KCX	C-CA-CB-CG
1	A	150	KCX	OQ2-CX-NZ-CE
1	B	150	KCX	OQ1-CX-NZ-CE
1	D	150	KCX	OQ1-CX-NZ-CE
1	D	150	KCX	OQ2-CX-NZ-CE
1	G	150	KCX	OQ1-CX-NZ-CE
1	G	150	KCX	OQ2-CX-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	H	150	KCX	OQ1-CX-NZ-CE
1	H	150	KCX	OQ2-CX-NZ-CE
1	A	150	KCX	C-CA-CB-CG
1	C	150	KCX	C-CA-CB-CG
1	B	150	KCX	OQ2-CX-NZ-CE
1	B	150	KCX	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	150	KCX	1	0
1	G	150	KCX	2	0
1	F	150	KCX	2	0
1	A	150	KCX	4	0
1	B	150	KCX	1	0
1	D	150	KCX	2	0
1	H	150	KCX	3	0
1	C	150	KCX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	459/460 (99%)	0.09	7 (1%) 72 49	33, 51, 75, 92	0
1	B	459/460 (99%)	0.14	6 (1%) 75 53	32, 51, 75, 92	0
1	C	459/460 (99%)	0.19	7 (1%) 72 49	32, 51, 75, 91	0
1	D	459/460 (99%)	0.22	8 (1%) 69 46	33, 53, 75, 92	0
1	E	459/460 (99%)	0.21	8 (1%) 69 46	32, 51, 75, 91	0
1	F	459/460 (99%)	0.33	12 (2%) 57 34	33, 53, 75, 91	0
1	G	459/460 (99%)	0.19	7 (1%) 72 49	33, 52, 76, 92	0
1	H	459/460 (99%)	0.11	6 (1%) 75 53	31, 52, 75, 91	0
All	All	3672/3680 (99%)	0.19	61 (1%) 69 46	31, 52, 75, 92	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	66	GLY	4.2
1	G	65	LEU	4.1
1	B	68	THR	4.0
1	D	67	GLY	4.0
1	G	68	THR	3.6
1	D	65	LEU	3.5
1	F	66	GLY	3.3
1	F	67	GLY	3.3
1	B	65	LEU	3.2
1	D	40	ALA	3.1
1	F	33	GLN	3.1
1	B	386	VAL	3.1
1	G	201	GLY	3.0
1	A	279	ASN	2.9
1	C	279	ASN	2.9
1	H	143	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	68	THR	2.8
1	F	65	LEU	2.8
1	C	69	VAL	2.8
1	E	407	GLU	2.8
1	H	65	LEU	2.8
1	A	65	LEU	2.7
1	F	41	GLU	2.7
1	H	41	GLU	2.7
1	A	143	GLU	2.6
1	F	106	GLU	2.6
1	C	459	GLY	2.6
1	C	65	LEU	2.6
1	F	127	SER	2.6
1	D	330	GLY	2.6
1	B	67	GLY	2.5
1	G	117	VAL	2.5
1	H	43	ILE	2.5
1	D	68	THR	2.5
1	E	279	ASN	2.4
1	A	39	GLY	2.4
1	E	65	LEU	2.4
1	D	192	TYR	2.4
1	A	386	VAL	2.3
1	B	33	GLN	2.3
1	B	278	PRO	2.2
1	C	278	PRO	2.2
1	F	96	ASN	2.2
1	H	460	THR	2.2
1	G	66	GLY	2.2
1	E	133	VAL	2.2
1	G	192	TYR	2.2
1	E	324	GLN	2.2
1	D	1	MET	2.2
1	E	277	LYS	2.2
1	E	401	GLU	2.1
1	C	35	LEU	2.1
1	E	41	GLU	2.1
1	H	400	ILE	2.1
1	A	337	ASN	2.1
1	C	277	LYS	2.0
1	F	285	TYR	2.0
1	F	323	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	67	GLY	2.0
1	F	278	PRO	2.0
1	F	407	GLU	2.0

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

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(Å ²)	Q<0.9
1	KCX	E	150	12/13	0.88	0.13	41,45,54,56	0
1	KCX	F	150	12/13	0.88	0.11	44,46,53,54	0
1	KCX	H	150	12/13	0.91	0.10	39,45,51,52	0
1	KCX	D	150	12/13	0.92	0.13	42,45,54,55	0
1	KCX	A	150	12/13	0.92	0.10	42,44,51,52	0
1	KCX	C	150	12/13	0.93	0.11	42,45,56,57	0
1	KCX	G	150	12/13	0.94	0.09	40,44,49,50	0
1	KCX	B	150	12/13	0.95	0.09	40,43,47,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	ZN	F	501	1/1	0.94	0.05	72,72,72,72	0
2	ZN	D	502	1/1	0.95	0.05	48,48,48,48	0
2	ZN	C	501	1/1	0.95	0.04	69,69,69,69	0
2	ZN	D	501	1/1	0.96	0.04	64,64,64,64	0
2	ZN	G	502	1/1	0.97	0.03	47,47,47,47	0
2	ZN	H	501	1/1	0.97	0.04	70,70,70,70	0
2	ZN	E	502	1/1	0.98	0.03	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	502	1/1	0.98	0.03	44,44,44,44	0
2	ZN	F	502	1/1	0.98	0.03	51,51,51,51	0
2	ZN	A	502	1/1	0.98	0.03	55,55,55,55	0
2	ZN	E	501	1/1	0.98	0.04	68,68,68,68	0
2	ZN	H	502	1/1	0.98	0.03	52,52,52,52	0
2	ZN	G	501	1/1	0.99	0.02	59,59,59,59	0
2	ZN	A	501	1/1	0.99	0.04	55,55,55,55	0
2	ZN	B	501	1/1	0.99	0.03	68,68,68,68	0
2	ZN	C	502	1/1	0.99	0.02	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.