



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:54 PM UTC

PDB ID : 2HU0 / pdb_00002hu0
Title : N1 neuraminidase in complex with oseltamivir 1
Authors : Russell, R.J.; Haire, L.F.; Stevens, D.J.; Collins, P.J.; Lin, Y.P.; Blackburn, G.M.; Hay, A.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2006-07-26
Resolution : 2.95 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

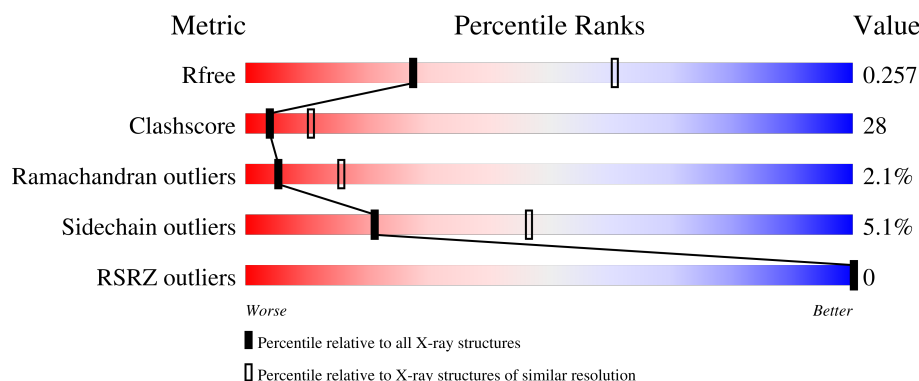
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	387	
1	B	387	
1	C	387	
1	D	387	
1	E	387	

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Mol	Chain	Length	Quality of chain
1	F	387	 56% 33% 10% ..
1	G	387	 51% 39% 8% ..
1	H	387	 52% 39% 7% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23716 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.

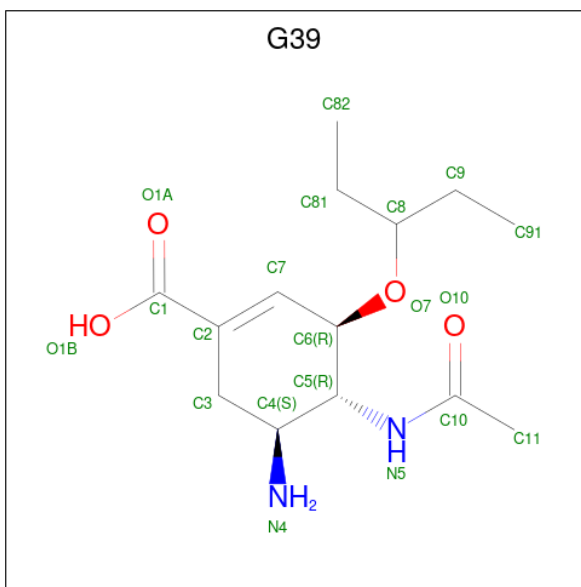
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	B	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	C	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	D	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	E	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	F	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	G	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	H	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
B	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
C	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
D	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
E	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
F	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
G	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
H	169A	TYR	HIS	engineered mutation	UNP Q6DPL2

- Molecule 2 is (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (CCD ID: G39) (formula: C₁₄H₂₄N₂O₄).

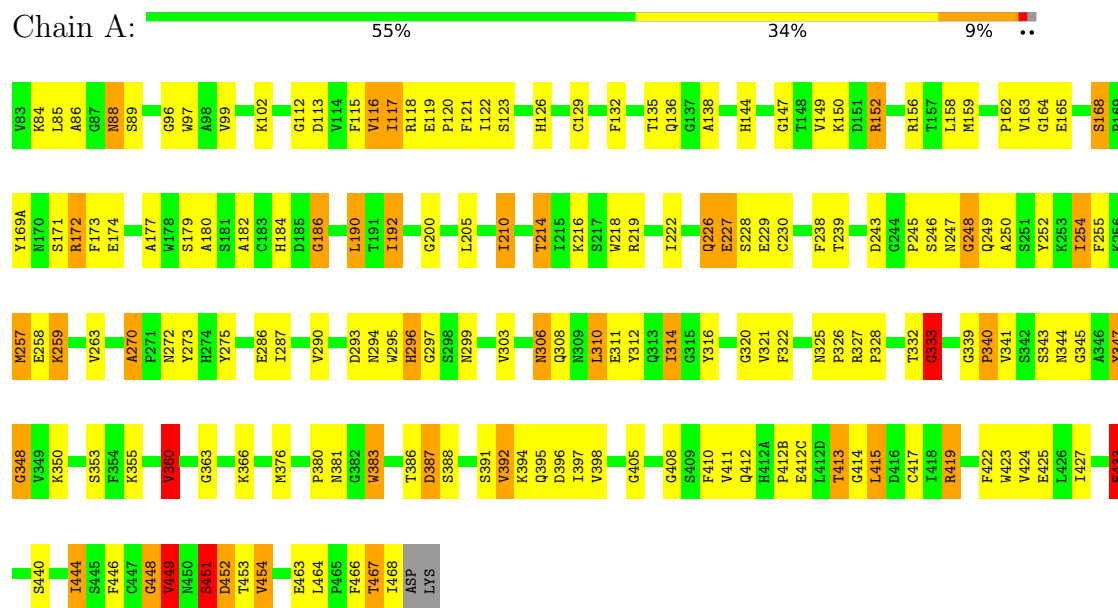


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	20	14	2	4	0	0

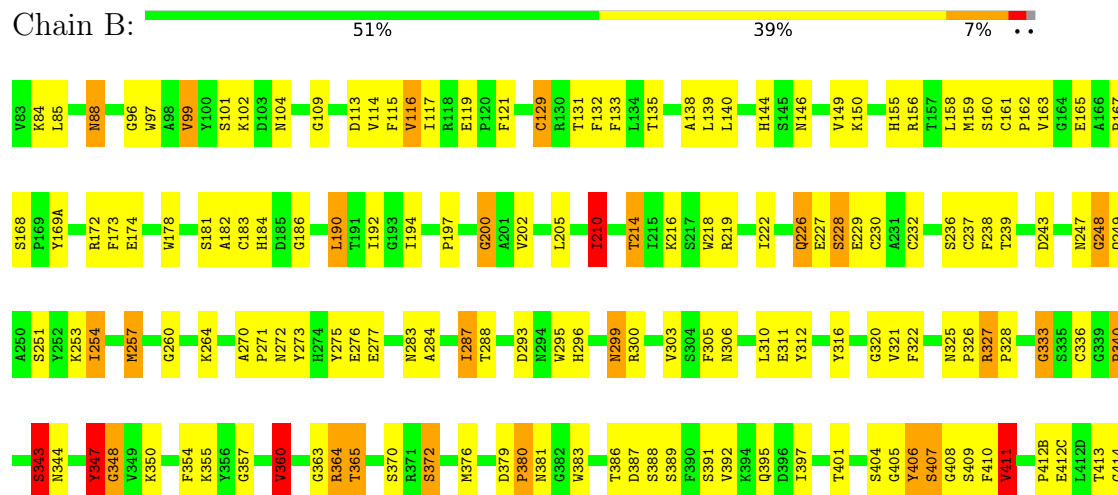
3 Residue-property plots

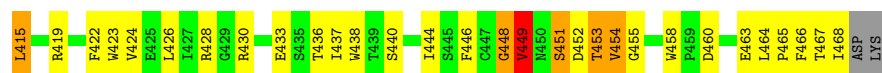
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



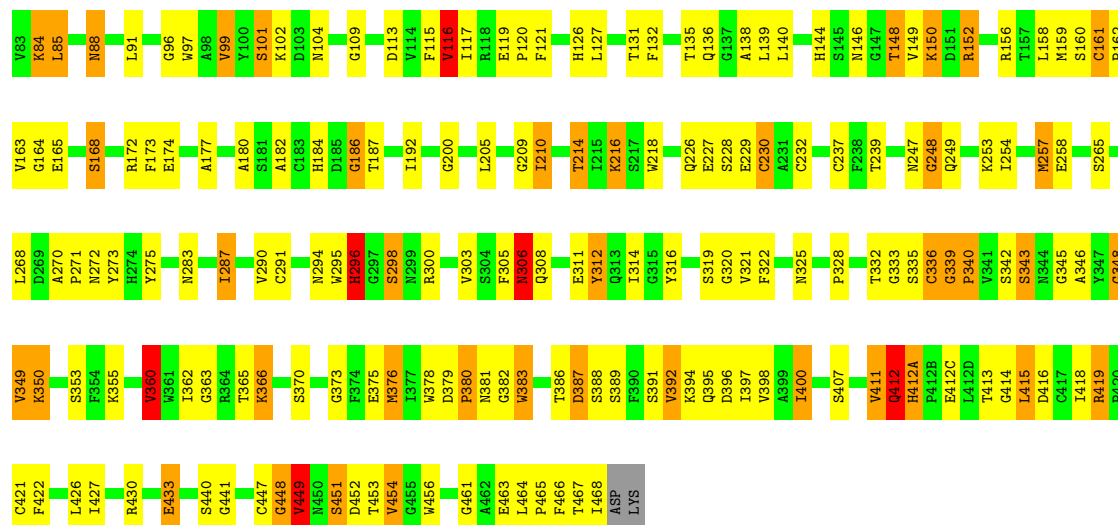
• Molecule 1: Neuraminidase





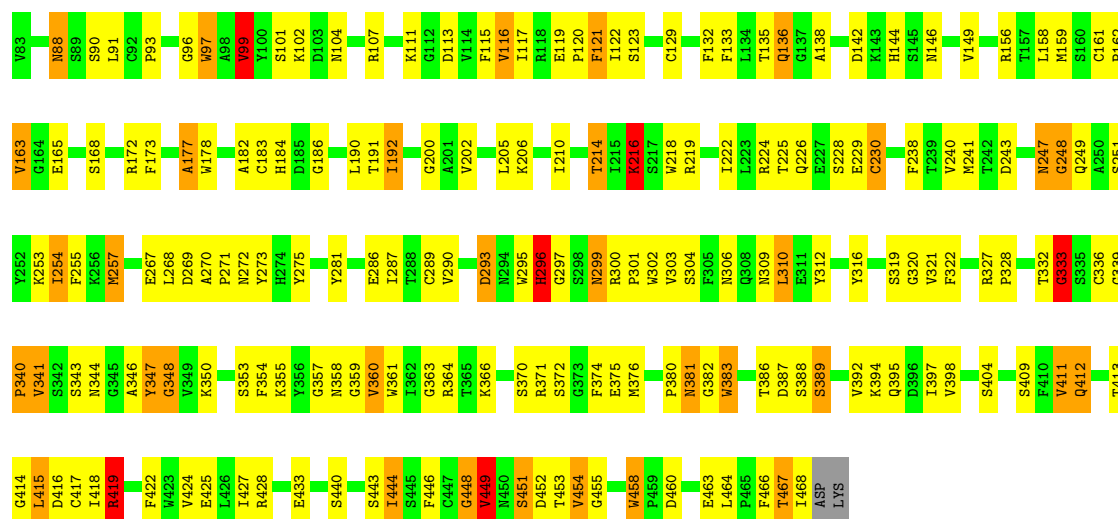
• Molecule 1: Neuraminidase

Chain C: 53% 34% 11% ..



• Molecule 1: Neuraminidase

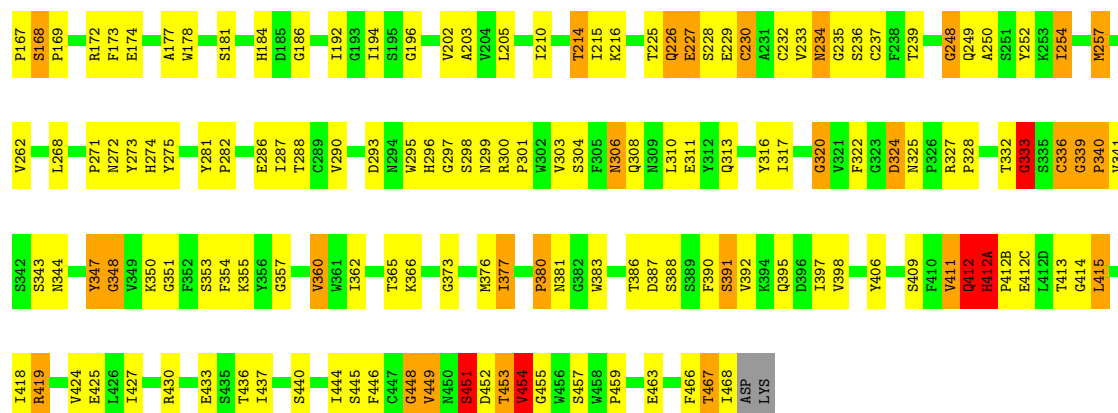
Chain D: 51% 39% 9% ..



• Molecule 1: Neuraminidase

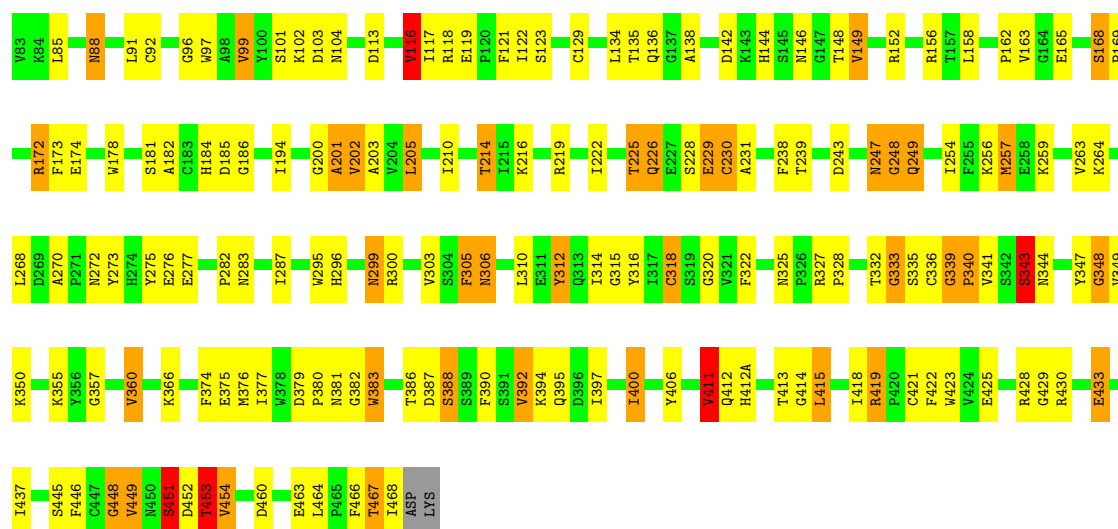
Chain E: 52% 37% 9% ..





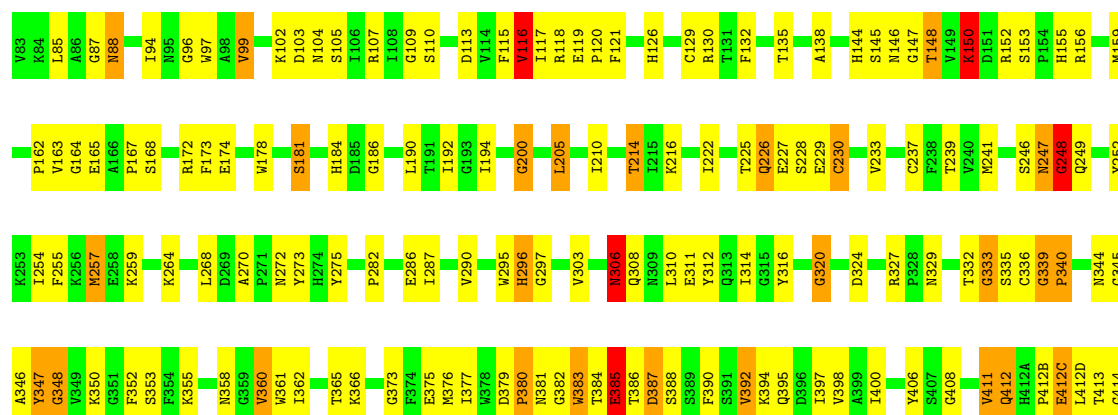
• Molecule 1: Neuraminidase

Chain F: 56% 33% 10% ..



• Molecule 1: Neuraminidase

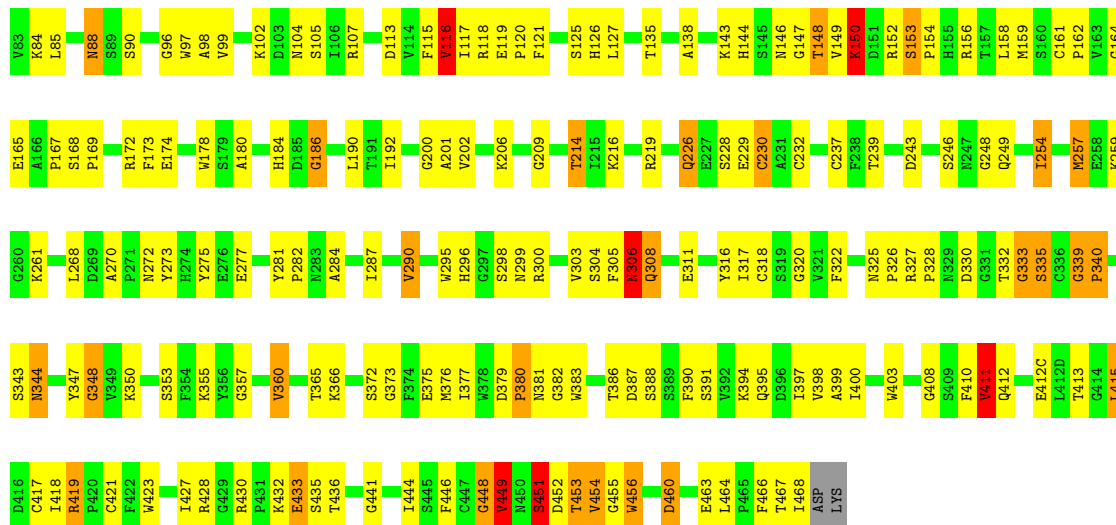
Chain G: 51% 39% 8% ..





• Molecule 1: Neuraminidase

Chain H: 52% 39% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	198.08Å 200.58Å 210.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	142.86 – 2.95 140.94 – 2.95	Depositor EDS
% Data completeness (in resolution range)	79.1 (142.86-2.95) 79.3 (140.94-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.295 0.257 , 0.257	Depositor DCC
R_{free} test set	3705 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23716	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G39

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.51	21/3045 (0.7%)	1.53	37/4141 (0.9%)
1	B	1.57	21/3045 (0.7%)	1.51	43/4141 (1.0%)
1	C	1.61	28/3045 (0.9%)	1.60	51/4141 (1.2%)
1	D	1.60	25/3045 (0.8%)	1.57	42/4141 (1.0%)
1	E	1.43	15/3045 (0.5%)	1.44	47/4141 (1.1%)
1	F	1.47	19/3045 (0.6%)	1.41	30/4141 (0.7%)
1	G	1.52	21/3045 (0.7%)	1.49	41/4141 (1.0%)
1	H	1.50	15/3045 (0.5%)	1.43	40/4141 (1.0%)
All	All	1.53	165/24360 (0.7%)	1.50	331/33128 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	4
1	D	0	2
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
All	All	0	21

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	306	ASN	C-N	16.35	1.58	1.33
1	E	333	GLY	C-N	14.85	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	333	GLY	C-N	13.72	1.51	1.33
1	C	336	CYS	C-N	13.26	1.53	1.33
1	F	411	VAL	C-N	13.01	1.50	1.33
1	B	333	GLY	C-N	12.83	1.49	1.33
1	B	392	VAL	C-N	12.79	1.49	1.33
1	G	392	VAL	C-N	12.58	1.49	1.33
1	H	333	GLY	C-N	12.33	1.49	1.33
1	H	150	LYS	CE-NZ	11.39	1.83	1.49
1	C	84	LYS	CG-CD	10.30	1.83	1.52
1	B	411	VAL	CB-CG2	10.18	1.86	1.52
1	B	336	CYS	C-N	9.89	1.48	1.33
1	D	346	ALA	CA-CB	9.82	1.66	1.52
1	F	433	GLU	C-N	9.75	1.46	1.33
1	B	149	VAL	CA-CB	9.37	1.63	1.54
1	A	392	VAL	C-N	9.15	1.45	1.33
1	A	149	VAL	CA-CB	9.12	1.63	1.54
1	E	392	VAL	C-N	8.99	1.46	1.33
1	C	339	GLY	N-CA	8.97	1.57	1.44
1	G	333	GLY	C-N	8.96	1.45	1.33
1	D	389	SER	C-O	8.95	1.34	1.23
1	H	150	LYS	CD-CE	8.75	1.78	1.52
1	C	392	VAL	C-N	8.72	1.44	1.33
1	D	392	VAL	C-N	8.48	1.44	1.33
1	E	411	VAL	CB-CG2	8.22	1.79	1.52
1	D	433	GLU	C-N	8.20	1.45	1.33
1	D	149	VAL	CA-CB	8.18	1.65	1.54
1	A	333	GLY	C-N	8.06	1.43	1.33
1	D	411	VAL	CB-CG2	7.89	1.78	1.52
1	D	254	ILE	CA-CB	-7.85	1.44	1.54
1	H	306	ASN	C-O	7.75	1.33	1.24
1	B	408	GLY	CA-C	-7.71	1.43	1.51
1	B	306	ASN	C-N	-7.68	1.23	1.33
1	D	411	VAL	C-N	7.39	1.43	1.33
1	C	411	VAL	CB-CG2	7.22	1.76	1.52
1	A	177	ALA	CA-CB	-7.16	1.42	1.53
1	H	433	GLU	C-N	7.14	1.43	1.33
1	D	336	CYS	C-N	7.13	1.44	1.33
1	C	148	THR	CA-CB	7.07	1.66	1.53
1	C	387	ASP	CA-C	-7.04	1.44	1.52
1	C	370	SER	CA-C	-7.00	1.43	1.52
1	B	433	GLU	C-N	6.83	1.42	1.33
1	E	134	LEU	N-CA	-6.77	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	456	TRP	C-O	6.76	1.29	1.24
1	F	336	CYS	C-N	6.65	1.43	1.33
1	D	333	GLY	C-N	6.59	1.41	1.33
1	C	412	GLN	C-N	-6.57	1.19	1.34
1	B	84	LYS	CG-CD	6.56	1.72	1.52
1	G	411	VAL	C-N	6.54	1.42	1.33
1	A	190	LEU	CA-C	-6.50	1.44	1.52
1	B	194	ILE	N-CA	-6.48	1.38	1.46
1	A	254	ILE	CA-CB	-6.45	1.46	1.54
1	A	387	ASP	CA-C	-6.45	1.47	1.53
1	E	297	GLY	C-O	6.44	1.32	1.23
1	B	364	ARG	N-CA	-6.42	1.38	1.46
1	F	306	ASN	C-N	6.42	1.43	1.33
1	D	177	ALA	CA-CB	-6.42	1.42	1.53
1	G	248	GLY	N-CA	6.42	1.54	1.45
1	H	290	VAL	C-O	-6.36	1.17	1.24
1	A	314	ILE	N-CA	-6.33	1.38	1.46
1	F	392	VAL	C-N	6.32	1.41	1.33
1	G	306	ASN	C-N	6.30	1.43	1.33
1	F	201	ALA	CA-CB	-6.29	1.42	1.53
1	C	216	LYS	CG-CD	6.25	1.71	1.52
1	A	424	VAL	N-CA	-6.23	1.38	1.46
1	B	129	CYS	N-CA	-6.22	1.38	1.46
1	C	150	LYS	C-O	6.21	1.31	1.23
1	D	247	ASN	N-CA	6.20	1.50	1.46
1	F	149	VAL	CA-CB	6.14	1.62	1.54
1	D	216	LYS	CG-CD	6.13	1.70	1.52
1	D	293	ASP	C-O	6.12	1.30	1.23
1	B	411	VAL	CB-CG1	-6.12	1.32	1.52
1	G	348	GLY	N-CA	6.07	1.50	1.45
1	D	216	LYS	CD-CE	6.06	1.70	1.52
1	G	148	THR	CA-CB	6.05	1.63	1.53
1	C	340	PRO	N-CA	-6.03	1.39	1.47
1	C	84	LYS	CD-CE	6.02	1.70	1.52
1	F	453	THR	C-O	-6.02	1.16	1.24
1	C	150	LYS	CA-C	5.97	1.60	1.52
1	C	350	LYS	C-O	5.95	1.31	1.23
1	H	335	SER	CA-C	-5.89	1.45	1.52
1	A	306	ASN	CG-OD1	5.85	1.34	1.23
1	C	152	ARG	C-O	5.83	1.31	1.23
1	E	148	THR	CA-CB	5.79	1.63	1.53
1	G	148	THR	N-CA	5.77	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	411	VAL	C-O	5.76	1.31	1.24
1	G	109	GLY	C-O	-5.75	1.17	1.23
1	A	152	ARG	C-O	5.71	1.31	1.23
1	E	377	ILE	C-O	-5.71	1.18	1.24
1	A	452	ASP	CA-C	-5.70	1.46	1.52
1	D	107	ARG	C-O	-5.70	1.17	1.24
1	C	149	VAL	CA-CB	5.69	1.62	1.54
1	B	453	THR	CA-C	-5.67	1.47	1.53
1	E	336	CYS	C-N	5.67	1.42	1.33
1	B	197	PRO	C-O	5.65	1.30	1.23
1	E	412	GLN	C-N	-5.64	1.21	1.34
1	H	201	ALA	CA-CB	-5.63	1.44	1.53
1	A	84	LYS	CG-CD	5.63	1.69	1.52
1	G	346	ALA	CA-CB	5.63	1.60	1.53
1	D	122	ILE	C-O	-5.61	1.17	1.24
1	F	168	SER	CA-CB	-5.60	1.47	1.53
1	A	306	ASN	C-N	5.58	1.41	1.33
1	G	412	GLN	CB-CG	5.58	1.69	1.52
1	D	121	PHE	C-O	5.58	1.30	1.23
1	E	150	LYS	CD-CE	5.58	1.69	1.52
1	H	84	LYS	C-O	5.57	1.30	1.23
1	C	412	GLN	C-O	-5.57	1.16	1.24
1	H	148	THR	CA-CB	5.53	1.62	1.53
1	B	458	TRP	N-CA	-5.51	1.40	1.46
1	G	150	LYS	CE-NZ	5.50	1.65	1.49
1	B	210	ILE	CA-CB	5.49	1.60	1.54
1	G	412(C)	GLU	C-O	-5.49	1.17	1.24
1	F	149	VAL	CA-C	5.47	1.59	1.52
1	G	167	PRO	C-O	-5.47	1.18	1.23
1	G	352	PHE	N-CA	5.47	1.52	1.46
1	C	177	ALA	CA-CB	-5.47	1.45	1.53
1	G	264	LYS	N-CA	5.46	1.52	1.46
1	G	150	LYS	CD-CE	5.45	1.68	1.52
1	B	306	ASN	CG-OD1	5.45	1.33	1.23
1	H	330	ASP	C-O	-5.43	1.17	1.24
1	E	324	ASP	CG-OD1	5.42	1.35	1.25
1	H	84	LYS	CG-CD	5.40	1.68	1.52
1	G	408	GLY	C-O	5.40	1.29	1.24
1	C	346	ALA	CA-CB	5.40	1.60	1.53
1	A	86	ALA	CA-CB	-5.39	1.45	1.53
1	C	161	CYS	CA-C	-5.36	1.46	1.52
1	A	192	ILE	C-O	-5.34	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	149	VAL	C-O	5.33	1.29	1.24
1	E	306	ASN	C-N	-5.33	1.26	1.33
1	E	116	VAL	C-O	-5.31	1.18	1.24
1	F	259	LYS	C-O	5.30	1.30	1.23
1	D	97	TRP	C-O	-5.30	1.18	1.24
1	B	405	GLY	N-CA	5.29	1.54	1.45
1	F	229	GLU	N-CA	-5.29	1.39	1.46
1	B	422	PHE	N-CA	-5.29	1.39	1.45
1	C	187	THR	CA-C	5.27	1.57	1.52
1	A	452	ASP	CB-CG	5.25	1.65	1.52
1	A	245	PRO	CA-C	5.24	1.59	1.52
1	D	225	THR	N-CA	-5.24	1.40	1.46
1	A	86	ALA	C-O	5.22	1.30	1.24
1	G	105	SER	N-CA	-5.22	1.40	1.46
1	E	83	VAL	N-CA	5.21	1.56	1.46
1	C	258	GLU	CA-C	-5.20	1.46	1.52
1	D	240	VAL	CA-CB	-5.19	1.47	1.54
1	C	348	GLY	C-N	5.18	1.38	1.33
1	D	458	TRP	N-CA	-5.18	1.40	1.46
1	D	412	GLN	CB-CG	5.17	1.68	1.52
1	G	94	ILE	C-O	5.17	1.29	1.23
1	A	321	VAL	CA-C	-5.17	1.48	1.52
1	G	387	ASP	CA-C	-5.17	1.45	1.52
1	F	247	ASN	N-CA	5.16	1.52	1.46
1	F	343	SER	CB-OG	5.16	1.52	1.42
1	F	349	VAL	CA-CB	-5.14	1.50	1.55
1	C	168	SER	N-CA	-5.11	1.41	1.45
1	D	404	SER	C-O	-5.10	1.17	1.24
1	B	347	TYR	C-O	5.09	1.30	1.24
1	D	99	VAL	C-O	-5.08	1.18	1.24
1	F	400	ILE	CG1-CD1	5.06	1.71	1.51
1	C	343	SER	CB-OG	5.05	1.52	1.42
1	E	351	GLY	N-CA	5.03	1.49	1.45
1	F	205	LEU	C-O	5.02	1.30	1.24
1	A	270	ALA	N-CA	-5.01	1.41	1.46
1	C	314	ILE	C-O	-5.01	1.17	1.23
1	H	149	VAL	CA-CB	5.01	1.59	1.54

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	306	ASN	O-C-N	-14.34	103.52	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	412	GLN	O-C-N	-13.38	101.30	122.70
1	D	388	SER	N-CA-C	-12.15	96.16	114.64
1	G	388	SER	N-CA-C	-12.02	99.61	114.75
1	C	336	CYS	CA-C-N	-10.86	104.83	121.87
1	C	336	CYS	C-N-CA	-10.86	104.83	121.87
1	C	388	SER	N-CA-C	-10.81	97.34	114.09
1	D	348	GLY	N-CA-C	10.47	125.25	110.38
1	E	412	GLN	O-C-N	-10.44	105.99	122.70
1	B	226	GLN	N-CA-C	10.40	122.62	111.28
1	A	388	SER	N-CA-C	-10.39	98.85	114.64
1	D	411	VAL	CA-CB-CG2	-10.37	92.77	110.40
1	E	388	SER	N-CA-C	-10.26	99.52	114.39
1	D	247	ASN	CB-CA-C	-10.18	102.42	117.07
1	A	433	GLU	CA-C-N	-10.09	108.04	122.06
1	A	433	GLU	C-N-CA	-10.09	108.04	122.06
1	B	405	GLY	CA-C-O	-9.86	114.11	120.91
1	G	226	GLN	N-CA-C	9.75	122.81	111.11
1	B	411	VAL	CA-CB-CG2	-9.60	94.08	110.40
1	C	350	LYS	N-CA-C	-9.58	95.82	110.10
1	A	383	TRP	N-CA-C	-9.58	101.72	113.41
1	B	336	CYS	CA-C-N	-9.55	106.88	121.87
1	B	336	CYS	C-N-CA	-9.55	106.88	121.87
1	F	306	ASN	O-C-N	-9.52	109.61	122.36
1	E	348	GLY	N-CA-C	9.44	123.78	110.38
1	B	388	SER	N-CA-C	-9.17	99.36	113.02
1	D	226	GLN	N-CA-C	9.13	120.84	111.07
1	F	226	GLN	N-CA-C	9.13	122.16	111.02
1	B	348	GLY	N-CA-C	9.07	121.99	110.38
1	H	333	GLY	O-C-N	9.02	131.45	122.88
1	C	349	VAL	CA-C-O	-8.97	112.52	120.96
1	A	387	ASP	CB-CA-C	-8.93	101.39	114.87
1	H	226	GLN	N-CA-C	8.90	122.10	111.33
1	E	414	GLY	N-CA-C	-8.87	102.92	115.43
1	D	336	CYS	CA-C-N	-8.84	108.00	121.87
1	D	336	CYS	C-N-CA	-8.84	108.00	121.87
1	D	383	TRP	N-CA-C	-8.84	101.33	112.90
1	C	296	HIS	N-CA-C	8.79	120.79	110.41
1	D	247	ASN	N-CA-C	-8.77	101.59	108.78
1	C	412	GLN	CA-C-N	8.70	136.34	117.20
1	E	226	GLN	N-CA-C	8.39	121.48	111.33
1	B	433	GLU	CA-C-N	-8.36	110.62	122.41
1	B	433	GLU	C-N-CA	-8.36	110.62	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	411	VAL	O-C-N	8.34	132.19	123.18
1	D	296	HIS	N-CA-C	8.26	120.15	110.41
1	F	339	GLY	CA-C-N	8.19	130.07	119.84
1	F	339	GLY	C-N-CA	8.19	130.07	119.84
1	D	467	THR	N-CA-C	-8.16	103.07	112.87
1	C	383	TRP	N-CA-C	-8.02	102.40	112.90
1	E	411	VAL	CA-CB-CG2	-7.97	96.86	110.40
1	C	411	VAL	CA-CB-CG2	-7.92	96.93	110.40
1	E	227	GLU	N-CA-C	-7.91	103.58	113.23
1	C	296	HIS	N-CA-CB	-7.89	102.32	111.79
1	A	405	GLY	CA-C-O	-7.82	115.51	120.91
1	H	427	ILE	N-CA-C	7.81	119.19	108.89
1	H	150	LYS	CD-CE-NZ	-7.80	86.93	111.90
1	F	392	VAL	O-C-N	7.79	131.88	123.00
1	A	117	ILE	N-CA-C	7.77	120.14	108.80
1	G	412	GLN	CA-CB-CG	-7.77	98.57	114.10
1	B	306	ASN	O-C-N	-7.75	111.93	122.23
1	G	247	ASN	CB-CA-C	-7.71	105.96	117.07
1	E	306	ASN	O-C-N	-7.67	112.68	122.20
1	E	339	GLY	CA-C-N	7.62	129.36	119.84
1	E	339	GLY	C-N-CA	7.62	129.36	119.84
1	C	209	GLY	CA-C-N	-7.60	113.29	123.10
1	C	209	GLY	C-N-CA	-7.60	113.29	123.10
1	D	433	GLU	CA-C-N	-7.57	108.99	122.32
1	D	433	GLU	C-N-CA	-7.57	108.99	122.32
1	F	414	GLY	N-CA-C	-7.51	105.16	114.92
1	C	407	SER	CA-C-O	-7.49	113.24	121.33
1	B	311	GLU	N-CA-C	-7.48	97.86	109.76
1	A	296	HIS	N-CA-C	7.45	119.20	110.41
1	D	411	VAL	CA-C-N	-7.36	112.74	123.05
1	D	411	VAL	C-N-CA	-7.36	112.74	123.05
1	F	467	THR	N-CA-C	-7.33	104.07	112.87
1	G	411	VAL	CA-C-N	-7.33	112.41	122.30
1	G	411	VAL	C-N-CA	-7.33	112.41	122.30
1	H	311	GLU	N-CA-C	-7.26	97.41	109.24
1	A	449	VAL	N-CA-C	7.25	124.41	109.34
1	C	349	VAL	N-CA-CB	-7.18	101.49	111.19
1	G	246	SER	N-CA-C	-7.17	103.69	113.30
1	F	312	TYR	N-CA-C	7.14	118.93	108.86
1	E	333	GLY	O-C-N	-7.11	115.92	122.96
1	C	346	ALA	N-CA-C	7.09	120.48	112.97
1	F	411	VAL	CA-C-N	-7.06	112.78	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	411	VAL	C-N-CA	-7.06	112.78	122.95
1	B	404	SER	CA-C-O	-7.01	110.48	120.51
1	E	306	ASN	CA-C-N	7.01	135.06	121.18
1	E	306	ASN	C-N-CA	7.01	135.06	121.18
1	D	363	GLY	N-CA-C	-7.00	98.72	111.25
1	E	412	GLN	CA-C-N	6.99	132.57	117.20
1	E	451	SER	CA-C-N	-6.98	110.56	123.05
1	E	451	SER	C-N-CA	-6.98	110.56	123.05
1	F	225	THR	N-CA-C	6.92	117.41	108.34
1	A	172	ARG	NE-CZ-NH1	-6.91	114.59	121.50
1	H	105	SER	N-CA-C	6.90	119.39	111.11
1	D	312	TYR	N-CA-C	6.88	119.60	109.69
1	D	136	GLN	N-CA-C	-6.84	105.01	113.15
1	G	348	GLY	N-CA-C	6.81	120.97	110.88
1	D	414	GLY	N-CA-C	-6.79	106.09	114.92
1	A	427	ILE	N-CA-C	6.78	117.79	108.84
1	E	136	GLN	N-CA-C	-6.78	105.34	112.93
1	G	126	HIS	N-CA-C	-6.77	104.89	113.02
1	C	363	GLY	N-CA-C	-6.75	98.69	110.71
1	B	379	ASP	CA-C-N	-6.75	112.55	120.11
1	B	379	ASP	C-N-CA	-6.75	112.55	120.11
1	H	116	VAL	N-CA-C	-6.75	99.98	108.89
1	B	411	VAL	CA-C-O	-6.73	113.48	121.28
1	D	419	ARG	CA-C-N	-6.72	111.17	120.25
1	D	419	ARG	C-N-CA	-6.72	111.17	120.25
1	A	444	ILE	N-CA-C	-6.72	98.81	108.42
1	H	180	ALA	N-CA-C	6.71	117.44	108.38
1	D	247	ASN	CA-C-O	6.69	121.82	117.94
1	G	247	ASN	N-CA-C	-6.63	103.34	108.78
1	A	363	GLY	N-CA-C	-6.62	99.39	111.25
1	B	254	ILE	CB-CA-C	-6.58	100.80	110.81
1	G	411	VAL	N-CA-C	6.57	117.36	108.17
1	D	230	CYS	N-CA-C	-6.55	101.09	110.59
1	F	315	GLY	N-CA-C	-6.55	101.57	110.80
1	H	306	ASN	CA-C-O	-6.54	111.16	120.51
1	A	408	GLY	CA-C-O	-6.53	114.36	121.48
1	E	168	SER	CA-C-N	6.53	126.22	119.82
1	E	168	SER	C-N-CA	6.53	126.22	119.82
1	B	300	ARG	CA-C-N	6.48	127.01	120.14
1	B	300	ARG	C-N-CA	6.48	127.01	120.14
1	C	298	SER	N-CA-C	-6.46	105.56	113.50
1	G	339	GLY	CA-C-N	6.46	127.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	339	GLY	C-N-CA	6.46	127.91	119.84
1	B	406	TYR	CB-CA-C	6.46	122.91	109.68
1	C	226	GLN	N-CA-C	6.42	118.81	111.11
1	B	380	PRO	N-CA-C	-6.41	102.17	111.33
1	G	116	VAL	N-CA-C	-6.41	99.35	108.58
1	B	236	SER	N-CA-C	-6.41	98.17	109.06
1	F	172	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	D	254	ILE	CB-CA-C	-6.37	102.00	110.98
1	H	308	GLN	N-CA-C	-6.33	105.56	113.28
1	G	383	TRP	N-CA-C	-6.29	104.66	112.90
1	F	306	ASN	CA-C-O	-6.29	115.41	122.01
1	B	363	GLY	N-CA-C	-6.27	101.12	110.71
1	B	306	ASN	CA-C-N	6.26	132.63	120.99
1	B	306	ASN	C-N-CA	6.26	132.63	120.99
1	C	427	ILE	CB-CA-C	-6.25	103.16	110.91
1	E	467	THR	N-CA-C	-6.22	105.40	112.87
1	C	350	LYS	CB-CA-C	6.22	119.60	109.90
1	G	333	GLY	O-C-N	-6.21	116.28	122.86
1	D	371	ARG	N-CA-C	-6.20	102.06	110.68
1	G	392	VAL	CA-C-N	-6.20	114.03	122.77
1	G	392	VAL	C-N-CA	-6.20	114.03	122.77
1	H	441	GLY	N-CA-C	6.20	120.39	110.90
1	E	411	VAL	CG1-CB-CG2	-6.20	97.17	110.80
1	B	455	GLY	N-CA-C	-6.18	103.72	112.37
1	E	380	PRO	CA-C-N	-6.17	114.05	122.82
1	E	380	PRO	C-N-CA	-6.17	114.05	122.82
1	H	348	GLY	N-CA-C	6.15	119.43	110.63
1	G	411	VAL	O-C-N	6.14	129.63	123.18
1	C	449	VAL	N-CA-C	6.13	122.09	109.34
1	G	332	THR	CA-C-N	-6.09	117.01	122.43
1	G	332	THR	C-N-CA	-6.09	117.01	122.43
1	C	321	VAL	N-CA-C	-6.06	96.74	109.34
1	F	336	CYS	O-C-N	6.04	129.99	122.19
1	H	449	VAL	N-CA-C	6.04	121.91	109.34
1	C	116	VAL	N-CA-C	-6.04	99.88	108.58
1	E	433	GLU	O-C-N	-6.03	115.82	123.24
1	D	192	ILE	CB-CA-C	-6.03	103.54	110.41
1	E	320	GLY	N-CA-C	-6.03	106.15	115.73
1	D	300	ARG	CA-C-N	6.03	126.53	120.14
1	D	300	ARG	C-N-CA	6.03	126.53	120.14
1	H	451	SER	CA-C-N	-6.01	112.28	123.05
1	H	451	SER	C-N-CA	-6.01	112.28	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	451	SER	CA-C-N	-5.99	112.33	123.05
1	G	451	SER	C-N-CA	-5.99	112.33	123.05
1	B	449	VAL	N-CA-C	5.96	121.73	109.34
1	A	126	HIS	N-CA-C	-5.94	105.79	113.16
1	C	412	GLN	C-N-CA	5.91	136.49	121.70
1	D	449	VAL	N-CA-C	5.91	121.64	109.34
1	A	312	TYR	N-CA-C	5.91	117.94	109.14
1	D	172	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	H	411	VAL	O-C-N	-5.90	116.62	122.76
1	E	454	VAL	CB-CA-C	-5.90	103.60	111.80
1	C	177	ALA	N-CA-C	5.90	117.36	108.46
1	F	172	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	H	365	THR	N-CA-C	-5.89	102.75	110.53
1	H	455	GLY	N-CA-C	-5.88	103.66	113.02
1	C	291	CYS	N-CA-C	5.87	117.57	109.29
1	C	306	ASN	O-C-N	-5.86	114.34	121.83
1	E	362	ILE	N-CA-C	5.85	116.73	108.36
1	F	299	ASN	N-CA-C	-5.84	101.88	110.52
1	E	298	SER	N-CA-C	-5.83	104.34	112.45
1	D	455	GLY	N-CA-C	-5.82	103.77	113.02
1	B	407	SER	N-CA-C	-5.80	99.89	108.99
1	D	444	ILE	N-CA-C	-5.77	99.46	108.81
1	C	294	ASN	CA-C-O	5.75	126.02	119.18
1	G	181	SER	N-CA-C	-5.74	99.42	108.14
1	A	179	SER	CA-C-O	-5.72	114.59	120.89
1	F	454	VAL	CB-CA-C	-5.71	100.89	111.18
1	F	116	VAL	N-CA-C	-5.71	99.49	108.23
1	H	153	SER	CA-C-N	-5.70	114.13	120.45
1	H	153	SER	C-N-CA	-5.70	114.13	120.45
1	C	163	VAL	N-CA-C	5.69	116.75	109.30
1	D	224	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	E	392	VAL	CA-C-N	-5.68	114.00	122.74
1	E	392	VAL	C-N-CA	-5.68	114.00	122.74
1	C	99	VAL	CB-CA-C	-5.67	102.07	111.32
1	E	365	THR	N-CA-C	-5.65	103.07	110.53
1	C	312	TYR	N-CA-C	5.65	118.45	109.81
1	H	125	SER	N-CA-C	-5.64	100.85	109.65
1	E	412(A)	HIS	N-CA-C	5.62	122.24	109.81
1	B	312	TYR	N-CA-C	5.62	116.79	108.86
1	E	177	ALA	N-CA-C	5.62	117.06	108.52
1	H	380	PRO	CA-C-N	-5.62	114.54	122.46
1	H	380	PRO	C-N-CA	-5.62	114.54	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	GLY	N-CA-C	-5.61	108.41	115.08
1	C	451	SER	CA-C-N	-5.60	113.11	122.64
1	C	451	SER	C-N-CA	-5.60	113.11	122.64
1	B	365	THR	N-CA-C	-5.58	103.33	110.53
1	A	263	VAL	N-CA-C	-5.57	106.90	113.42
1	B	327	ARG	CA-C-N	-5.56	112.89	119.84
1	B	327	ARG	C-N-CA	-5.56	112.89	119.84
1	H	209	GLY	CA-C-N	-5.56	115.39	123.06
1	H	209	GLY	C-N-CA	-5.56	115.39	123.06
1	C	376	MET	N-CA-C	-5.52	100.18	109.07
1	G	312	TYR	N-CA-C	5.51	117.78	109.41
1	B	414	GLY	N-CA-C	-5.49	108.08	115.21
1	D	93	PRO	CA-C-N	-5.47	115.60	123.03
1	D	93	PRO	C-N-CA	-5.47	115.60	123.03
1	G	380	PRO	N-CA-C	-5.46	103.21	111.41
1	H	84	LYS	N-CA-C	5.46	117.94	110.24
1	G	311	GLU	N-CA-C	-5.46	100.39	109.46
1	F	388	SER	N-CA-C	-5.45	99.19	110.80
1	D	321	VAL	N-CA-C	-5.45	98.65	106.55
1	B	343	SER	CA-C-N	-5.45	118.31	126.86
1	B	343	SER	C-N-CA	-5.45	118.31	126.86
1	F	383	TRP	N-CA-C	-5.45	106.48	113.23
1	G	361	TRP	N-CA-C	-5.44	98.90	108.20
1	E	336	CYS	CA-C-N	-5.42	113.36	121.87
1	E	336	CYS	C-N-CA	-5.42	113.36	121.87
1	G	99	VAL	CB-CA-C	-5.41	103.16	111.71
1	A	171	SER	N-CA-C	5.41	118.92	110.32
1	H	388	SER	N-CA-C	-5.41	99.29	110.80
1	H	281	TYR	CA-C-N	5.40	125.82	119.99
1	H	281	TYR	C-N-CA	5.40	125.82	119.99
1	H	347	TYR	N-CA-C	-5.39	99.32	110.80
1	H	339	GLY	CA-C-N	5.38	126.57	119.84
1	H	339	GLY	C-N-CA	5.38	126.57	119.84
1	A	226	GLN	N-CA-C	5.38	120.24	111.37
1	E	339	GLY	N-CA-C	-5.37	101.38	112.34
1	F	348	GLY	N-CA-C	5.34	117.39	110.45
1	E	196	GLY	CA-C-N	5.33	125.63	119.92
1	E	196	GLY	C-N-CA	5.33	125.63	119.92
1	C	362	ILE	CB-CA-C	-5.33	102.71	110.81
1	D	341	VAL	N-CA-C	-5.33	100.08	108.23
1	A	451	SER	CA-C-N	-5.32	113.56	122.92
1	A	451	SER	C-N-CA	-5.32	113.56	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	VAL	CB-CA-C	-5.32	102.66	111.32
1	F	92	CYS	CA-C-N	-5.31	114.45	119.76
1	F	92	CYS	C-N-CA	-5.31	114.45	119.76
1	E	311	GLU	N-CA-C	-5.31	101.32	109.76
1	C	311	GLU	N-CA-C	-5.30	100.53	108.96
1	H	339	GLY	N-CA-C	-5.30	101.53	112.34
1	B	161	CYS	CA-C-N	-5.26	114.36	119.78
1	B	161	CYS	C-N-CA	-5.26	114.36	119.78
1	G	148	THR	CA-C-N	5.26	128.22	120.91
1	G	148	THR	C-N-CA	5.26	128.22	120.91
1	B	254	ILE	N-CA-C	-5.26	100.91	108.53
1	E	427	ILE	CB-CA-C	-5.25	104.32	111.15
1	A	348	GLY	N-CA-C	5.25	117.83	110.38
1	G	320	GLY	N-CA-C	-5.24	107.40	115.73
1	D	222	ILE	N-CA-C	5.23	120.21	109.34
1	B	360	VAL	CB-CA-C	-5.22	101.47	110.65
1	E	411	VAL	CA-CB-CG1	-5.21	101.54	110.40
1	E	254	ILE	CB-CA-C	-5.21	103.76	110.84
1	A	259	LYS	CB-CA-C	-5.20	104.34	111.73
1	C	216	LYS	CB-CA-C	-5.20	100.61	109.51
1	E	412	GLN	N-CA-C	5.20	119.73	113.17
1	B	401	THR	N-CA-C	5.20	119.38	113.19
1	D	269	ASP	N-CA-C	-5.20	98.83	108.24
1	A	333	GLY	O-C-N	-5.20	118.19	122.92
1	H	246	SER	N-CA-C	-5.19	106.63	113.17
1	C	186	GLY	N-CA-C	-5.19	107.83	114.37
1	E	455	GLY	N-CA-C	-5.17	105.68	112.82
1	C	370	SER	CA-C-N	-5.17	114.40	122.16
1	C	370	SER	C-N-CA	-5.17	114.40	122.16
1	C	380	PRO	N-CA-C	-5.17	103.93	111.33
1	F	305	PHE	N-CA-C	5.16	116.91	109.07
1	H	186	GLY	N-CA-C	-5.14	107.89	114.37
1	B	406	TYR	N-CA-CB	-5.14	103.00	110.36
1	G	259	LYS	CG-CD-CE	-5.14	99.48	111.30
1	B	84	LYS	CB-CG-CD	-5.14	99.48	111.30
1	G	110	SER	N-CA-C	-5.13	105.69	111.28
1	C	412(A)	HIS	N-CA-C	5.13	121.15	109.81
1	F	101	SER	N-CA-C	5.13	116.09	108.60
1	C	366	LYS	N-CA-C	-5.12	106.71	113.12
1	A	186	GLY	N-CA-C	-5.12	108.39	114.48
1	A	311	GLU	N-CA-C	-5.12	101.62	109.76
1	E	126	HIS	N-CA-C	-5.12	106.79	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	344	ASN	N-CA-CB	-5.12	108.98	114.10
1	A	413	THR	N-CA-C	5.12	119.60	112.90
1	A	387	ASP	N-CA-CB	5.10	114.71	109.51
1	C	365	THR	N-CA-C	-5.09	103.96	110.53
1	G	247	ASN	CA-C-O	5.09	120.89	117.94
1	A	246	SER	N-CA-C	-5.09	106.76	113.17
1	A	452	ASP	N-CA-C	5.09	118.02	110.14
1	C	414	GLY	N-CA-C	-5.09	108.31	114.92
1	D	361	TRP	N-CA-C	-5.09	100.44	108.73
1	D	299	ASN	N-CA-C	-5.08	102.94	110.46
1	G	145	SER	N-CA-C	-5.08	107.37	113.21
1	C	373	GLY	CA-C-O	-5.08	117.67	122.39
1	A	345	GLY	CA-C-N	-5.07	115.61	123.17
1	A	345	GLY	C-N-CA	-5.07	115.61	123.17
1	H	254	ILE	CA-C-N	-5.07	114.72	122.62
1	H	254	ILE	C-N-CA	-5.07	114.72	122.62
1	E	427	ILE	N-CA-C	5.06	115.57	108.89
1	H	259	LYS	N-CA-C	-5.05	105.16	111.92
1	G	329	ASN	CA-C-O	-5.04	116.02	121.87
1	C	360	VAL	CB-CA-C	-5.04	101.98	110.71
1	G	150	LYS	CD-CE-NZ	-5.04	95.79	111.90
1	A	227	GLU	N-CA-C	-5.03	106.44	112.58
1	E	391	SER	N-CA-C	5.03	119.55	113.41
1	F	451	SER	CA-C-N	-5.03	114.07	122.92
1	F	451	SER	C-N-CA	-5.03	114.07	122.92
1	F	306	ASN	CA-C-N	5.03	133.28	121.52
1	F	306	ASN	C-N-CA	5.03	133.28	121.52
1	G	414	GLY	N-CA-C	-5.03	108.67	115.21
1	A	245	PRO	N-CA-C	5.02	119.19	111.21
1	B	408	GLY	O-C-N	5.02	128.16	123.54
1	G	362	ILE	CB-CA-C	-5.02	104.02	110.84
1	C	101	SER	N-CA-C	5.01	115.76	108.14
1	A	360	VAL	CB-CA-C	-5.00	102.05	111.30
1	C	433	GLU	O-C-N	-5.00	116.40	123.11
1	G	385	GLU	N-CA-C	5.00	117.56	109.40
1	C	84	LYS	CG-CD-CE	-5.00	99.80	111.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	433	GLU	Mainchain
1	B	411	VAL	Mainchain
1	C	306	ASN	Mainchain
1	C	336	CYS	Mainchain
1	C	412	GLN	Peptide,Mainchain
1	D	306	ASN	Mainchain
1	D	333	GLY	Mainchain
1	E	333	GLY	Mainchain
1	E	336	CYS	Mainchain
1	E	412	GLN	Peptide
1	F	306	ASN	Mainchain
1	F	333	GLY	Mainchain
1	F	411	VAL	Mainchain
1	G	306	ASN	Mainchain
1	G	336	CYS	Mainchain
1	G	392	VAL	Mainchain
1	H	306	ASN	Mainchain
1	H	411	VAL	Mainchain
1	H	433	GLU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2962	0	2783	166	0
1	B	2962	0	2783	175	0
1	C	2962	0	2782	185	5
1	D	2962	0	2783	185	8
1	E	2962	0	2782	200	0
1	F	2962	0	2783	180	0
1	G	2962	0	2783	175	3
1	H	2962	0	2783	171	0
2	B	20	0	23	4	0
All	All	23716	0	22285	1287	8

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 28.

All (1287) 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:E:411:VAL:CG2	1:E:411:VAL:CB	1.79	1.58
1:H:150:LYS:CE	1:H:150:LYS:CD	1.78	1.56
1:C:411:VAL:CG2	1:C:411:VAL:CB	1.76	1.56
1:D:411:VAL:CB	1:D:411:VAL:CG2	1.78	1.56
1:C:84:LYS:CD	1:C:84:LYS:CG	1.83	1.53
1:B:411:VAL:CB	1:B:411:VAL:CG2	1.86	1.48
1:H:150:LYS:CE	1:H:150:LYS:NZ	1.83	1.40
1:C:412:GLN:NE2	1:C:421:CYS:SG	2.03	1.32
1:B:452:ASP:HB3	1:D:216:LYS:HD3	1.21	1.19
1:G:453:THR:HG22	1:G:454:VAL:H	1.07	1.18
1:A:216:LYS:HD3	1:D:452:ASP:HB3	1.21	1.15
1:C:228:SER:HB3	1:C:350:LYS:HE2	1.13	1.13
1:E:413:THR:HG21	1:E:415:LEU:HD22	1.32	1.11
1:C:228:SER:HB3	1:C:350:LYS:CE	1.81	1.11
1:F:216:LYS:HD3	1:G:452:ASP:HB3	1.18	1.11
1:E:412:GLN:HG3	1:E:419:ARG:CB	1.81	1.10
1:B:97:TRP:O	1:B:453:THR:HG21	1.54	1.07
1:H:376:MET:HG2	1:H:397:ILE:HD11	1.37	1.07
1:D:453:THR:HG22	1:D:454:VAL:H	1.20	1.06
1:E:452:ASP:HB3	1:G:216:LYS:HD3	1.12	1.06
1:F:452:ASP:HB3	1:H:216:LYS:HD3	1.37	1.05
1:D:97:TRP:O	1:D:453:THR:HG21	1.59	1.02
1:E:452:ASP:HB3	1:G:216:LYS:CD	1.90	1.01
1:G:228:SER:HB3	1:G:350:LYS:HE2	1.41	1.01
1:A:453:THR:HG22	1:A:454:VAL:H	1.24	1.01
1:A:413:THR:HG21	1:A:415:LEU:HD22	1.41	1.00
1:B:333:GLY:H	1:B:386:THR:CG2	1.73	1.00
1:E:412:GLN:CG	1:E:419:ARG:CB	2.38	1.00
1:E:88:ASN:HD22	1:E:88:ASN:H	1.09	0.99
1:C:249:GLN:NE2	1:C:272:ASN:H	1.58	0.99
1:E:113:ASP:O	1:E:168:SER:HB2	1.63	0.99
1:E:412:GLN:CG	1:E:419:ARG:HB3	1.93	0.98
1:A:97:TRP:O	1:A:453:THR:HG21	1.64	0.98
1:G:453:THR:CG2	1:G:454:VAL:H	1.77	0.97
1:H:413:THR:HG21	1:H:415:LEU:HD22	1.46	0.96
1:B:276:GLU:OE2	2:B:800:G39:H92	1.65	0.96
1:B:144:HIS:HE1	1:C:463:GLU:H	1.00	0.96
1:E:412:GLN:HG3	1:E:419:ARG:HB3	1.45	0.96
1:D:411:VAL:CG2	1:D:411:VAL:CA	2.43	0.96
1:F:184:HIS:HD2	1:F:186:GLY:H	1.12	0.96
1:F:216:LYS:CD	1:G:452:ASP:HB3	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:THR:HG22	1:C:415:LEU:H	1.31	0.94
1:C:453:THR:HG22	1:C:454:VAL:H	1.33	0.94
1:B:85:LEU:HD12	1:B:412(C):GLU:HG3	1.46	0.93
1:C:412:GLN:CG	1:C:419:ARG:HB3	1.98	0.93
1:C:411:VAL:CG2	1:C:411:VAL:CA	2.46	0.93
1:D:249:GLN:HE21	1:D:272:ASN:H	1.13	0.93
1:D:411:VAL:CG2	1:D:411:VAL:CG1	2.46	0.93
1:B:463:GLU:H	1:D:144:HIS:HE1	1.17	0.92
1:A:88:ASN:H	1:A:88:ASN:HD22	1.17	0.92
1:A:463:GLU:H	1:C:144:HIS:HE1	0.98	0.92
1:E:249:GLN:NE2	1:E:272:ASN:H	1.67	0.92
1:B:411:VAL:CG2	1:B:411:VAL:CA	2.47	0.92
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.51	0.92
1:A:144:HIS:HE1	1:D:463:GLU:H	1.12	0.92
1:C:249:GLN:HE21	1:C:272:ASN:H	0.97	0.92
1:F:375:GLU:OE1	1:F:394:LYS:HE3	1.71	0.91
1:B:452:ASP:HB3	1:D:216:LYS:CD	1.99	0.91
1:H:320:GLY:HA3	1:H:387:ASP:O	1.72	0.90
1:F:463:GLU:H	1:H:144:HIS:HE1	1.19	0.89
1:E:412:GLN:CG	1:E:419:ARG:HB2	2.01	0.89
1:E:411:VAL:CG2	1:E:411:VAL:CA	2.49	0.89
1:E:249:GLN:HE21	1:E:272:ASN:H	1.20	0.89
1:B:453:THR:HG22	1:B:454:VAL:H	1.37	0.88
1:D:359:GLY:CA	1:D:381:ASN:H	1.86	0.88
1:B:144:HIS:CE1	1:C:463:GLU:H	1.91	0.88
1:C:97:TRP:O	1:C:453:THR:HG21	1.73	0.88
1:D:333:GLY:H	1:D:386:THR:HG23	1.39	0.88
1:D:359:GLY:HA2	1:D:381:ASN:H	1.37	0.88
1:E:412:GLN:CB	1:E:419:ARG:HB2	2.04	0.88
1:G:282:PRO:HD2	1:G:411:VAL:HG21	1.55	0.88
1:A:216:LYS:CD	1:D:452:ASP:HB3	2.02	0.87
1:G:85:LEU:HD12	1:G:412(C):GLU:HG3	1.55	0.87
1:E:412:GLN:HB2	1:E:419:ARG:HB2	1.56	0.87
1:E:411:VAL:CG2	1:E:411:VAL:CG1	2.53	0.86
1:B:333:GLY:H	1:B:386:THR:HG23	1.40	0.86
1:B:448:GLY:O	1:B:449:VAL:HB	1.73	0.86
1:F:214:THR:HB	1:G:451:SER:OG	1.75	0.86
1:B:249:GLN:HE21	1:B:272:ASN:H	1.19	0.86
1:E:463:GLU:H	1:G:144:HIS:HE1	1.23	0.86
1:B:360:VAL:HG22	1:B:383:TRP:HB2	1.58	0.85
1:G:453:THR:HG22	1:G:454:VAL:N	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:GLY:HA2	1:D:381:ASN:N	1.90	0.85
1:B:214:THR:HG21	1:C:452:ASP:O	1.75	0.85
1:F:413:THR:HG21	1:F:415:LEU:HD22	1.59	0.84
1:F:214:THR:HG21	1:G:452:ASP:O	1.77	0.84
1:A:216:LYS:NZ	1:D:452:ASP:HB2	1.92	0.84
1:C:412:GLN:HG3	1:C:419:ARG:HB3	1.60	0.84
1:E:453:THR:HG22	1:E:454:VAL:H	1.42	0.84
1:F:184:HIS:CD2	1:F:186:GLY:H	1.94	0.84
1:A:448:GLY:O	1:A:449:VAL:HB	1.77	0.83
1:B:333:GLY:N	1:B:386:THR:CG2	2.42	0.83
1:E:452:ASP:O	1:G:214:THR:HG21	1.79	0.83
1:C:411:VAL:CG2	1:C:411:VAL:CG1	2.57	0.82
1:A:463:GLU:H	1:C:144:HIS:CE1	1.91	0.82
1:B:216:LYS:HD3	1:C:452:ASP:HB3	1.60	0.82
1:C:249:GLN:NE2	1:C:272:ASN:N	2.27	0.82
1:A:214:THR:HG21	1:D:452:ASP:O	1.79	0.82
1:F:452:ASP:O	1:H:214:THR:HG21	1.79	0.82
1:A:452:ASP:HB3	1:C:216:LYS:HD3	1.59	0.82
1:G:85:LEU:CD1	1:G:412(C):GLU:HG3	2.10	0.82
1:C:162:PRO:HG2	1:C:165:GLU:CD	2.05	0.82
1:G:275:TYR:CE2	1:G:303:VAL:HG23	2.14	0.82
1:E:214:THR:HG21	1:H:452:ASP:O	1.80	0.82
1:F:97:TRP:O	1:F:453:THR:HG21	1.81	0.81
1:B:249:GLN:NE2	1:B:272:ASN:H	1.78	0.81
1:F:366:LYS:HD3	1:F:400:ILE:HG12	1.62	0.81
1:G:249:GLN:NE2	1:G:272:ASN:H	1.78	0.81
1:D:249:GLN:NE2	1:D:272:ASN:H	1.78	0.80
1:G:306:ASN:CG	1:G:308:GLN:H	1.89	0.80
1:G:320:GLY:HA3	1:G:387:ASP:O	1.81	0.80
1:C:184:HIS:CD2	1:C:186:GLY:H	2.00	0.80
1:E:376:MET:HG2	1:E:397:ILE:HD11	1.63	0.80
1:B:452:ASP:O	1:D:214:THR:HG21	1.82	0.79
1:H:376:MET:HG2	1:H:397:ILE:CD1	2.12	0.79
1:B:85:LEU:CD1	1:B:412(C):GLU:HG3	2.12	0.79
1:D:113:ASP:O	1:D:168:SER:HB2	1.82	0.79
1:F:91:LEU:HG	1:F:283:ASN:ND2	1.96	0.79
1:D:376:MET:HG2	1:D:397:ILE:HD11	1.64	0.79
1:E:97:TRP:O	1:E:453:THR:HG21	1.82	0.79
1:E:144:HIS:HE1	1:H:463:GLU:H	1.30	0.78
1:F:316:TYR:CE1	1:F:340:PRO:HD3	2.18	0.78
1:D:466:PHE:C	1:D:468:ILE:H	1.91	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:448:GLY:O	1:H:449:VAL:HB	1.81	0.78
1:A:192:ILE:HG12	1:A:205:LEU:HD22	1.65	0.78
1:B:413:THR:HG21	1:B:415:LEU:HD22	1.65	0.78
1:A:452:ASP:HB2	1:C:216:LYS:NZ	1.98	0.78
1:H:316:TYR:CE1	1:H:340:PRO:HD3	2.19	0.78
1:F:144:HIS:HE1	1:G:463:GLU:H	1.32	0.78
1:G:229:GLU:HG2	1:G:230:CYS:O	1.84	0.78
1:F:249:GLN:NE2	1:F:272:ASN:H	1.83	0.77
1:H:306:ASN:CG	1:H:308:GLN:H	1.91	0.77
1:G:316:TYR:CE1	1:G:340:PRO:HD3	2.20	0.77
1:C:413:THR:HG21	1:C:415:LEU:HD22	1.67	0.77
1:D:358:ASN:O	1:D:381:ASN:HA	1.85	0.77
1:H:333:GLY:H	1:H:386:THR:HG23	1.49	0.77
1:H:411:VAL:CG1	1:H:418:ILE:HG23	2.15	0.77
1:B:264:LYS:HG2	1:B:310:LEU:HD22	1.66	0.76
1:A:144:HIS:CE1	1:D:463:GLU:H	2.01	0.76
1:C:275:TYR:CE2	1:C:303:VAL:HG23	2.21	0.76
1:D:448:GLY:O	1:D:449:VAL:HB	1.85	0.76
1:G:88:ASN:HD22	1:G:88:ASN:H	1.33	0.76
1:A:136:GLN:HE21	1:A:156:ARG:CD	1.99	0.76
1:C:412:GLN:HG2	1:C:419:ARG:HB3	1.68	0.76
1:D:453:THR:HG22	1:D:454:VAL:N	2.00	0.76
1:B:162:PRO:HG2	1:B:165:GLU:CD	2.11	0.75
1:A:229:GLU:OE1	1:A:410:PHE:HA	1.86	0.75
1:B:466:PHE:C	1:B:468:ILE:H	1.94	0.75
1:G:333:GLY:H	1:G:386:THR:CG2	1.99	0.75
1:B:411:VAL:CG2	1:B:411:VAL:CG1	2.61	0.75
1:E:216:LYS:HD3	1:H:452:ASP:HB3	1.68	0.75
1:D:184:HIS:CD2	1:D:186:GLY:H	2.04	0.75
1:D:248:GLY:HA2	1:D:295:TRP:CE2	2.22	0.75
1:E:254:ILE:HD11	1:E:268:LEU:HD21	1.68	0.75
1:A:184:HIS:HD2	1:A:186:GLY:H	1.34	0.75
1:G:287:ILE:HD12	1:G:287:ILE:N	2.01	0.75
1:H:150:LYS:CD	1:H:150:LYS:NZ	2.49	0.75
1:D:316:TYR:CE1	1:D:340:PRO:HD3	2.22	0.75
1:G:117:ILE:HG22	1:G:135:THR:HG22	1.69	0.75
1:A:97:TRP:H	1:A:395:GLN:HE22	1.34	0.74
1:A:248:GLY:HA2	1:A:295:TRP:CE2	2.22	0.74
1:B:454:VAL:HG21	1:D:200:GLY:O	1.86	0.74
1:F:453:THR:HG22	1:F:454:VAL:H	1.52	0.74
1:A:249:GLN:HE21	1:A:272:ASN:H	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:ASN:ND2	1:F:316:TYR:HB3	2.03	0.74
1:C:228:SER:CB	1:C:350:LYS:HE2	2.07	0.74
1:H:228:SER:HB3	1:H:350:LYS:HE2	1.69	0.74
1:B:192:ILE:HG12	1:B:205:LEU:HD22	1.68	0.73
1:H:333:GLY:H	1:H:386:THR:CG2	2.01	0.73
1:E:412:GLN:HG2	1:E:419:ARG:HB3	1.69	0.73
1:C:270:ALA:HB1	1:C:273:TYR:HB2	1.71	0.73
1:C:115:PHE:CZ	1:C:159:MET:HE1	2.22	0.73
1:A:116:VAL:HG23	1:A:440:SER:HB2	1.71	0.73
1:F:228:SER:HB3	1:F:350:LYS:HE2	1.70	0.73
1:D:413:THR:HG21	1:D:415:LEU:HD22	1.70	0.73
1:F:248:GLY:HA2	1:F:295:TRP:CE2	2.24	0.73
1:C:88:ASN:H	1:C:88:ASN:HD22	1.34	0.72
1:D:287:ILE:N	1:D:287:ILE:HD12	2.04	0.72
1:G:121:PHE:CG	1:G:228:SER:HA	2.24	0.72
1:H:248:GLY:HA2	1:H:295:TRP:CE2	2.24	0.72
1:B:463:GLU:H	1:D:144:HIS:CE1	2.06	0.72
1:D:333:GLY:N	1:D:386:THR:HG23	2.04	0.72
1:B:156:ARG:HG2	1:B:178:TRP:HA	1.72	0.72
1:C:150:LYS:HD3	1:C:152:ARG:O	1.88	0.72
1:C:412:GLN:HG3	1:C:419:ARG:CB	2.20	0.72
1:B:452:ASP:HB2	1:D:216:LYS:NZ	2.04	0.72
1:G:270:ALA:HB1	1:G:273:TYR:HB2	1.71	0.72
1:D:376:MET:HG2	1:D:397:ILE:CD1	2.19	0.72
1:G:397:ILE:HG22	1:G:398:VAL:HG23	1.72	0.72
1:G:412:GLN:HB2	1:G:419:ARG:HB2	1.72	0.72
1:H:97:TRP:O	1:H:453:THR:HG21	1.89	0.72
1:C:412:GLN:CG	1:C:419:ARG:CB	2.67	0.71
1:F:88:ASN:H	1:F:88:ASN:HD22	1.36	0.71
1:A:184:HIS:CD2	1:A:186:GLY:H	2.08	0.71
1:G:306:ASN:CG	1:G:308:GLN:N	2.48	0.71
1:D:97:TRP:H	1:D:395:GLN:HE22	1.39	0.71
1:F:275:TYR:CE2	1:F:303:VAL:HG23	2.25	0.71
1:G:249:GLN:NE2	1:G:272:ASN:N	2.38	0.71
1:A:249:GLN:NE2	1:A:272:ASN:H	1.88	0.71
1:C:287:ILE:HD12	1:C:287:ILE:N	2.06	0.71
1:H:254:ILE:HD11	1:H:268:LEU:HD21	1.72	0.71
1:D:333:GLY:H	1:D:386:THR:CG2	2.04	0.70
1:G:413:THR:HG21	1:G:415:LEU:HD22	1.72	0.70
1:A:320:GLY:HA3	1:A:387:ASP:O	1.91	0.70
1:A:380:PRO:O	1:A:381:ASN:C	2.33	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:THR:HG22	1:A:415:LEU:H	1.57	0.70
1:D:453:THR:CG2	1:D:454:VAL:H	2.02	0.70
1:B:287:ILE:N	1:B:287:ILE:HD12	2.06	0.70
1:C:84:LYS:CG	1:C:84:LYS:CE	2.70	0.70
1:G:448:GLY:O	1:G:449:VAL:HB	1.90	0.70
1:A:102:LYS:HG3	1:A:444:ILE:HG22	1.74	0.70
1:B:109:GLY:HA3	1:B:140:LEU:HD12	1.72	0.70
1:A:228:SER:HB3	1:A:350:LYS:CE	2.22	0.69
1:E:214:THR:HB	1:H:451:SER:OG	1.91	0.69
1:C:248:GLY:HA2	1:C:295:TRP:CE2	2.27	0.69
1:D:192:ILE:HG12	1:D:205:LEU:HD22	1.74	0.69
1:F:228:SER:HB3	1:F:350:LYS:CE	2.21	0.69
1:H:150:LYS:CE	1:H:150:LYS:CG	2.69	0.69
1:B:214:THR:HB	1:C:451:SER:CB	2.22	0.69
1:D:162:PRO:HG2	1:D:165:GLU:CD	2.16	0.69
1:D:184:HIS:HD2	1:D:186:GLY:H	1.37	0.69
1:D:247:ASN:O	1:D:248:GLY:O	2.10	0.69
1:D:375:GLU:OE1	1:D:394:LYS:HE3	1.92	0.69
1:A:451:SER:OG	1:C:214:THR:HB	1.93	0.69
1:B:115:PHE:CE1	1:B:159:MET:HE1	2.27	0.69
1:D:320:GLY:HA3	1:D:387:ASP:O	1.93	0.68
1:C:333:GLY:H	1:C:386:THR:HG23	1.58	0.68
1:F:88:ASN:HD22	1:F:88:ASN:N	1.88	0.68
1:E:121:PHE:CG	1:E:228:SER:HA	2.28	0.68
1:D:411:VAL:HG13	1:D:418:ILE:HG23	1.75	0.68
1:E:316:TYR:CE1	1:E:340:PRO:HD3	2.27	0.68
1:D:210:ILE:O	1:D:210:ILE:HG13	1.92	0.68
1:D:249:GLN:HE21	1:D:272:ASN:N	1.89	0.68
1:E:239:THR:HG22	1:E:257:MET:HE1	1.74	0.68
1:F:320:GLY:HA3	1:F:387:ASP:O	1.94	0.68
1:G:97:TRP:H	1:G:395:GLN:HE22	1.42	0.68
1:C:380:PRO:O	1:C:381:ASN:C	2.35	0.68
1:H:397:ILE:HG22	1:H:398:VAL:HG23	1.76	0.68
1:D:228:SER:HB3	1:D:350:LYS:HE2	1.74	0.68
1:D:249:GLN:NE2	1:D:272:ASN:N	2.42	0.68
1:E:320:GLY:HA3	1:E:387:ASP:O	1.94	0.68
1:H:184:HIS:CD2	1:H:186:GLY:H	2.11	0.68
1:B:466:PHE:C	1:B:468:ILE:N	2.50	0.67
1:E:249:GLN:NE2	1:E:272:ASN:N	2.41	0.67
1:C:413:THR:HG21	1:C:415:LEU:HB2	1.77	0.67
1:D:466:PHE:C	1:D:468:ILE:N	2.48	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:376:MET:HG2	1:E:397:ILE:CD1	2.23	0.67
1:F:380:PRO:O	1:F:381:ASN:C	2.35	0.67
1:G:248:GLY:HA2	1:G:295:TRP:CE2	2.29	0.67
1:H:282:PRO:HD2	1:H:411:VAL:HG21	1.76	0.67
1:E:412:GLN:HG3	1:E:419:ARG:HB2	1.62	0.67
1:F:376:MET:HG2	1:F:397:ILE:HD11	1.76	0.67
1:A:150:LYS:HD3	1:A:152:ARG:O	1.93	0.67
1:D:88:ASN:HD22	1:D:88:ASN:N	1.92	0.67
1:A:88:ASN:HD22	1:A:88:ASN:N	1.84	0.67
1:A:136:GLN:HE21	1:A:156:ARG:HD2	1.58	0.67
1:E:85:LEU:HD12	1:E:412(C):GLU:HG3	1.76	0.67
1:F:113:ASP:O	1:F:168:SER:HB2	1.95	0.67
1:C:413:THR:HG22	1:C:415:LEU:N	2.08	0.67
1:B:117:ILE:HG22	1:B:135:THR:HG22	1.77	0.67
1:H:411:VAL:HG13	1:H:418:ILE:HG23	1.76	0.66
1:D:270:ALA:O	1:D:273:TYR:HB2	1.95	0.66
1:E:463:GLU:H	1:G:144:HIS:CE1	2.09	0.66
1:F:116:VAL:HG12	1:F:138:ALA:O	1.96	0.66
1:E:88:ASN:HD22	1:E:88:ASN:N	1.81	0.66
1:G:118:ARG:O	1:G:119:GLU:HG3	1.96	0.66
1:G:333:GLY:N	1:G:386:THR:CG2	2.58	0.66
1:C:413:THR:CG2	1:C:415:LEU:HB2	2.26	0.66
1:H:466:PHE:C	1:H:468:ILE:H	2.03	0.66
1:C:117:ILE:HG22	1:C:135:THR:HG22	1.77	0.66
1:D:88:ASN:HD22	1:D:88:ASN:H	1.41	0.66
1:D:102:LYS:HZ2	1:D:104:ASN:HD21	1.44	0.66
1:F:377:ILE:HG23	1:F:390:PHE:CD1	2.29	0.66
1:D:254:ILE:CD1	1:D:268:LEU:HD21	2.26	0.66
1:G:88:ASN:HD22	1:G:88:ASN:N	1.89	0.66
1:G:97:TRP:O	1:G:453:THR:HG21	1.96	0.66
1:B:113:ASP:O	1:B:168:SER:HB2	1.96	0.66
1:C:113:ASP:O	1:C:168:SER:HB2	1.95	0.66
1:E:413:THR:HG21	1:E:415:LEU:CD2	2.19	0.66
1:E:162:PRO:HG2	1:E:165:GLU:CD	2.20	0.66
1:F:463:GLU:H	1:H:144:HIS:CE1	2.09	0.66
1:H:226:GLN:NE2	1:H:239:THR:OG1	2.24	0.66
1:A:453:THR:CG2	1:A:454:VAL:H	2.03	0.65
1:F:162:PRO:HG2	1:F:165:GLU:CD	2.22	0.65
1:H:156:ARG:HG2	1:H:178:TRP:HA	1.77	0.65
1:B:380:PRO:O	1:B:381:ASN:C	2.40	0.65
1:F:156:ARG:HG2	1:F:178:TRP:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:184:HIS:HD2	1:H:186:GLY:H	1.42	0.65
1:C:333:GLY:N	1:C:386:THR:HG23	2.12	0.65
1:E:286:GLU:C	1:E:287:ILE:HD12	2.21	0.65
1:E:287:ILE:HD12	1:E:287:ILE:N	2.11	0.65
1:F:322:PHE:HB2	1:F:327:ARG:HD2	1.79	0.65
1:H:116:VAL:HG12	1:H:138:ALA:O	1.97	0.65
1:A:113:ASP:O	1:A:168:SER:HB2	1.96	0.65
1:B:214:THR:HB	1:C:451:SER:OG	1.97	0.65
1:B:216:LYS:CD	1:C:452:ASP:HB3	2.25	0.65
1:C:320:GLY:HA3	1:C:387:ASP:O	1.96	0.65
1:B:144:HIS:HE1	1:C:463:GLU:N	1.85	0.65
1:F:332:THR:HG23	1:F:386:THR:CG2	2.27	0.65
1:C:325:ASN:O	1:C:348:GLY:HA2	1.97	0.65
1:A:290:VAL:HG21	1:A:353:SER:HB2	1.79	0.64
1:A:303:VAL:HG22	1:A:314:ILE:HG22	1.79	0.64
1:C:161:CYS:HB2	1:C:162:PRO:HD2	1.77	0.64
1:D:117:ILE:HG22	1:D:135:THR:HG22	1.78	0.64
1:A:135:THR:O	1:A:156:ARG:HA	1.98	0.64
1:B:249:GLN:NE2	1:B:272:ASN:N	2.43	0.64
1:A:162:PRO:HG2	1:A:165:GLU:CD	2.22	0.64
1:E:184:HIS:HD2	1:E:186:GLY:H	1.46	0.64
1:F:452:ASP:HB3	1:H:216:LYS:CD	2.22	0.64
1:G:228:SER:HB3	1:G:350:LYS:CE	2.24	0.64
1:A:452:ASP:O	1:C:214:THR:HG21	1.97	0.64
1:B:248:GLY:HA2	1:B:295:TRP:CE2	2.32	0.64
1:C:184:HIS:HD2	1:C:186:GLY:H	1.44	0.64
1:F:247:ASN:O	1:F:248:GLY:O	2.15	0.64
1:G:412:GLN:HB2	1:G:419:ARG:CB	2.27	0.64
1:B:376:MET:HG2	1:B:397:ILE:CD1	2.27	0.64
1:C:88:ASN:HD22	1:C:88:ASN:N	1.92	0.64
1:C:192:ILE:HG12	1:C:205:LEU:HD22	1.79	0.64
1:F:287:ILE:N	1:F:287:ILE:HD12	2.12	0.64
1:B:406:TYR:OH	2:B:800:G39:C2	2.46	0.64
1:B:270:ALA:HB1	1:B:273:TYR:HB2	1.79	0.63
1:B:214:THR:HB	1:C:451:SER:HB2	1.79	0.63
1:E:148:THR:HG22	1:E:430:ARG:HH22	1.64	0.63
1:E:411:VAL:CG2	1:E:411:VAL:HA	2.28	0.63
1:H:300:ARG:HB2	1:H:317:ILE:HD12	1.80	0.63
1:A:451:SER:CB	1:C:214:THR:HB	2.28	0.63
1:F:136:GLN:HE21	1:F:156:ARG:CD	2.10	0.63
1:H:333:GLY:N	1:H:386:THR:HG23	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:CG	1:A:228:SER:HA	2.33	0.63
1:A:214:THR:HB	1:D:451:SER:OG	1.99	0.63
1:B:316:TYR:CE1	1:B:340:PRO:HD3	2.33	0.63
1:H:375:GLU:OE1	1:H:394:LYS:HE3	1.99	0.63
1:A:316:TYR:CE1	1:A:340:PRO:HD3	2.34	0.63
1:B:115:PHE:CZ	1:B:159:MET:HE1	2.34	0.63
1:B:376:MET:HG2	1:B:397:ILE:HD11	1.80	0.63
1:C:412:GLN:HB2	1:C:419:ARG:HB2	1.81	0.63
1:B:333:GLY:N	1:B:386:THR:HG21	2.14	0.63
1:F:144:HIS:CE1	1:G:463:GLU:H	2.15	0.63
1:C:376:MET:HG2	1:C:397:ILE:CD1	2.29	0.63
1:G:156:ARG:HG2	1:G:178:TRP:HA	1.81	0.63
1:E:413:THR:CG2	1:E:415:LEU:HD22	2.21	0.62
1:F:181:SER:HB2	1:F:228:SER:O	1.99	0.62
1:H:202:VAL:CG2	1:H:214:THR:HG23	2.28	0.62
1:D:190:LEU:HD21	1:D:257:MET:HE3	1.80	0.62
1:F:411:VAL:HG13	1:F:418:ILE:HG23	1.80	0.62
1:A:466:PHE:C	1:A:468:ILE:H	2.06	0.62
1:G:249:GLN:HE21	1:G:272:ASN:H	1.45	0.62
1:C:453:THR:CG2	1:C:454:VAL:H	2.11	0.62
1:D:116:VAL:HG12	1:D:138:ALA:O	1.98	0.62
1:F:256:LYS:HB2	1:F:310:LEU:HD11	1.81	0.62
1:F:327:ARG:HB2	1:F:328:PRO:HD2	1.81	0.62
1:G:148:THR:HG22	1:G:430:ARG:HH22	1.63	0.62
1:A:466:PHE:C	1:A:468:ILE:N	2.56	0.62
1:B:129:CYS:O	1:B:163:VAL:HG23	1.99	0.62
1:B:343:SER:O	1:B:344:ASN:CB	2.47	0.62
1:E:192:ILE:HG12	1:E:205:LEU:HD22	1.80	0.62
1:C:411:VAL:HG13	1:C:418:ILE:HG23	1.81	0.62
1:B:333:GLY:N	1:B:386:THR:HG23	2.12	0.62
1:B:411:VAL:CG2	1:B:411:VAL:HA	2.29	0.62
1:F:249:GLN:HE21	1:F:272:ASN:H	1.47	0.62
1:D:88:ASN:H	1:D:88:ASN:ND2	1.98	0.62
1:H:102:LYS:HG3	1:H:444:ILE:HG22	1.82	0.62
1:H:306:ASN:CG	1:H:308:GLN:N	2.58	0.62
1:H:412:GLN:HB2	1:H:419:ARG:HB2	1.81	0.62
1:F:202:VAL:HG11	1:G:454:VAL:HG23	1.82	0.62
1:F:316:TYR:CZ	1:F:340:PRO:HD3	2.34	0.62
1:G:275:TYR:CE2	1:G:303:VAL:CG2	2.82	0.62
1:A:452:ASP:HB2	1:C:216:LYS:HZ3	1.62	0.61
1:E:452:ASP:HB2	1:G:216:LYS:NZ	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:CYS:O	1:F:163:VAL:HG23	2.00	0.61
1:A:453:THR:HG22	1:A:454:VAL:N	2.06	0.61
1:E:216:LYS:CD	1:H:452:ASP:HB3	2.28	0.61
1:F:88:ASN:H	1:F:88:ASN:ND2	1.98	0.61
1:B:229:GLU:OE1	1:B:410:PHE:HA	2.00	0.61
1:C:84:LYS:CD	1:C:84:LYS:CB	2.75	0.61
1:D:411:VAL:CG2	1:D:411:VAL:HA	2.29	0.61
1:E:168:SER:HB2	1:E:169:PRO:HD2	1.82	0.61
1:F:184:HIS:HD2	1:F:186:GLY:N	1.91	0.61
1:F:412:GLN:HB2	1:F:419:ARG:CB	2.31	0.61
1:G:103:ASP:O	1:G:104:ASN:HB2	2.00	0.61
1:D:254:ILE:HD11	1:D:268:LEU:HD21	1.81	0.61
1:G:184:HIS:CD2	1:G:186:GLY:H	2.18	0.61
1:G:333:GLY:H	1:G:386:THR:HG23	1.65	0.61
1:E:248:GLY:HA2	1:E:295:TRP:CE2	2.35	0.61
1:E:239:THR:CG2	1:E:257:MET:HE1	2.30	0.61
1:E:466:PHE:C	1:E:468:ILE:N	2.58	0.61
1:C:343:SER:C	1:C:345:GLY:H	2.07	0.61
1:C:411:VAL:CG2	1:C:411:VAL:HA	2.30	0.61
1:E:333:GLY:H	1:E:386:THR:HG23	1.65	0.61
1:H:333:GLY:N	1:H:386:THR:CG2	2.63	0.61
1:E:117:ILE:HG22	1:E:135:THR:HG22	1.82	0.60
1:A:216:LYS:HZ3	1:D:452:ASP:HB2	1.64	0.60
1:E:184:HIS:CD2	1:E:186:GLY:H	2.19	0.60
1:F:282:PRO:HD2	1:F:411:VAL:HG21	1.83	0.60
1:A:216:LYS:NZ	1:D:452:ASP:CB	2.64	0.60
1:D:115:PHE:CZ	1:D:159:MET:HE1	2.36	0.60
1:E:250:ALA:HB3	1:E:252:TYR:CE2	2.36	0.60
1:G:466:PHE:C	1:G:468:ILE:H	2.10	0.60
1:A:413:THR:HG21	1:A:415:LEU:CD2	2.25	0.60
1:C:387:ASP:HB3	1:C:389:SER:H	1.66	0.60
1:F:451:SER:OG	1:H:214:THR:HB	2.02	0.60
1:H:161:CYS:HB2	1:H:162:PRO:HD2	1.83	0.60
1:H:379:ASP:OD2	1:H:382:GLY:HA3	2.02	0.60
1:A:250:ALA:HB3	1:A:252:TYR:CE2	2.36	0.60
1:G:290:VAL:HG21	1:G:353:SER:HB2	1.83	0.60
1:G:113:ASP:O	1:G:168:SER:HB2	2.01	0.60
1:H:228:SER:HB3	1:H:350:LYS:CE	2.32	0.60
1:H:254:ILE:CD1	1:H:268:LEU:HD21	2.32	0.60
1:B:452:ASP:CB	1:D:216:LYS:NZ	2.65	0.60
1:E:322:PHE:HB2	1:E:327:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:LYS:HD3	1:C:400:ILE:HG12	1.83	0.60
1:D:121:PHE:CG	1:D:228:SER:HA	2.36	0.60
1:E:144:HIS:CE1	1:H:463:GLU:H	2.17	0.60
1:F:299:ASN:HD22	1:F:316:TYR:HB3	1.66	0.60
1:A:216:LYS:HD3	1:D:452:ASP:CB	2.13	0.59
1:G:88:ASN:H	1:G:88:ASN:ND2	2.00	0.59
1:A:115:PHE:CZ	1:A:159:MET:HE1	2.36	0.59
1:A:158:LEU:O	1:A:174:GLU:HB2	2.01	0.59
1:D:275:TYR:CE2	1:D:303:VAL:CG2	2.85	0.59
1:F:194:ILE:HG12	1:F:203:ALA:HB2	1.83	0.59
1:G:194:ILE:HD11	1:G:241:MET:HE2	1.84	0.59
1:H:162:PRO:HG2	1:H:165:GLU:CD	2.27	0.59
1:F:332:THR:HG23	1:F:386:THR:HG21	1.84	0.59
1:A:144:HIS:HE1	1:D:463:GLU:N	1.93	0.59
1:B:364:ARG:HG3	1:B:365:THR:O	2.01	0.59
1:F:412:GLN:HB2	1:F:419:ARG:HB2	1.84	0.59
1:A:216:LYS:HZ2	1:D:452:ASP:HB2	1.65	0.59
1:B:452:ASP:HB2	1:D:216:LYS:HZ2	1.67	0.59
1:E:96:GLY:O	1:E:448:GLY:O	2.20	0.59
1:F:96:GLY:O	1:F:448:GLY:O	2.19	0.59
1:H:355:LYS:HD2	1:H:383:TRP:CE2	2.38	0.59
1:C:464:LEU:HB3	1:C:465:PRO:HA	1.83	0.59
1:F:172:ARG:HD2	1:F:174:GLU:OE1	2.03	0.59
1:E:229:GLU:HG2	1:E:230:CYS:O	2.03	0.59
1:H:118:ARG:HB2	1:H:156:ARG:HH11	1.68	0.59
1:D:97:TRP:N	1:D:395:GLN:HE22	2.00	0.59
1:E:210:ILE:HG13	1:E:210:ILE:O	2.03	0.59
1:E:451:SER:HB2	1:G:214:THR:CG2	2.33	0.59
1:F:325:ASN:O	1:F:348:GLY:HA2	2.03	0.59
1:H:148:THR:HG23	1:H:430:ARG:HH12	1.68	0.59
1:A:454:VAL:HG21	1:C:200:GLY:O	2.02	0.58
1:F:229:GLU:HG2	1:F:230:CYS:O	2.03	0.58
1:B:116:VAL:HG12	1:B:138:ALA:O	2.04	0.58
1:E:148:THR:HG23	1:E:430:ARG:HH12	1.68	0.58
1:E:413:THR:CG2	1:E:415:LEU:HB2	2.32	0.58
1:F:216:LYS:CE	1:G:452:ASP:HB3	2.32	0.58
1:C:88:ASN:H	1:C:88:ASN:ND2	2.01	0.58
1:C:249:GLN:NE2	1:C:271:PRO:HA	2.18	0.58
1:A:451:SER:HB2	1:C:214:THR:CG2	2.33	0.58
1:A:466:PHE:O	1:A:468:ILE:N	2.36	0.58
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:HD12	1:C:412(C):GLU:HG3	1.85	0.58
1:E:320:GLY:CA	1:E:387:ASP:O	2.52	0.58
1:E:355:LYS:HD2	1:E:383:TRP:CE2	2.39	0.58
1:B:228:SER:HB3	1:B:350:LYS:NZ	2.17	0.58
1:B:247:ASN:O	1:B:248:GLY:O	2.21	0.58
1:D:182:ALA:O	1:D:229:GLU:HA	2.04	0.58
1:F:202:VAL:CG1	1:G:454:VAL:HG23	2.34	0.58
1:B:97:TRP:H	1:B:395:GLN:HE22	1.50	0.58
1:E:271:PRO:O	1:E:272:ASN:CB	2.51	0.58
1:F:168:SER:HB2	1:F:169:PRO:HD2	1.85	0.58
1:H:229:GLU:OE1	1:H:410:PHE:HA	2.04	0.58
1:F:451:SER:CB	1:H:214:THR:HB	2.34	0.58
1:H:88:ASN:N	1:H:88:ASN:HD22	2.02	0.58
1:H:113:ASP:O	1:H:168:SER:HB2	2.04	0.58
1:F:254:ILE:HD11	1:F:268:LEU:HD21	1.85	0.57
1:G:466:PHE:C	1:G:468:ILE:N	2.62	0.57
1:G:411:VAL:HG13	1:G:418:ILE:HG23	1.85	0.57
1:H:190:LEU:HD21	1:H:257:MET:HE3	1.85	0.57
1:A:249:GLN:NE2	1:A:272:ASN:N	2.52	0.57
1:B:249:GLN:HE21	1:B:272:ASN:N	1.93	0.57
1:E:466:PHE:C	1:E:468:ILE:H	2.11	0.57
1:G:254:ILE:HD11	1:G:268:LEU:HD21	1.85	0.57
1:A:120:PRO:HA	1:A:132:PHE:O	2.04	0.57
1:B:453:THR:CG2	1:B:454:VAL:H	2.10	0.57
1:E:411:VAL:CG1	1:E:412:GLN:N	2.66	0.57
1:F:316:TYR:CD1	1:F:340:PRO:HD3	2.39	0.57
1:B:275:TYR:CE2	1:B:303:VAL:CG2	2.88	0.57
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.86	0.57
1:E:343:SER:O	1:E:344:ASN:CB	2.53	0.57
1:F:216:LYS:NZ	1:G:452:ASP:CB	2.67	0.57
1:G:135:THR:O	1:G:156:ARG:HA	2.05	0.57
1:G:172:ARG:HD2	1:G:174:GLU:OE1	2.05	0.57
1:E:227:GLU:HA	1:E:227:GLU:OE1	2.04	0.57
1:H:97:TRP:HD1	1:H:395:GLN:NE2	2.03	0.57
1:D:156:ARG:HB3	1:D:177:ALA:O	2.04	0.57
1:H:453:THR:HG22	1:H:454:VAL:H	1.70	0.57
1:F:152:ARG:CZ	1:F:222:ILE:HD13	2.35	0.57
1:F:173:PHE:CG	1:G:164:GLY:HA3	2.39	0.57
1:A:366:LYS:NZ	1:A:396:ASP:OD1	2.38	0.57
1:E:216:LYS:CE	1:H:452:ASP:HB3	2.35	0.57
1:B:119:GLU:HG3	1:B:119:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:SER:HB2	1:D:214:THR:CG2	2.35	0.56
1:F:332:THR:CG2	1:F:386:THR:HG21	2.34	0.56
1:A:452:ASP:CB	1:C:216:LYS:NZ	2.67	0.56
1:E:457:SER:OG	1:E:459:PRO:HD3	2.05	0.56
1:G:355:LYS:HD2	1:G:383:TRP:CE2	2.39	0.56
1:A:88:ASN:H	1:A:88:ASN:ND2	1.94	0.56
1:A:316:TYR:CZ	1:A:340:PRO:HD3	2.40	0.56
1:D:102:LYS:HZ2	1:D:104:ASN:ND2	2.03	0.56
1:F:210:ILE:HD13	1:G:413:THR:HA	1.87	0.56
1:H:88:ASN:O	1:H:284:ALA:HA	2.05	0.56
1:F:249:GLN:NE2	1:F:272:ASN:N	2.52	0.56
1:F:411:VAL:HG11	1:F:412(A):HIS:CD2	2.41	0.56
1:C:121:PHE:CG	1:C:228:SER:HA	2.41	0.56
1:D:299:ASN:ND2	1:D:316:TYR:HB3	2.19	0.56
1:F:318:CYS:HA	1:F:335:SER:O	2.05	0.56
1:H:277:GLU:OE1	1:H:350:LYS:HB2	2.04	0.56
1:A:162:PRO:HG2	1:A:165:GLU:OE1	2.05	0.56
1:C:239:THR:HG22	1:C:257:MET:HE1	1.88	0.56
1:D:360:VAL:HG13	1:D:383:TRP:HE3	1.71	0.56
1:F:97:TRP:H	1:F:395:GLN:HE22	1.53	0.56
1:D:228:SER:HB3	1:D:350:LYS:CE	2.36	0.56
1:F:347:TYR:CG	1:F:348:GLY:N	2.74	0.56
1:F:466:PHE:C	1:F:468:ILE:N	2.63	0.56
1:G:247:ASN:O	1:G:248:GLY:O	2.23	0.56
1:B:370:SER:HB2	1:B:372:SER:OG	2.05	0.56
1:F:118:ARG:O	1:F:119:GLU:HG3	2.06	0.56
1:H:88:ASN:HD22	1:H:88:ASN:H	1.53	0.56
1:A:247:ASN:O	1:A:248:GLY:O	2.24	0.56
1:F:254:ILE:CD1	1:F:268:LEU:HD21	2.36	0.56
1:C:96:GLY:O	1:C:448:GLY:O	2.24	0.56
1:E:325:ASN:O	1:E:348:GLY:HA2	2.06	0.56
1:F:355:LYS:NZ	1:F:357:GLY:O	2.36	0.56
1:A:376:MET:HG2	1:A:397:ILE:HD11	1.86	0.55
1:A:413:THR:CG2	1:A:415:LEU:HD22	2.27	0.55
1:B:406:TYR:OH	2:B:800:G39:C1	2.54	0.55
1:B:413:THR:HG22	1:B:415:LEU:H	1.70	0.55
1:D:116:VAL:HG23	1:D:440:SER:HB2	1.88	0.55
1:E:88:ASN:H	1:E:88:ASN:ND2	1.91	0.55
1:E:275:TYR:CE2	1:E:303:VAL:HG23	2.40	0.55
1:F:397:ILE:HD13	1:F:422:PHE:HZ	1.70	0.55
1:A:299:ASN:ND2	1:A:316:TYR:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HG22	1:B:135:THR:CG2	2.37	0.55
1:F:219:ARG:HB2	1:F:243:ASP:CG	2.31	0.55
1:F:452:ASP:O	1:H:214:THR:CG2	2.52	0.55
1:G:162:PRO:HG2	1:G:165:GLU:CD	2.31	0.55
1:H:97:TRP:H	1:H:395:GLN:HE22	1.55	0.55
1:E:397:ILE:HG22	1:E:398:VAL:HG23	1.87	0.55
1:G:118:ARG:C	1:G:119:GLU:CG	2.80	0.55
1:B:360:VAL:CG2	1:B:383:TRP:HB2	2.35	0.55
1:C:466:PHE:C	1:C:468:ILE:H	2.14	0.55
1:E:380:PRO:O	1:E:381:ASN:C	2.49	0.55
1:G:97:TRP:N	1:G:395:GLN:HE22	2.02	0.55
1:G:287:ILE:N	1:G:287:ILE:CD1	2.69	0.55
1:E:116:VAL:HG23	1:E:440:SER:HB2	1.88	0.55
1:E:252:TYR:HB2	1:E:268:LEU:HD12	1.87	0.55
1:E:412(B):PRO:HB3	1:E:415:LEU:O	2.07	0.55
1:A:136:GLN:HE21	1:A:156:ARG:HD3	1.71	0.55
1:B:321:VAL:HG13	1:B:364:ARG:NH2	2.22	0.55
1:D:290:VAL:HG11	1:D:353:SER:HB2	1.89	0.55
1:G:241:MET:HB2	1:G:255:PHE:HE1	1.72	0.55
1:A:96:GLY:O	1:A:448:GLY:O	2.25	0.55
1:C:412:GLN:NE2	1:C:447:CYS:SG	2.78	0.55
1:D:412:GLN:HB2	1:D:419:ARG:HB2	1.89	0.55
1:F:136:GLN:HE21	1:F:156:ARG:HD3	1.70	0.55
1:A:275:TYR:CE2	1:A:303:VAL:HG23	2.42	0.54
1:A:452:ASP:HB3	1:C:216:LYS:CD	2.33	0.54
1:B:85:LEU:HD12	1:B:412(C):GLU:CG	2.30	0.54
1:B:133:PHE:O	1:B:158:LEU:HD12	2.07	0.54
1:E:210:ILE:CD1	1:H:413:THR:HG23	2.37	0.54
1:A:180:ALA:HB1	1:A:192:ILE:O	2.08	0.54
1:B:466:PHE:O	1:B:468:ILE:N	2.40	0.54
1:A:216:LYS:HE2	1:D:452:ASP:H	1.72	0.54
1:A:452:ASP:HB2	1:C:216:LYS:HZ2	1.71	0.54
1:B:413:THR:HA	1:D:210:ILE:HD13	1.88	0.54
1:C:290:VAL:HG11	1:C:353:SER:HB2	1.88	0.54
1:D:97:TRP:HD1	1:D:395:GLN:NE2	2.05	0.54
1:D:218:TRP:CZ2	1:D:253:LYS:HG3	2.42	0.54
1:H:366:LYS:HD2	1:H:398:VAL:O	2.08	0.54
1:F:118:ARG:C	1:F:119:GLU:CG	2.80	0.54
1:H:322:PHE:HB2	1:H:327:ARG:HD2	1.89	0.54
1:H:428:ARG:NH2	1:H:460:ASP:OD1	2.40	0.54
1:A:333:GLY:N	1:A:386:THR:HG23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:411:VAL:HG13	1:H:418:ILE:CG2	2.38	0.54
1:A:333:GLY:H	1:A:386:THR:HG23	1.73	0.54
1:D:358:ASN:C	1:D:381:ASN:HA	2.33	0.54
1:D:411:VAL:CG2	1:D:411:VAL:HG13	2.37	0.54
1:F:102:LYS:HZ2	1:F:104:ASN:HD21	1.55	0.54
1:G:226:GLN:NE2	1:G:239:THR:OG1	2.38	0.54
1:H:436:THR:HG21	1:H:464:LEU:HD13	1.90	0.54
1:C:239:THR:CG2	1:C:257:MET:HE1	2.38	0.54
1:B:202:VAL:CG2	1:B:214:THR:HG23	2.37	0.54
1:E:452:ASP:HB3	1:G:216:LYS:CE	2.37	0.54
1:F:216:LYS:NZ	1:G:452:ASP:HB2	2.23	0.54
1:F:248:GLY:O	1:F:249:GLN:C	2.51	0.54
1:H:355:LYS:NZ	1:H:357:GLY:O	2.38	0.54
1:H:412:GLN:HB2	1:H:419:ARG:CB	2.37	0.54
1:C:148:THR:HG23	1:C:430:ARG:HH12	1.72	0.54
1:D:184:HIS:HD2	1:D:186:GLY:N	2.05	0.54
1:E:85:LEU:CD1	1:E:412(C):GLU:HG3	2.37	0.54
1:F:467:THR:O	1:F:468:ILE:HB	2.07	0.54
1:B:190:LEU:HD21	1:B:257:MET:HE3	1.90	0.53
1:D:466:PHE:O	1:D:468:ILE:N	2.42	0.53
1:H:466:PHE:C	1:H:468:ILE:N	2.65	0.53
1:H:229:GLU:HG2	1:H:230:CYS:O	2.08	0.53
1:C:120:PRO:HA	1:C:132:PHE:O	2.08	0.53
1:D:413:THR:HG22	1:D:415:LEU:H	1.73	0.53
1:H:275:TYR:CE2	1:H:303:VAL:HG23	2.43	0.53
1:B:343:SER:O	1:B:344:ASN:HB2	2.07	0.53
1:C:270:ALA:HB1	1:C:273:TYR:CB	2.37	0.53
1:C:343:SER:C	1:C:345:GLY:N	2.64	0.53
1:C:397:ILE:HG22	1:C:398:VAL:HG23	1.89	0.53
1:B:454:VAL:HG23	1:D:202:VAL:CG1	2.38	0.53
1:D:101:SER:O	1:D:444:ILE:HA	2.09	0.53
1:H:290:VAL:HG21	1:H:353:SER:HB2	1.91	0.53
1:A:360:VAL:HG13	1:A:383:TRP:HE3	1.73	0.53
1:C:360:VAL:HG22	1:C:383:TRP:HB2	1.89	0.53
1:E:448:GLY:O	1:E:449:VAL:HB	2.08	0.53
1:E:454:VAL:HG21	1:G:200:GLY:O	2.08	0.53
1:B:463:GLU:N	1:D:144:HIS:HE1	1.97	0.53
1:C:332:THR:CG2	1:C:386:THR:HG21	2.39	0.53
1:C:416:ASP:OD1	1:C:416:ASP:N	2.36	0.53
1:G:413:THR:HG22	1:G:415:LEU:H	1.74	0.53
1:C:227:GLU:O	1:C:350:LYS:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:GLU:OE1	1:C:394:LYS:HE3	2.09	0.53
1:D:129:CYS:O	1:D:163:VAL:HG23	2.09	0.53
1:D:316:TYR:CZ	1:D:340:PRO:HD3	2.44	0.53
1:F:452:ASP:HB2	1:H:216:LYS:NZ	2.23	0.53
1:G:144:HIS:C	1:G:146:ASN:H	2.17	0.53
1:A:173:PHE:CZ	1:D:101:SER:HA	2.43	0.53
1:B:96:GLY:O	1:B:448:GLY:O	2.26	0.53
1:D:467:THR:O	1:D:468:ILE:HB	2.08	0.53
1:F:299:ASN:OD1	1:F:341:VAL:HG23	2.08	0.53
1:A:97:TRP:N	1:A:395:GLN:HE22	2.06	0.52
1:G:442:SER:OG	1:G:460:ASP:OD2	2.27	0.52
1:G:466:PHE:O	1:G:468:ILE:N	2.42	0.52
1:B:101:SER:HA	1:D:173:PHE:CZ	2.44	0.52
1:C:467:THR:O	1:C:468:ILE:HB	2.08	0.52
1:E:105:SER:HB3	1:E:167:PRO:HD2	1.91	0.52
1:A:249:GLN:HE21	1:A:272:ASN:N	2.05	0.52
1:G:184:HIS:HD2	1:G:186:GLY:H	1.55	0.52
1:H:172:ARG:HD2	1:H:174:GLU:OE1	2.10	0.52
1:H:270:ALA:HB1	1:H:273:TYR:HB2	1.91	0.52
1:B:133:PHE:CD2	1:B:133:PHE:N	2.77	0.52
1:D:136:GLN:NE2	1:D:156:ARG:HD2	2.24	0.52
1:D:229:GLU:HG2	1:D:230:CYS:O	2.09	0.52
1:F:162:PRO:HG2	1:F:165:GLU:OE2	2.09	0.52
1:C:119:GLU:OE1	1:C:227:GLU:HB3	2.10	0.52
1:D:192:ILE:HD11	1:D:257:MET:HE1	1.89	0.52
1:H:411:VAL:HG11	1:H:418:ILE:HG23	1.90	0.52
1:E:232:CYS:HA	1:E:236:SER:O	2.10	0.52
1:F:463:GLU:N	1:H:144:HIS:HE1	2.00	0.52
1:G:115:PHE:CZ	1:G:159:MET:HE1	2.45	0.52
1:E:332:THR:HG23	1:E:386:THR:HG21	1.91	0.52
1:E:333:GLY:H	1:E:386:THR:CG2	2.23	0.52
1:C:397:ILE:HD13	1:C:422:PHE:HZ	1.74	0.52
1:C:466:PHE:C	1:C:468:ILE:N	2.67	0.52
1:E:99:VAL:HG13	1:E:446:PHE:CE2	2.44	0.52
1:G:406:TYR:HB2	1:G:425:GLU:OE1	2.10	0.52
1:D:333:GLY:N	1:D:386:THR:CG2	2.69	0.52
1:F:117:ILE:HG22	1:F:135:THR:HG22	1.91	0.52
1:F:231:ALA:HB1	1:F:282:PRO:HD3	1.92	0.52
1:F:428:ARG:NH2	1:F:460:ASP:OD1	2.42	0.52
1:B:387:ASP:HB3	1:B:389:SER:H	1.76	0.52
1:C:376:MET:HG2	1:C:397:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:GLY:HA2	1:D:341:VAL:O	2.11	0.52
1:F:397:ILE:CD1	1:F:422:PHE:HZ	2.23	0.52
1:D:397:ILE:HD13	1:D:422:PHE:HZ	1.74	0.51
1:E:129:CYS:O	1:E:163:VAL:HG23	2.09	0.51
1:H:115:PHE:CZ	1:H:159:MET:HE1	2.46	0.51
1:H:339:GLY:O	1:H:340:PRO:C	2.52	0.51
1:A:117:ILE:HG22	1:A:135:THR:HG22	1.91	0.51
1:E:136:GLN:HE21	1:E:156:ARG:CD	2.23	0.51
1:H:380:PRO:O	1:H:381:ASN:C	2.51	0.51
1:A:467:THR:O	1:A:468:ILE:HB	2.11	0.51
1:B:355:LYS:NZ	1:B:357:GLY:O	2.41	0.51
1:D:133:PHE:O	1:D:158:LEU:HD12	2.11	0.51
1:G:333:GLY:N	1:G:386:THR:HG23	2.24	0.51
1:H:97:TRP:N	1:H:395:GLN:HE22	2.07	0.51
1:H:135:THR:O	1:H:156:ARG:HA	2.10	0.51
1:B:113:ASP:HB3	1:B:139:LEU:HD13	1.92	0.51
1:D:413:THR:CG2	1:D:415:LEU:HD13	2.40	0.51
1:E:91:LEU:HD11	1:E:281:TYR:CE2	2.46	0.51
1:G:129:CYS:O	1:G:163:VAL:HG23	2.11	0.51
1:G:379:ASP:OD2	1:G:382:GLY:HA3	2.11	0.51
1:H:249:GLN:HE21	1:H:272:ASN:H	1.57	0.51
1:B:248:GLY:O	1:B:249:GLN:C	2.51	0.51
1:C:342:SER:O	1:C:343:SER:C	2.53	0.51
1:E:452:ASP:CB	1:G:216:LYS:NZ	2.74	0.51
1:A:129:CYS:O	1:A:163:VAL:HG23	2.11	0.51
1:A:287:ILE:N	1:A:287:ILE:HD12	2.26	0.51
1:A:413:THR:CG2	1:A:415:LEU:HB2	2.40	0.51
1:B:155:HIS:HD2	1:C:102:LYS:HE3	1.75	0.51
1:H:316:TYR:CZ	1:H:340:PRO:HD3	2.45	0.51
1:B:184:HIS:HD2	1:B:186:GLY:H	1.57	0.51
1:B:452:ASP:HB2	1:D:216:LYS:HZ3	1.74	0.51
1:D:428:ARG:HB3	1:D:464:LEU:HD11	1.93	0.51
1:H:126:HIS:O	1:H:127:LEU:HD23	2.10	0.51
1:A:322:PHE:CE2	1:A:341:VAL:HG21	2.45	0.51
1:D:287:ILE:O	1:D:304:SER:HA	2.11	0.51
1:D:309:ASN:O	1:D:310:LEU:HB2	2.11	0.51
1:D:332:THR:HG22	1:D:386:THR:HG21	1.91	0.51
1:E:172:ARG:HD2	1:E:174:GLU:OE1	2.11	0.51
1:H:268:LEU:HD11	1:H:303:VAL:HG21	1.91	0.51
1:B:102:LYS:HG3	1:B:444:ILE:HG22	1.93	0.51
1:D:380:PRO:HB2	1:D:381:ASN:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ALA:O	1:F:229:GLU:HA	2.10	0.51
1:A:136:GLN:NE2	1:A:156:ARG:HD2	2.23	0.51
1:A:226:GLN:NE2	1:A:239:THR:OG1	2.43	0.51
1:C:227:GLU:HB2	1:C:350:LYS:HD2	1.93	0.51
1:G:85:LEU:HD12	1:G:412(C):GLU:CG	2.33	0.51
1:G:87:GLY:HA3	1:G:233:VAL:HG22	1.93	0.51
1:A:397:ILE:CD1	1:A:422:PHE:HZ	2.24	0.50
1:C:218:TRP:CE2	1:C:253:LYS:HE3	2.46	0.50
1:C:366:LYS:HD2	1:C:398:VAL:O	2.12	0.50
1:D:119:GLU:O	1:D:119:GLU:HG3	2.11	0.50
1:D:366:LYS:HD2	1:D:398:VAL:O	2.10	0.50
1:F:282:PRO:HD2	1:F:411:VAL:CG2	2.41	0.50
1:B:114:VAL:HG13	1:B:167:PRO:O	2.12	0.50
1:D:286:GLU:C	1:D:287:ILE:HD12	2.36	0.50
1:D:290:VAL:HG21	1:D:353:SER:HB2	1.92	0.50
1:F:448:GLY:O	1:F:449:VAL:HB	2.10	0.50
1:A:376:MET:HG2	1:A:397:ILE:CD1	2.41	0.50
1:D:287:ILE:N	1:D:287:ILE:CD1	2.74	0.50
1:H:104:ASN:HD22	1:H:107:ARG:HD3	1.76	0.50
1:A:89:SER:HB2	1:A:417:CYS:HA	1.92	0.50
1:C:116:VAL:O	1:C:116:VAL:HG13	2.11	0.50
1:E:119:GLU:HG3	1:E:119:GLU:O	2.11	0.50
1:E:412:GLN:HG3	1:E:419:ARG:CG	2.39	0.50
1:G:118:ARG:HB2	1:G:156:ARG:HH11	1.77	0.50
1:B:219:ARG:HB2	1:B:243:ASP:CG	2.37	0.50
1:B:249:GLN:NE2	1:B:271:PRO:HA	2.26	0.50
1:C:392:VAL:HG12	1:C:394:LYS:N	2.26	0.50
1:A:325:ASN:HA	1:A:326:PRO:C	2.36	0.50
1:C:229:GLU:HG2	1:C:230:CYS:O	2.12	0.50
1:C:275:TYR:CE2	1:C:303:VAL:CG2	2.93	0.50
1:F:451:SER:HB2	1:H:214:THR:HB	1.93	0.50
1:H:118:ARG:O	1:H:119:GLU:HG3	2.12	0.50
1:A:116:VAL:HG12	1:A:138:ALA:O	2.11	0.50
1:A:293:ASP:OD2	1:A:293:ASP:C	2.52	0.50
1:B:216:LYS:CE	1:C:452:ASP:HB3	2.42	0.50
1:F:122:ILE:HG22	1:F:123:SER:N	2.26	0.50
1:F:135:THR:O	1:F:156:ARG:HA	2.12	0.50
1:H:249:GLN:NE2	1:H:272:ASN:H	2.10	0.50
1:B:347:TYR:CG	1:B:348:GLY:N	2.75	0.50
1:C:91:LEU:HG	1:C:283:ASN:ND2	2.27	0.50
1:D:183:CYS:HB3	1:D:230:CYS:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:VAL:CG1	1:H:454:VAL:HG23	2.42	0.50
1:D:354:PHE:CZ	1:D:409:SER:HB2	2.47	0.49
1:D:241:MET:HB2	1:D:255:PHE:HE1	1.76	0.49
1:E:194:ILE:HG12	1:E:203:ALA:HB2	1.93	0.49
1:E:453:THR:CG2	1:E:454:VAL:H	2.08	0.49
1:C:109:GLY:HA3	1:C:140:LEU:HD12	1.94	0.49
1:D:123:SER:OG	1:D:229:GLU:HG3	2.13	0.49
1:G:116:VAL:HG23	1:G:440:SER:HB2	1.94	0.49
1:G:296:HIS:HA	1:G:345:GLY:O	2.12	0.49
1:H:318:CYS:HA	1:H:335:SER:O	2.11	0.49
1:E:102:LYS:HG3	1:E:444:ILE:HG22	1.94	0.49
1:H:448:GLY:O	1:H:449:VAL:CB	2.55	0.49
1:F:119:GLU:CD	1:F:134:LEU:HD12	2.38	0.49
1:G:366:LYS:HD2	1:G:398:VAL:O	2.12	0.49
1:D:425:GLU:OE1	1:D:427:ILE:HD11	2.12	0.49
1:E:123:SER:OG	1:E:229:GLU:HG3	2.12	0.49
1:E:202:VAL:CG2	1:E:214:THR:HG23	2.43	0.49
1:A:216:LYS:CE	1:D:452:ASP:CB	2.91	0.49
1:C:249:GLN:HE21	1:C:272:ASN:N	1.81	0.49
1:E:135:THR:O	1:E:156:ARG:HA	2.12	0.49
1:E:463:GLU:N	1:G:144:HIS:HE1	2.00	0.49
1:F:136:GLN:O	1:G:107:ARG:NH1	2.43	0.49
1:F:343:SER:O	1:F:344:ASN:CB	2.59	0.49
1:G:376:MET:HG2	1:G:397:ILE:HD11	1.95	0.49
1:B:412(B):PRO:HB3	1:B:415:LEU:O	2.13	0.49
1:F:91:LEU:HG	1:F:283:ASN:HD22	1.75	0.49
1:G:303:VAL:HG22	1:G:314:ILE:HG22	1.95	0.49
1:B:275:TYR:CE2	1:B:303:VAL:HG23	2.47	0.49
1:F:454:VAL:HG21	1:H:200:GLY:O	2.12	0.49
1:D:413:THR:HG21	1:D:415:LEU:HB2	1.95	0.48
1:F:85:LEU:HD21	1:F:412(A):HIS:CD2	2.48	0.48
1:F:360:VAL:HG13	1:F:383:TRP:HE3	1.78	0.48
1:F:466:PHE:C	1:F:468:ILE:H	2.21	0.48
1:C:162:PRO:HG2	1:C:165:GLU:OE1	2.14	0.48
1:C:355:LYS:HD2	1:C:383:TRP:CE2	2.47	0.48
1:E:327:ARG:HB2	1:E:328:PRO:HD2	1.95	0.48
1:E:452:ASP:H	1:G:216:LYS:HE2	1.79	0.48
1:G:286:GLU:C	1:G:287:ILE:HD12	2.38	0.48
1:B:216:LYS:NZ	1:C:452:ASP:CB	2.77	0.48
1:F:103:ASP:O	1:F:104:ASN:HB2	2.12	0.48
1:G:335:SER:OG	1:G:339:GLY:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:SER:HB3	1:B:350:LYS:HZ3	1.79	0.48
1:D:299:ASN:HD22	1:D:316:TYR:HB3	1.76	0.48
1:F:264:LYS:HG2	1:F:310:LEU:HD22	1.94	0.48
1:G:192:ILE:HG23	1:G:205:LEU:CD2	2.44	0.48
1:A:112:GLY:O	1:D:111:LYS:NZ	2.46	0.48
1:D:319:SER:HB2	1:D:382:GLY:O	2.14	0.48
1:E:105:SER:CB	1:E:167:PRO:HD2	2.43	0.48
1:E:168:SER:CB	1:E:169:PRO:HD2	2.40	0.48
1:F:102:LYS:HZ2	1:F:104:ASN:ND2	2.11	0.48
1:H:287:ILE:O	1:H:304:SER:HA	2.14	0.48
1:H:325:ASN:O	1:H:348:GLY:HA2	2.13	0.48
1:A:190:LEU:HD21	1:A:257:MET:HE3	1.95	0.48
1:B:173:PHE:CZ	1:C:101:SER:HA	2.48	0.48
1:D:293:ASP:OD2	1:D:293:ASP:C	2.56	0.48
1:H:408:GLY:HA3	1:H:423:TRP:CZ2	2.49	0.48
1:A:295:TRP:CD1	1:A:295:TRP:C	2.90	0.48
1:A:463:GLU:N	1:C:144:HIS:HE1	1.84	0.48
1:B:184:HIS:CD2	1:B:186:GLY:H	2.32	0.48
1:F:216:LYS:NZ	1:G:452:ASP:HB3	2.29	0.48
1:B:226:GLN:O	1:B:227:GLU:HB2	2.13	0.48
1:E:333:GLY:N	1:E:386:THR:HG23	2.28	0.48
1:E:424:VAL:HG12	1:E:425:GLU:N	2.28	0.48
1:F:136:GLN:NE2	1:F:156:ARG:CD	2.76	0.48
1:A:332:THR:HG23	1:A:386:THR:HG21	1.95	0.48
1:B:135:THR:O	1:B:156:ARG:HA	2.13	0.48
1:E:287:ILE:N	1:E:287:ILE:CD1	2.77	0.48
1:G:146:ASN:O	1:G:148:THR:N	2.47	0.48
1:C:228:SER:CB	1:C:350:LYS:CE	2.73	0.47
1:D:413:THR:CG2	1:D:415:LEU:HB2	2.44	0.47
1:E:101:SER:HA	1:G:173:PHE:CZ	2.49	0.47
1:E:406:TYR:HB2	1:E:425:GLU:OE1	2.14	0.47
1:E:411:VAL:HG13	1:E:418:ILE:HG23	1.95	0.47
1:E:467:THR:O	1:E:468:ILE:HB	2.14	0.47
1:F:202:VAL:HG23	1:F:214:THR:HG23	1.95	0.47
1:G:297:GLY:N	1:G:345:GLY:O	2.47	0.47
1:A:164:GLY:HA3	1:C:173:PHE:CG	2.48	0.47
1:B:216:LYS:NZ	1:C:452:ASP:HB3	2.29	0.47
1:F:88:ASN:N	1:F:88:ASN:ND2	2.58	0.47
1:G:380:PRO:O	1:G:381:ASN:C	2.57	0.47
1:E:228:SER:HB3	1:E:350:LYS:CE	2.44	0.47
1:F:148:THR:HG23	1:F:430:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:412:GLN:HB2	1:F:419:ARG:HB3	1.97	0.47
1:F:429:GLY:O	1:F:433:GLU:N	2.46	0.47
1:G:190:LEU:HD21	1:G:257:MET:HE3	1.96	0.47
1:A:99:VAL:HG12	1:A:446:PHE:CE2	2.50	0.47
1:B:413:THR:CG2	1:B:415:LEU:HB2	2.43	0.47
1:B:283:ASN:O	1:B:284:ALA:C	2.54	0.47
1:G:120:PRO:HA	1:G:132:PHE:O	2.13	0.47
1:H:85:LEU:HA	1:H:412(C):GLU:OE1	2.13	0.47
1:B:183:CYS:SG	1:B:190:LEU:HD23	2.54	0.47
1:A:297:GLY:HA2	1:A:341:VAL:O	2.14	0.47
1:B:228:SER:HB3	1:B:350:LYS:CE	2.44	0.47
1:F:366:LYS:CD	1:F:400:ILE:HG12	2.40	0.47
1:G:121:PHE:CB	1:G:228:SER:HA	2.45	0.47
1:H:254:ILE:HD11	1:H:303:VAL:HG11	1.95	0.47
1:H:332:THR:HG23	1:H:386:THR:HG21	1.96	0.47
1:B:321:VAL:HG12	1:B:321:VAL:O	2.13	0.47
1:G:347:TYR:CG	1:G:348:GLY:N	2.83	0.47
1:A:412:GLN:HB2	1:A:419:ARG:HB2	1.97	0.47
1:B:182:ALA:O	1:B:229:GLU:HA	2.15	0.47
1:C:332:THR:HG23	1:C:386:THR:HG21	1.97	0.47
1:D:102:LYS:NZ	1:D:104:ASN:ND2	2.63	0.47
1:E:290:VAL:HG21	1:E:353:SER:HB2	1.97	0.47
1:E:366:LYS:HD2	1:E:398:VAL:O	2.15	0.47
1:F:397:ILE:HD13	1:F:422:PHE:CZ	2.49	0.47
1:A:451:SER:HB2	1:C:214:THR:HB	1.97	0.47
1:E:136:GLN:HE21	1:E:156:ARG:HD3	1.80	0.47
1:E:228:SER:HB3	1:E:350:LYS:HE2	1.96	0.47
1:E:451:SER:CB	1:G:214:THR:HB	2.45	0.47
1:A:216:LYS:CE	1:D:452:ASP:HB3	2.44	0.46
1:A:392:VAL:HG12	1:A:394:LYS:N	2.30	0.46
1:C:300:ARG:HH12	1:C:349:VAL:HG13	1.81	0.46
1:E:162:PRO:HG2	1:E:165:GLU:OE2	2.15	0.46
1:E:444:ILE:HG13	1:E:444:ILE:O	2.16	0.46
1:G:152:ARG:HH21	1:G:152:ARG:HG3	1.78	0.46
1:A:273:TYR:CD2	1:A:316:TYR:CE1	3.03	0.46
1:A:294:ASN:HA	1:A:347:TYR:O	2.16	0.46
1:A:327:ARG:O	1:A:344:ASN:ND2	2.48	0.46
1:B:218:TRP:CE2	1:B:253:LYS:HE3	2.50	0.46
1:E:216:LYS:NZ	1:H:452:ASP:HB3	2.30	0.46
1:E:354:PHE:CZ	1:E:409:SER:HB2	2.49	0.46
1:F:216:LYS:HZ3	1:G:452:ASP:HB2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:TYR:CD1	1:G:340:PRO:HD3	2.50	0.46
1:A:451:SER:HB2	1:C:214:THR:HG22	1.96	0.46
1:B:88:ASN:N	1:B:88:ASN:HD22	2.13	0.46
1:B:173:PHE:CG	1:C:164:GLY:HA3	2.51	0.46
1:B:287:ILE:HG22	1:B:288:THR:N	2.29	0.46
1:C:136:GLN:HE21	1:C:156:ARG:CD	2.28	0.46
1:D:136:GLN:HE21	1:D:156:ARG:HD2	1.79	0.46
1:E:287:ILE:HG22	1:E:288:THR:N	2.31	0.46
1:E:377:ILE:HG23	1:E:390:PHE:CD1	2.51	0.46
1:E:453:THR:HG22	1:E:454:VAL:N	2.20	0.46
1:G:102:LYS:HG3	1:G:444:ILE:HG22	1.96	0.46
1:H:411:VAL:HG12	1:H:412:GLN:N	2.30	0.46
1:H:413:THR:HB	1:H:415:LEU:HB2	1.97	0.46
1:A:325:ASN:O	1:A:348:GLY:HA2	2.15	0.46
1:B:115:PHE:CE1	1:B:159:MET:CE	2.96	0.46
1:B:135:THR:OG1	1:B:159:MET:HE2	2.15	0.46
1:D:397:ILE:HG22	1:D:398:VAL:HG23	1.97	0.46
1:F:102:LYS:NZ	1:F:104:ASN:ND2	2.64	0.46
1:F:411:VAL:HG13	1:F:418:ILE:CG2	2.44	0.46
1:F:419:ARG:NH1	1:F:419:ARG:HG3	2.31	0.46
1:H:88:ASN:H	1:H:88:ASN:ND2	2.12	0.46
1:C:453:THR:HG22	1:C:454:VAL:N	2.16	0.46
1:E:250:ALA:HB3	1:E:252:TYR:HE2	1.79	0.46
1:E:332:THR:HG23	1:E:386:THR:CG2	2.45	0.46
1:E:415:LEU:HD12	1:E:415:LEU:HA	1.71	0.46
1:G:249:GLN:HE21	1:G:272:ASN:N	2.09	0.46
1:G:397:ILE:HD11	1:G:422:PHE:HZ	1.79	0.46
1:H:150:LYS:NZ	1:H:150:LYS:HD2	2.31	0.46
1:A:88:ASN:N	1:A:88:ASN:ND2	2.57	0.46
1:A:172:ARG:HD2	1:A:174:GLU:OE1	2.15	0.46
1:B:254:ILE:HD13	1:B:305:PHE:CD2	2.51	0.46
1:B:407:SER:HA	1:B:423:TRP:O	2.16	0.46
1:C:115:PHE:CE1	1:C:159:MET:HE1	2.50	0.46
1:C:433:GLU:CD	1:C:464:LEU:HD12	2.41	0.46
1:E:271:PRO:O	1:E:272:ASN:HB3	2.15	0.46
1:F:239:THR:CG2	1:F:257:MET:HE1	2.45	0.46
1:B:277:GLU:OE1	1:B:350:LYS:HB2	2.16	0.46
1:C:305:PHE:HB3	1:C:312:TYR:HB3	1.97	0.46
1:C:332:THR:HG23	1:C:386:THR:CG2	2.45	0.46
1:C:379:ASP:C	1:C:380:PRO:O	2.58	0.46
1:H:355:LYS:HB2	1:H:383:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:CD2	1:A:316:TYR:HE1	2.33	0.46
1:C:136:GLN:NE2	1:C:156:ARG:HD2	2.30	0.46
1:C:343:SER:O	1:C:345:GLY:N	2.49	0.46
1:E:413:THR:HG23	1:G:210:ILE:HD12	1.98	0.46
1:F:390:PHE:CD2	1:F:390:PHE:N	2.83	0.46
1:G:412(B):PRO:HB3	1:G:415:LEU:O	2.16	0.46
1:B:121:PHE:CG	1:B:228:SER:HA	2.51	0.46
1:C:144:HIS:C	1:C:146:ASN:H	2.24	0.46
1:G:152:ARG:HG3	1:G:152:ARG:NH2	2.31	0.46
1:D:96:GLY:O	1:D:448:GLY:O	2.34	0.45
1:E:324:ASP:O	1:E:327:ARG:HD3	2.15	0.45
1:F:97:TRP:CE2	1:F:376:MET:HE2	2.51	0.45
1:C:254:ILE:HD11	1:C:268:LEU:HD21	1.97	0.45
1:E:452:ASP:CB	1:G:216:LYS:CE	2.94	0.45
1:G:181:SER:OG	1:G:192:ILE:HD12	2.16	0.45
1:H:411:VAL:CG1	1:H:418:ILE:CG2	2.91	0.45
1:A:339:GLY:O	1:A:340:PRO:C	2.60	0.45
1:D:219:ARG:HB2	1:D:243:ASP:CG	2.41	0.45
1:E:97:TRP:H	1:E:395:GLN:HE22	1.64	0.45
1:E:227:GLU:OE1	1:E:227:GLU:CA	2.64	0.45
1:G:467:THR:HG22	1:G:467:THR:O	2.15	0.45
1:E:274:HIS:HB3	1:E:293:ASP:OD2	2.15	0.45
1:E:320:GLY:N	1:E:387:ASP:O	2.49	0.45
1:F:136:GLN:NE2	1:F:156:ARG:HD3	2.31	0.45
1:F:275:TYR:CE2	1:F:303:VAL:CG2	2.95	0.45
1:G:237:CYS:O	1:G:257:MET:HG2	2.16	0.45
1:H:153:SER:HB2	1:H:154:PRO:HD2	1.97	0.45
1:H:219:ARG:HB2	1:H:243:ASP:CG	2.41	0.45
1:A:270:ALA:O	1:A:273:TYR:HB2	2.17	0.45
1:A:433:GLU:OE2	1:A:464:LEU:HD12	2.15	0.45
1:B:146:ASN:O	1:B:437:ILE:O	2.35	0.45
1:B:287:ILE:N	1:B:287:ILE:CD1	2.78	0.45
1:B:354:PHE:CZ	1:B:409:SER:HB2	2.51	0.45
1:E:254:ILE:CD1	1:E:268:LEU:HD21	2.41	0.45
1:H:320:GLY:CA	1:H:387:ASP:O	2.56	0.45
1:H:453:THR:CG2	1:H:454:VAL:H	2.30	0.45
1:A:328:PRO:HD3	1:A:343:SER:O	2.17	0.45
1:D:136:GLN:HE21	1:D:156:ARG:CD	2.30	0.45
1:E:300:ARG:HB2	1:E:317:ILE:HD12	1.99	0.45
1:F:366:LYS:HG3	1:F:374:PHE:N	2.32	0.45
1:A:136:GLN:NE2	1:A:156:ARG:CD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HD13	1:D:413:THR:HA	1.99	0.45
1:A:226:GLN:O	1:A:227:GLU:HB2	2.17	0.45
1:A:397:ILE:HG22	1:A:398:VAL:HG23	1.98	0.45
1:B:232:CYS:HA	1:B:237:CYS:HA	1.97	0.45
1:B:424:VAL:HB	1:B:444:ILE:HG13	1.98	0.45
1:E:233:VAL:O	1:E:235:GLY:N	2.50	0.45
1:E:332:THR:CG2	1:E:386:THR:HG21	2.47	0.45
1:E:412(B):PRO:HD3	1:E:418:ILE:HA	1.98	0.45
1:F:287:ILE:N	1:F:287:ILE:CD1	2.78	0.45
1:G:467:THR:O	1:G:468:ILE:HB	2.16	0.45
1:A:397:ILE:HG23	1:A:446:PHE:CZ	2.52	0.45
1:B:226:GLN:NE2	1:B:239:THR:OG1	2.39	0.45
1:D:156:ARG:HG2	1:D:178:TRP:HA	1.98	0.45
1:G:275:TYR:HE2	1:G:303:VAL:HG23	1.76	0.45
1:H:96:GLY:O	1:H:448:GLY:O	2.34	0.45
1:H:150:LYS:CE	1:H:150:LYS:CB	2.94	0.45
1:B:426:LEU:HD13	1:B:460:ASP:N	2.32	0.45
1:E:85:LEU:HD21	1:E:412(A):HIS:CD2	2.52	0.45
1:H:202:VAL:HG21	1:H:214:THR:HG23	1.98	0.45
1:H:360:VAL:HG13	1:H:383:TRP:HE3	1.81	0.45
1:H:375:GLU:OE1	1:H:394:LYS:CE	2.65	0.45
1:A:343:SER:O	1:A:344:ASN:HB3	2.17	0.45
1:C:113:ASP:HB3	1:C:139:LEU:HD13	1.99	0.45
1:G:360:VAL:HG13	1:G:383:TRP:HE3	1.82	0.45
1:H:98:ALA:O	1:H:446:PHE:HA	2.17	0.45
1:A:413:THR:HG21	1:A:415:LEU:HB2	1.98	0.44
1:C:159:MET:HA	1:C:174:GLU:HG2	1.99	0.44
1:D:99:VAL:HG13	1:D:446:PHE:CE2	2.52	0.44
1:D:322:PHE:CE1	1:D:328:PRO:HG2	2.51	0.44
1:E:343:SER:O	1:E:344:ASN:HB2	2.16	0.44
1:F:113:ASP:O	1:F:169:PRO:HD2	2.17	0.44
1:H:118:ARG:C	1:H:119:GLU:CG	2.89	0.44
1:C:306:ASN:CG	1:C:308:GLN:H	2.24	0.44
1:E:306:ASN:CG	1:E:308:GLN:H	2.26	0.44
1:E:339:GLY:O	1:E:340:PRO:C	2.60	0.44
1:F:210:ILE:CD1	1:G:413:THR:HA	2.46	0.44
1:G:152:ARG:NH1	1:G:222:ILE:HD13	2.32	0.44
1:H:377:ILE:HG23	1:H:390:PHE:CD1	2.52	0.44
1:A:113:ASP:OD2	1:A:169(A):TYR:OH	2.33	0.44
1:B:430:ARG:HD2	1:B:436:THR:O	2.16	0.44
1:E:411:VAL:HG13	1:E:418:ILE:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:VAL:O	1:F:116:VAL:HG13	2.16	0.44
1:F:121:PHE:CG	1:F:228:SER:HA	2.53	0.44
1:F:144:HIS:HE1	1:G:463:GLU:N	2.08	0.44
1:F:276:GLU:O	1:F:277:GLU:C	2.60	0.44
1:F:419:ARG:HG3	1:F:419:ARG:HH11	1.82	0.44
1:G:375:GLU:OE1	1:G:394:LYS:HE3	2.17	0.44
1:H:117:ILE:HD13	1:H:167:PRO:HG3	1.98	0.44
1:H:355:LYS:HB2	1:H:383:TRP:CZ3	2.53	0.44
1:A:320:GLY:CA	1:A:387:ASP:O	2.63	0.44
1:C:306:ASN:CG	1:C:308:GLN:N	2.75	0.44
1:D:97:TRP:CE2	1:D:376:MET:HE2	2.52	0.44
1:E:373:GLY:HA2	1:E:398:VAL:O	2.17	0.44
1:G:226:GLN:O	1:G:227:GLU:HB2	2.17	0.44
1:H:172:ARG:HG2	1:H:173:PHE:N	2.31	0.44
1:H:232:CYS:HA	1:H:237:CYS:HA	1.99	0.44
1:D:347:TYR:CG	1:D:348:GLY:N	2.77	0.44
1:E:328:PRO:HD3	1:E:343:SER:O	2.18	0.44
1:E:411:VAL:HG12	1:E:412:GLN:N	2.28	0.44
1:F:300:ARG:HG2	1:F:300:ARG:HH21	1.82	0.44
1:G:377:ILE:HG23	1:G:390:PHE:CD1	2.52	0.44
1:A:85:LEU:HD12	1:A:412(C):GLU:HG3	1.99	0.44
1:A:118:ARG:O	1:A:119:GLU:HG3	2.17	0.44
1:B:132:PHE:HB3	1:B:158:LEU:HD11	2.00	0.44
1:C:192:ILE:HG23	1:C:205:LEU:CD2	2.48	0.44
1:E:452:ASP:O	1:G:214:THR:CG2	2.56	0.44
1:G:413:THR:CG2	1:G:415:LEU:HD13	2.47	0.44
1:A:433:GLU:CD	1:A:464:LEU:HD12	2.43	0.44
1:B:451:SER:CB	1:D:214:THR:HB	2.48	0.44
1:C:355:LYS:HB2	1:C:383:TRP:CZ3	2.52	0.44
1:F:406:TYR:HB2	1:F:425:GLU:OE1	2.18	0.44
1:H:85:LEU:HD12	1:H:412(C):GLU:HG3	2.00	0.44
1:C:254:ILE:CD1	1:C:268:LEU:HD21	2.48	0.44
1:C:412:GLN:CB	1:C:419:ARG:HB2	2.46	0.44
1:D:249:GLN:NE2	1:D:271:PRO:HA	2.33	0.44
1:E:451:SER:HB2	1:G:214:THR:HG22	1.99	0.44
1:G:152:ARG:CZ	1:G:222:ILE:HD13	2.46	0.44
1:G:365:THR:HA	1:G:373:GLY:O	2.18	0.44
1:H:148:THR:HG22	1:H:430:ARG:HH22	1.82	0.44
1:A:238:PHE:HA	1:A:255:PHE:O	2.18	0.44
1:D:251:SER:OG	1:D:267:GLU:OE2	2.34	0.44
1:E:115:PHE:CZ	1:E:159:MET:HE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ALA:HB1	1:F:273:TYR:HB2	1.99	0.44
1:G:397:ILE:CD1	1:G:422:PHE:HZ	2.31	0.44
1:H:146:ASN:O	1:H:148:THR:N	2.50	0.44
1:D:270:ALA:HB1	1:D:273:TYR:HB2	1.99	0.43
1:D:328:PRO:HD3	1:D:343:SER:O	2.18	0.43
1:D:339:GLY:O	1:D:340:PRO:C	2.61	0.43
1:E:164:GLY:HA3	1:G:173:PHE:CG	2.53	0.43
1:E:360:VAL:HG22	1:E:383:TRP:HB2	2.00	0.43
1:F:248:GLY:HA2	1:F:295:TRP:CZ2	2.53	0.43
1:B:116:VAL:HG23	1:B:440:SER:HB2	2.01	0.43
1:B:210:ILE:HD13	1:C:413:THR:HA	2.00	0.43
1:B:397:ILE:HG23	1:B:446:PHE:CZ	2.53	0.43
1:F:247:ASN:O	1:F:248:GLY:C	2.58	0.43
1:F:332:THR:HG23	1:F:386:THR:HG22	2.01	0.43
1:F:421:CYS:HB3	1:F:446:PHE:O	2.18	0.43
1:G:366:LYS:HB3	1:G:400:ILE:HG12	2.00	0.43
1:H:85:LEU:CD1	1:H:412(C):GLU:HG3	2.48	0.43
1:H:117:ILE:HD12	1:H:120:PRO:HB3	2.00	0.43
1:D:161:CYS:HB2	1:D:162:PRO:HD2	2.00	0.43
1:D:184:HIS:CD2	1:D:186:GLY:N	2.80	0.43
1:G:324:ASP:O	1:G:327:ARG:HD3	2.19	0.43
1:H:152:ARG:HG3	1:H:152:ARG:HH21	1.82	0.43
1:A:412(B):PRO:HB3	1:A:415:LEU:O	2.19	0.43
1:B:299:ASN:OD1	1:B:299:ASN:N	2.38	0.43
1:C:136:GLN:HE21	1:C:156:ARG:HD2	1.84	0.43
1:C:158:LEU:O	1:C:174:GLU:HB2	2.18	0.43
1:E:210:ILE:HD13	1:H:413:THR:HG23	2.00	0.43
1:E:282:PRO:HD2	1:E:411:VAL:HG21	1.99	0.43
1:E:413:THR:HG21	1:E:415:LEU:HB2	2.01	0.43
1:F:397:ILE:HG23	1:F:446:PHE:CZ	2.54	0.43
1:G:150:LYS:HD3	1:G:152:ARG:O	2.17	0.43
1:G:411:VAL:HG13	1:G:418:ILE:CG2	2.48	0.43
1:G:412(D):LEU:O	1:G:412(D):LEU:HD12	2.19	0.43
1:B:190:LEU:HD13	1:B:260:GLY:HA2	2.00	0.43
1:C:335:SER:OG	1:C:339:GLY:O	2.36	0.43
1:F:453:THR:CG2	1:F:454:VAL:H	2.22	0.43
1:G:118:ARG:C	1:G:119:GLU:HG3	2.42	0.43
1:H:190:LEU:HA	1:H:206:LYS:O	2.18	0.43
1:H:248:GLY:O	1:H:249:GLN:C	2.62	0.43
1:B:172:ARG:HD2	1:B:174:GLU:OE1	2.18	0.43
1:B:438:TRP:CZ2	1:B:464:LEU:HD22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:TRP:H	1:C:395:GLN:HE22	1.65	0.43
1:B:88:ASN:HD22	1:B:88:ASN:H	1.65	0.43
1:D:364:ARG:O	1:D:374:PHE:HA	2.19	0.43
1:E:451:SER:OG	1:G:214:THR:HB	2.19	0.43
1:F:445:SER:C	1:F:446:PHE:CD1	2.96	0.43
1:G:358:ASN:HB3	1:G:381:ASN:HA	2.00	0.43
1:A:116:VAL:HG23	1:A:440:SER:CB	2.45	0.43
1:A:449:VAL:HG13	1:A:451:SER:OG	2.19	0.43
1:B:325:ASN:HA	1:B:326:PRO:C	2.43	0.43
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.75	0.43
1:E:316:TYR:CZ	1:E:340:PRO:HD3	2.54	0.43
1:H:421:CYS:HB3	1:H:446:PHE:O	2.19	0.43
1:D:248:GLY:O	1:D:249:GLN:C	2.61	0.43
1:D:413:THR:HG22	1:D:415:LEU:HD13	2.00	0.43
1:E:156:ARG:HG2	1:E:178:TRP:HA	2.00	0.43
1:F:263:VAL:O	1:F:264:LYS:HB2	2.19	0.43
1:H:428:ARG:NH1	1:H:464:LEU:HG	2.34	0.43
1:A:343:SER:O	1:A:344:ASN:CB	2.66	0.43
1:B:451:SER:HB2	1:D:214:THR:HG22	2.01	0.43
1:C:116:VAL:HG12	1:C:138:ALA:O	2.19	0.43
1:E:210:ILE:HD12	1:H:413:THR:HG23	2.00	0.43
1:G:355:LYS:HB2	1:G:383:TRP:CZ3	2.53	0.43
1:G:428:ARG:NH1	1:G:464:LEU:HG	2.34	0.43
1:G:430:ARG:HD2	1:G:436:THR:O	2.18	0.43
1:H:90:SER:O	1:H:417:CYS:HB2	2.19	0.43
1:B:228:SER:HB3	1:B:350:LYS:HE2	2.00	0.42
1:B:238:PHE:N	1:B:238:PHE:CD1	2.87	0.42
1:E:154:PRO:HB3	1:H:456:TRP:CZ3	2.54	0.42
1:E:225:THR:OG1	1:E:226:GLN:N	2.52	0.42
1:E:452:ASP:HB2	1:G:216:LYS:HZ3	1.84	0.42
1:H:158:LEU:HG	1:H:174:GLU:HB2	2.00	0.42
1:H:343:SER:O	1:H:344:ASN:CB	2.66	0.42
1:A:397:ILE:HD13	1:A:422:PHE:HZ	1.83	0.42
1:B:320:GLY:HA3	1:B:387:ASP:O	2.19	0.42
1:C:287:ILE:N	1:C:287:ILE:CD1	2.77	0.42
1:C:312:TYR:CD1	1:C:312:TYR:C	2.98	0.42
1:C:319:SER:HB2	1:C:382:GLY:O	2.19	0.42
1:D:289:CYS:O	1:D:302:TRP:HA	2.19	0.42
1:E:85:LEU:CD2	1:E:412(A):HIS:CD2	3.02	0.42
1:G:116:VAL:HG12	1:G:138:ALA:O	2.19	0.42
1:A:306:ASN:OD1	1:A:308:GLN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:PRO:HA	1:D:132:PHE:O	2.19	0.42
1:D:191:THR:OG1	1:D:206:LYS:HB2	2.20	0.42
1:D:355:LYS:NZ	1:D:357:GLY:O	2.51	0.42
1:E:202:VAL:HG23	1:E:214:THR:HG23	2.02	0.42
1:E:233:VAL:O	1:E:234:ASN:C	2.63	0.42
1:E:273:TYR:CD2	1:E:316:TYR:HE1	2.37	0.42
1:E:301:PRO:HB3	1:E:316:TYR:CZ	2.55	0.42
1:G:421:CYS:HA	1:G:447:CYS:HA	2.01	0.42
1:H:102:LYS:HG3	1:H:444:ILE:CG2	2.47	0.42
1:H:316:TYR:CD1	1:H:340:PRO:HD3	2.54	0.42
1:H:379:ASP:CG	1:H:382:GLY:HA3	2.44	0.42
1:A:347:TYR:CG	1:A:348:GLY:N	2.83	0.42
1:B:452:ASP:O	1:D:214:THR:CG2	2.62	0.42
1:E:226:GLN:HE22	1:E:230:CYS:HA	1.85	0.42
1:E:412(C):GLU:H	1:E:412(C):GLU:HG2	1.64	0.42
1:F:85:LEU:HB2	1:F:185:ASP:O	2.19	0.42
1:H:430:ARG:HD2	1:H:436:THR:O	2.19	0.42
1:B:131:THR:O	1:B:160:SER:HA	2.18	0.42
1:D:142:ASP:OD2	1:D:144:HIS:HD2	2.03	0.42
1:E:333:GLY:N	1:E:386:THR:CG2	2.83	0.42
1:E:411:VAL:CG2	1:E:411:VAL:HG13	2.44	0.42
1:A:182:ALA:O	1:A:229:GLU:HA	2.20	0.42
1:B:322:PHE:CE1	1:B:328:PRO:HG2	2.54	0.42
1:B:467:THR:HG22	1:B:467:THR:O	2.20	0.42
1:C:426:LEU:O	1:C:441:GLY:HA2	2.20	0.42
1:E:129:CYS:C	1:E:163:VAL:HG23	2.45	0.42
1:F:122:ILE:HD12	1:F:445:SER:HB3	2.02	0.42
1:H:403:TRP:CH2	1:H:432:LYS:HB3	2.54	0.42
1:B:200:GLY:O	1:C:454:VAL:HG21	2.19	0.42
1:B:438:TRP:HZ2	1:B:464:LEU:HD22	1.84	0.42
1:E:347:TYR:CG	1:E:348:GLY:N	2.88	0.42
1:F:303:VAL:HG22	1:F:314:ILE:HG22	2.00	0.42
1:G:148:THR:HG23	1:G:430:ARG:HH12	1.85	0.42
1:A:115:PHE:CE1	1:A:159:MET:HE1	2.54	0.42
1:C:339:GLY:O	1:C:340:PRO:C	2.63	0.42
1:D:91:LEU:HD11	1:D:281:TYR:CE2	2.54	0.42
1:D:301:PRO:HB3	1:D:316:TYR:CZ	2.55	0.42
1:D:366:LYS:HG3	1:D:374:PHE:N	2.35	0.42
1:D:380:PRO:C	1:D:381:ASN:HD22	2.27	0.42
1:E:202:VAL:HG11	1:H:454:VAL:HG23	2.02	0.42
1:F:99:VAL:HG13	1:F:446:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:VAL:CG1	1:G:454:VAL:CG2	2.97	0.42
1:F:433:GLU:CD	1:F:464:LEU:HD12	2.45	0.42
1:H:299:ASN:ND2	1:H:316:TYR:HB3	2.35	0.42
1:A:120:PRO:HD2	1:A:425:GLU:HB2	2.00	0.42
1:A:355:LYS:HD2	1:A:383:TRP:CE2	2.55	0.42
1:C:119:GLU:OE1	1:C:227:GLU:OE1	2.38	0.42
1:C:135:THR:O	1:C:156:ARG:HA	2.19	0.42
1:C:378:TRP:HB3	1:C:392:VAL:HB	2.02	0.42
1:D:397:ILE:HD13	1:D:422:PHE:CZ	2.55	0.42
1:F:392:VAL:HG12	1:F:394:LYS:N	2.34	0.42
1:F:452:ASP:HB2	1:H:216:LYS:HZ3	1.85	0.42
1:H:257:MET:HA	1:H:261:LYS:O	2.19	0.42
1:A:258:GLU:O	1:A:259:LYS:HB2	2.20	0.42
1:C:102:LYS:NZ	1:C:104:ASN:ND2	2.68	0.42
1:C:270:ALA:O	1:C:273:TYR:HB2	2.20	0.42
1:E:181:SER:HB2	1:E:228:SER:O	2.20	0.42
1:E:216:LYS:NZ	1:H:452:ASP:CB	2.82	0.42
1:E:232:CYS:HA	1:E:237:CYS:HA	2.02	0.42
1:H:327:ARG:HB2	1:H:328:PRO:HD2	2.01	0.42
1:A:180:ALA:CB	1:A:192:ILE:O	2.68	0.41
1:A:286:GLU:C	1:A:287:ILE:HD12	2.45	0.41
2:B:800:G39:H811	2:B:800:G39:H912	1.86	0.41
1:C:158:LEU:HD22	1:C:180:ALA:HB1	2.02	0.41
1:C:182:ALA:O	1:C:229:GLU:HA	2.20	0.41
1:D:370:SER:HB2	1:D:372:SER:OG	2.21	0.41
1:F:142:ASP:OD2	1:F:144:HIS:HB2	2.20	0.41
1:F:452:ASP:CB	1:H:216:LYS:NZ	2.83	0.41
1:H:325:ASN:HA	1:H:326:PRO:C	2.45	0.41
1:C:316:TYR:CE1	1:C:340:PRO:HD3	2.55	0.41
1:E:155:HIS:HB3	1:H:104:ASN:HD21	1.85	0.41
1:E:287:ILE:O	1:E:304:SER:HA	2.20	0.41
1:E:453:THR:C	1:E:454:VAL:CG2	2.93	0.41
1:G:192:ILE:HG23	1:G:205:LEU:HD22	2.01	0.41
1:G:339:GLY:O	1:G:340:PRO:C	2.62	0.41
1:A:248:GLY:HA2	1:A:295:TRP:NE1	2.35	0.41
1:B:428:ARG:HB3	1:B:464:LEU:HD11	2.01	0.41
1:C:254:ILE:O	1:C:265:SER:HA	2.20	0.41
1:C:320:GLY:CA	1:C:387:ASP:O	2.67	0.41
1:C:322:PHE:CD1	1:C:328:PRO:HG2	2.55	0.41
1:C:379:ASP:OD2	1:C:382:GLY:HA3	2.19	0.41
1:E:132:PHE:CD2	1:E:160:SER:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HB2	1:A:243:ASP:CG	2.46	0.41
1:B:226:GLN:O	1:B:227:GLU:CB	2.66	0.41
1:B:321:VAL:CG1	1:B:364:ARG:NH2	2.83	0.41
1:B:453:THR:HG22	1:B:454:VAL:N	2.20	0.41
1:C:172:ARG:HD2	1:C:174:GLU:OE1	2.21	0.41
1:D:99:VAL:HG11	1:D:458:TRP:CE2	2.56	0.41
1:D:238:PHE:CD1	1:D:238:PHE:N	2.89	0.41
1:E:116:VAL:O	1:E:116:VAL:HG13	2.21	0.41
1:F:339:GLY:HA2	1:F:340:PRO:HD2	1.67	0.41
1:G:184:HIS:HD2	1:G:186:GLY:N	2.18	0.41
1:G:445:SER:C	1:G:446:PHE:CD1	2.98	0.41
1:H:373:GLY:HA2	1:H:399:ALA:O	2.20	0.41
1:A:250:ALA:HB3	1:A:252:TYR:HE2	1.85	0.41
1:B:169(A):TYR:CD2	1:B:169(A):TYR:N	2.84	0.41
1:B:293:ASP:C	1:B:293:ASP:OD2	2.62	0.41
1:D:142:ASP:OD2	1:D:144:HIS:CD2	2.73	0.41
1:D:343:SER:O	1:D:344:ASN:HB2	2.21	0.41
1:E:174:GLU:HA	1:E:174:GLU:OE2	2.20	0.41
1:F:202:VAL:HG12	1:G:454:VAL:CG2	2.51	0.41
1:H:121:PHE:CG	1:H:228:SER:HA	2.55	0.41
1:B:102:LYS:NZ	1:B:104:ASN:ND2	2.69	0.41
1:B:155:HIS:CE1	1:C:461:GLY:HA3	2.56	0.41
1:B:181:SER:OG	1:B:192:ILE:HD12	2.21	0.41
1:C:448:GLY:O	1:C:449:VAL:HB	2.19	0.41
1:A:218:TRP:N	1:A:243:ASP:OD1	2.52	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.87	0.41
1:B:448:GLY:O	1:B:449:VAL:CB	2.50	0.41
1:C:116:VAL:HG23	1:C:440:SER:HB2	2.02	0.41
1:E:299:ASN:CG	1:E:341:VAL:HG23	2.45	0.41
1:E:355:LYS:NZ	1:E:357:GLY:O	2.54	0.41
1:F:122:ILE:CG2	1:F:123:SER:N	2.83	0.41
1:A:102:LYS:HG3	1:A:444:ILE:CG2	2.47	0.41
1:A:159:MET:HA	1:A:174:GLU:HG2	2.02	0.41
1:B:155:HIS:NE2	1:C:461:GLY:HA3	2.36	0.41
1:B:454:VAL:HG23	1:D:202:VAL:HG11	2.02	0.41
1:C:332:THR:HG22	1:C:386:THR:HG21	2.03	0.41
1:D:90:SER:O	1:D:417:CYS:HB2	2.21	0.41
1:A:210:ILE:HD12	1:D:413:THR:HG23	2.02	0.41
1:A:332:THR:CG2	1:A:386:THR:HG21	2.50	0.41
1:B:264:LYS:HG2	1:B:310:LEU:CD2	2.45	0.41
1:B:451:SER:HB2	1:D:214:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:CD	1:C:227:GLU:HB3	2.46	0.41
1:C:247:ASN:O	1:C:248:GLY:O	2.39	0.41
1:D:102:LYS:HG3	1:D:444:ILE:HG22	2.03	0.41
1:D:327:ARG:HB2	1:D:328:PRO:HD2	2.03	0.41
1:E:146:ASN:O	1:E:437:ILE:O	2.38	0.41
1:E:430:ARG:HD2	1:E:436:THR:O	2.21	0.41
1:F:152:ARG:HB3	1:F:178:TRP:CG	2.55	0.41
1:F:238:PHE:CD1	1:F:238:PHE:N	2.89	0.41
1:F:256:LYS:HG2	1:F:263:VAL:CG2	2.51	0.41
1:G:225:THR:OG1	1:G:226:GLN:N	2.53	0.41
1:G:420:PRO:O	1:G:448:GLY:N	2.48	0.41
1:H:192:ILE:HD11	1:H:257:MET:HE3	2.03	0.41
1:H:366:LYS:HB3	1:H:400:ILE:HG12	2.02	0.41
1:A:122:ILE:CG2	1:A:123:SER:N	2.84	0.41
1:B:464:LEU:HB3	1:B:465:PRO:HA	2.02	0.41
1:D:380:PRO:O	1:D:381:ASN:C	2.63	0.41
1:F:226:GLN:HE22	1:F:230:CYS:HB3	1.86	0.41
1:F:300:ARG:HG2	1:F:300:ARG:NH2	2.36	0.41
1:H:254:ILE:HD13	1:H:305:PHE:CD2	2.56	0.41
1:A:121:PHE:HB3	1:A:423:TRP:CZ2	2.56	0.40
1:B:219:ARG:HE	1:B:251:SER:HB2	1.86	0.40
1:B:295:TRP:CD1	1:B:295:TRP:C	2.98	0.40
1:D:360:VAL:CG1	1:D:383:TRP:HE3	2.34	0.40
1:E:445:SER:C	1:E:446:PHE:CD1	2.99	0.40
1:F:158:LEU:O	1:F:174:GLU:HB2	2.21	0.40
1:H:113:ASP:O	1:H:169:PRO:HD2	2.21	0.40
1:A:270:ALA:HB1	1:A:273:TYR:HB2	2.02	0.40
1:B:218:TRP:CD1	1:B:219:ARG:HG2	2.56	0.40
1:C:126:HIS:CD2	1:C:127:LEU:HG	2.55	0.40
1:E:313:GLN:HE21	1:E:313:GLN:HB3	1.65	0.40
1:F:379:ASP:OD2	1:F:382:GLY:HA3	2.20	0.40
1:G:96:GLY:O	1:G:448:GLY:O	2.39	0.40
1:G:400:ILE:H	1:G:400:ILE:HG13	1.49	0.40
1:G:426:LEU:O	1:G:441:GLY:HA2	2.21	0.40
1:H:466:PHE:O	1:H:468:ILE:N	2.54	0.40
1:A:254:ILE:HD13	1:A:254:ILE:HG21	1.89	0.40
1:A:413:THR:HA	1:C:210:ILE:HD13	2.02	0.40
1:C:232:CYS:HA	1:C:237:CYS:HA	2.02	0.40
1:C:366:LYS:NZ	1:C:396:ASP:OD1	2.52	0.40
1:D:387:ASP:HB3	1:D:389:SER:H	1.86	0.40
1:F:144:HIS:CE1	1:G:462:ALA:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:GLU:HB2	1:H:143:LYS:HE3	2.04	0.40
1:G:130:ARG:HG2	1:G:130:ARG:HH21	1.87	0.40
1:G:153:SER:C	1:G:155:HIS:H	2.28	0.40
1:D:424:VAL:O	1:D:443:SER:HA	2.21	0.40
1:E:173:PHE:CG	1:H:164:GLY:HA3	2.56	0.40
1:F:122:ILE:H	1:F:423:TRP:CD1	2.40	0.40
1:F:225:THR:OG1	1:F:226:GLN:N	2.48	0.40
1:F:305:PHE:HB3	1:F:312:TYR:HB3	2.02	0.40
1:G:118:ARG:HD2	1:G:118:ARG:HA	1.77	0.40
1:H:287:ILE:HD12	1:H:287:ILE:N	2.36	0.40
1:B:438:TRP:CD1	1:B:438:TRP:N	2.90	0.40
1:C:131:THR:O	1:C:160:SER:HA	2.21	0.40
1:C:453:THR:CG2	1:C:454:VAL:N	2.81	0.40
1:E:215:ILE:HD11	1:E:262:VAL:CG2	2.51	0.40
1:E:446:PHE:CD1	1:E:446:PHE:N	2.89	0.40
1:F:202:VAL:HG12	1:G:454:VAL:HG21	2.04	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:HIS:CD2	1:D:272:ASN:OD1[8_456]	1.92	0.28
1:D:381:ASN:OD1	1:G:384:THR:O[3_565]	1.93	0.27
1:D:416:ASP:OD2	1:G:344:ASN:N[3_565]	2.05	0.15
1:C:332:THR:OG1	1:D:332:THR:OG1[8_456]	2.12	0.08
1:C:272:ASN:OD1	1:D:296:HIS:CD2[8_456]	2.15	0.05
1:C:342:SER:OG	1:D:339:GLY:C[8_456]	2.18	0.02
1:C:342:SER:OG	1:D:339:GLY:O[8_456]	2.19	0.01
1:D:381:ASN:ND2	1:G:385:GLU:CB[3_565]	2.19	0.01

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	383/387 (99%)	339 (88%)	34 (9%)	10 (3%)	4	12
1	B	383/387 (99%)	345 (90%)	30 (8%)	8 (2%)	5	16
1	C	383/387 (99%)	339 (88%)	40 (10%)	4 (1%)	12	32
1	D	383/387 (99%)	341 (89%)	36 (9%)	6 (2%)	7	21
1	E	383/387 (99%)	344 (90%)	31 (8%)	8 (2%)	5	16
1	F	383/387 (99%)	339 (88%)	32 (8%)	12 (3%)	3	8
1	G	383/387 (99%)	345 (90%)	29 (8%)	9 (2%)	5	14
1	H	383/387 (99%)	339 (88%)	36 (9%)	8 (2%)	5	16
All	All	3064/3096 (99%)	2731 (89%)	268 (9%)	65 (2%)	5	16

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	412(A)	HIS
1	C	448	GLY
1	D	248	GLY
1	D	448	GLY
1	E	412(A)	HIS
1	F	201	ALA
1	F	340	PRO
1	F	448	GLY
1	F	451	SER
1	G	248	GLY
1	A	147	GLY
1	A	248	GLY
1	A	448	GLY
1	A	449	VAL
1	A	451	SER
1	A	467	THR
1	B	248	GLY
1	B	448	GLY
1	B	449	VAL
1	C	248	GLY
1	D	340	PRO
1	E	234	ASN
1	E	248	GLY
1	E	340	PRO
1	E	448	GLY
1	F	248	GLY
1	F	343	SER

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Mol	Chain	Res	Type
1	G	147	GLY
1	G	340	PRO
1	G	448	GLY
1	G	451	SER
1	H	306	ASN
1	H	340	PRO
1	H	448	GLY
1	H	451	SER
1	A	340	PRO
1	C	449	VAL
1	D	146	ASN
1	D	449	VAL
1	E	449	VAL
1	F	449	VAL
1	G	449	VAL
1	G	467	THR
1	H	435	SER
1	H	449	VAL
1	H	467	THR
1	B	200	GLY
1	B	343	SER
1	B	347	TYR
1	D	347	TYR
1	E	347	TYR
1	F	249	GLN
1	F	388	SER
1	A	347	TYR
1	F	146	ASN
1	G	347	TYR
1	B	340	PRO
1	E	451	SER
1	H	147	GLY
1	G	200	GLY
1	A	200	GLY
1	F	149	VAL
1	B	222	ILE
1	F	200	GLY
1	A	222	ILE

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	329/331 (99%)	314 (95%)	15 (5%)	24	50
1	B	329/331 (99%)	308 (94%)	21 (6%)	16	38
1	C	329/331 (99%)	312 (95%)	17 (5%)	21	46
1	D	329/331 (99%)	313 (95%)	16 (5%)	22	48
1	E	329/331 (99%)	314 (95%)	15 (5%)	24	50
1	F	329/331 (99%)	313 (95%)	16 (5%)	22	48
1	G	329/331 (99%)	313 (95%)	16 (5%)	22	48
1	H	329/331 (99%)	311 (94%)	18 (6%)	19	43
All	All	2632/2648 (99%)	2498 (95%)	134 (5%)	21	47

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	116	VAL
1	A	168	SER
1	A	210	ILE
1	A	214	THR
1	A	230	CYS
1	A	257	MET
1	A	296	HIS
1	A	310	LEU
1	A	360	VAL
1	A	391	SER
1	A	411	VAL
1	A	415	LEU
1	A	419	ARG
1	A	454	VAL
1	B	88	ASN
1	B	99	VAL
1	B	116	VAL
1	B	150	LYS

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Mol	Chain	Res	Type
1	B	190	LEU
1	B	210	ILE
1	B	214	THR
1	B	228	SER
1	B	230	CYS
1	B	257	MET
1	B	287	ILE
1	B	296	HIS
1	B	299	ASN
1	B	360	VAL
1	B	372	SER
1	B	391	SER
1	B	411	VAL
1	B	415	LEU
1	B	419	ARG
1	B	451	SER
1	B	454	VAL
1	C	85	LEU
1	C	88	ASN
1	C	99	VAL
1	C	116	VAL
1	C	210	ILE
1	C	214	THR
1	C	230	CYS
1	C	257	MET
1	C	287	ILE
1	C	296	HIS
1	C	298	SER
1	C	360	VAL
1	C	391	SER
1	C	400	ILE
1	C	415	LEU
1	C	419	ARG
1	C	454	VAL
1	D	88	ASN
1	D	99	VAL
1	D	116	VAL
1	D	163	VAL
1	D	214	THR
1	D	216	LYS
1	D	257	MET
1	D	296	HIS

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Mol	Chain	Res	Type
1	D	310	LEU
1	D	360	VAL
1	D	381	ASN
1	D	415	LEU
1	D	419	ARG
1	D	451	SER
1	D	454	VAL
1	D	460	ASP
1	E	85	LEU
1	E	88	ASN
1	E	99	VAL
1	E	214	THR
1	E	230	CYS
1	E	257	MET
1	E	296	HIS
1	E	310	LEU
1	E	360	VAL
1	E	391	SER
1	E	415	LEU
1	E	419	ARG
1	E	451	SER
1	E	453	THR
1	E	454	VAL
1	F	88	ASN
1	F	99	VAL
1	F	116	VAL
1	F	202	VAL
1	F	205	LEU
1	F	214	THR
1	F	230	CYS
1	F	257	MET
1	F	296	HIS
1	F	318	CYS
1	F	343	SER
1	F	360	VAL
1	F	415	LEU
1	F	419	ARG
1	F	437	ILE
1	F	453	THR
1	G	88	ASN
1	G	99	VAL
1	G	116	VAL

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Mol	Chain	Res	Type
1	G	150	LYS
1	G	205	LEU
1	G	214	THR
1	G	230	CYS
1	G	252	TYR
1	G	257	MET
1	G	296	HIS
1	G	310	LEU
1	G	360	VAL
1	G	385	GLU
1	G	415	LEU
1	G	419	ARG
1	G	454	VAL
1	H	88	ASN
1	H	99	VAL
1	H	116	VAL
1	H	150	LYS
1	H	214	THR
1	H	230	CYS
1	H	257	MET
1	H	296	HIS
1	H	298	SER
1	H	360	VAL
1	H	372	SER
1	H	391	SER
1	H	415	LEU
1	H	419	ARG
1	H	453	THR
1	H	454	VAL
1	H	456	TRP
1	H	460	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	104	ASN
1	A	136	GLN
1	A	144	HIS
1	A	146	ASN
1	A	155	HIS
1	A	184	HIS

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Mol	Chain	Res	Type
1	A	226	GLN
1	A	249	GLN
1	A	296	HIS
1	A	313	GLN
1	A	358	ASN
1	A	395	GLN
1	B	88	ASN
1	B	104	ASN
1	B	144	HIS
1	B	155	HIS
1	B	184	HIS
1	B	226	GLN
1	B	249	GLN
1	B	313	GLN
1	B	358	ASN
1	B	395	GLN
1	C	88	ASN
1	C	104	ASN
1	C	136	GLN
1	C	144	HIS
1	C	155	HIS
1	C	184	HIS
1	C	226	GLN
1	C	249	GLN
1	C	274	HIS
1	C	313	GLN
1	C	358	ASN
1	C	395	GLN
1	D	88	ASN
1	D	104	ASN
1	D	136	GLN
1	D	144	HIS
1	D	184	HIS
1	D	226	GLN
1	D	249	GLN
1	D	313	GLN
1	D	344	ASN
1	D	381	ASN
1	D	395	GLN
1	E	88	ASN
1	E	104	ASN
1	E	136	GLN

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Mol	Chain	Res	Type
1	E	144	HIS
1	E	184	HIS
1	E	208	ASN
1	E	220	ASN
1	E	226	GLN
1	E	249	GLN
1	E	296	HIS
1	E	313	GLN
1	E	344	ASN
1	E	358	ASN
1	E	395	GLN
1	E	412(A)	HIS
1	F	88	ASN
1	F	104	ASN
1	F	136	GLN
1	F	144	HIS
1	F	155	HIS
1	F	184	HIS
1	F	226	GLN
1	F	249	GLN
1	F	313	GLN
1	F	344	ASN
1	F	395	GLN
1	F	412(A)	HIS
1	G	88	ASN
1	G	104	ASN
1	G	136	GLN
1	G	144	HIS
1	G	184	HIS
1	G	249	GLN
1	G	313	GLN
1	G	344	ASN
1	G	381	ASN
1	G	395	GLN
1	H	88	ASN
1	H	104	ASN
1	H	144	HIS
1	H	146	ASN
1	H	155	HIS
1	H	184	HIS
1	H	226	GLN
1	H	249	GLN

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Mol	Chain	Res	Type
1	H	272	ASN
1	H	313	GLN
1	H	395	GLN
1	H	450	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	G39	B	800	-	19,20,20	1.27	2 (10%)	20,27,27	1.54	4 (20%)

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
2	G39	B	800	-	-	7/16/32/32	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	G39	C6-C7	2.88	1.54	1.50
2	B	800	G39	C3-C2	2.31	1.55	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	G39	C3-C2-C1	3.42	123.25	116.99
2	B	800	G39	C3-C2-C7	-3.13	118.39	122.25
2	B	800	G39	C4-C3-C2	2.95	113.06	109.72
2	B	800	G39	C3-C4-N4	2.21	115.14	110.76

There are no chirality outliers.

All (7) torsion outliers are listed below:

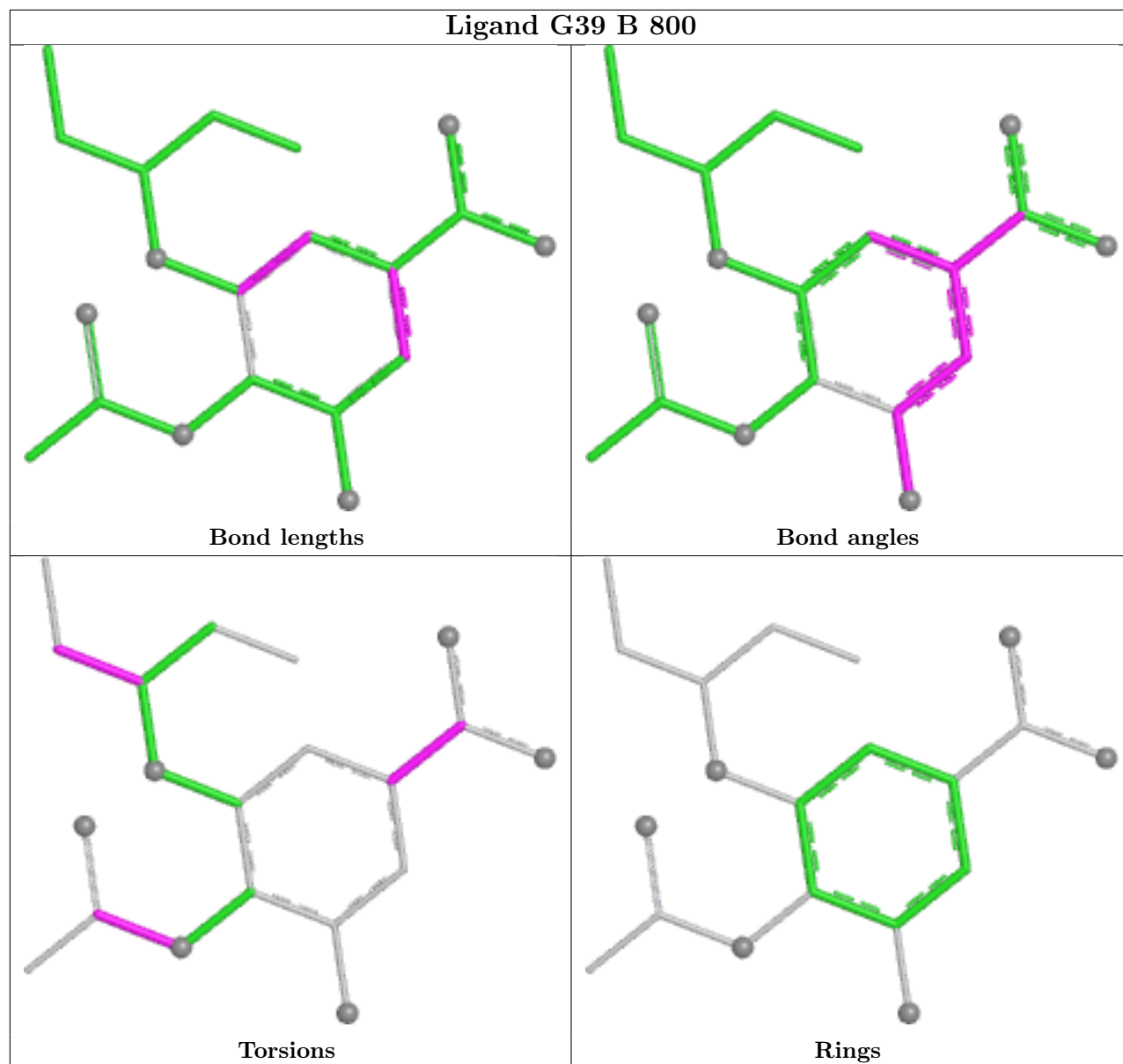
Mol	Chain	Res	Type	Atoms
2	B	800	G39	C11-C10-N5-C5
2	B	800	G39	O10-C10-N5-C5
2	B	800	G39	O7-C8-C81-C82
2	B	800	G39	O1A-C1-C2-C3
2	B	800	G39	O1B-C1-C2-C3
2	B	800	G39	C9-C8-C81-C82
2	B	800	G39	O1A-C1-C2-C7

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	G39	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	412:GLN	C	412(A):HIS	N	1.18

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

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

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	385/387 (99%)	-1.80	0 100 100	4, 17, 33, 51	0
1	B	385/387 (99%)	-1.79	0 100 100	3, 19, 34, 60	0
1	C	385/387 (99%)	-1.78	0 100 100	8, 17, 33, 60	0
1	D	385/387 (99%)	-1.77	0 100 100	3, 17, 30, 57	0
1	E	385/387 (99%)	-1.77	0 100 100	14, 28, 40, 74	0
1	F	385/387 (99%)	-1.72	0 100 100	19, 32, 49, 68	0
1	G	385/387 (99%)	-1.77	0 100 100	10, 23, 38, 66	0
1	H	385/387 (99%)	-1.75	0 100 100	18, 32, 47, 71	0
All	All	3080/3096 (99%)	-1.77	0 100 100	3, 23, 41, 74	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

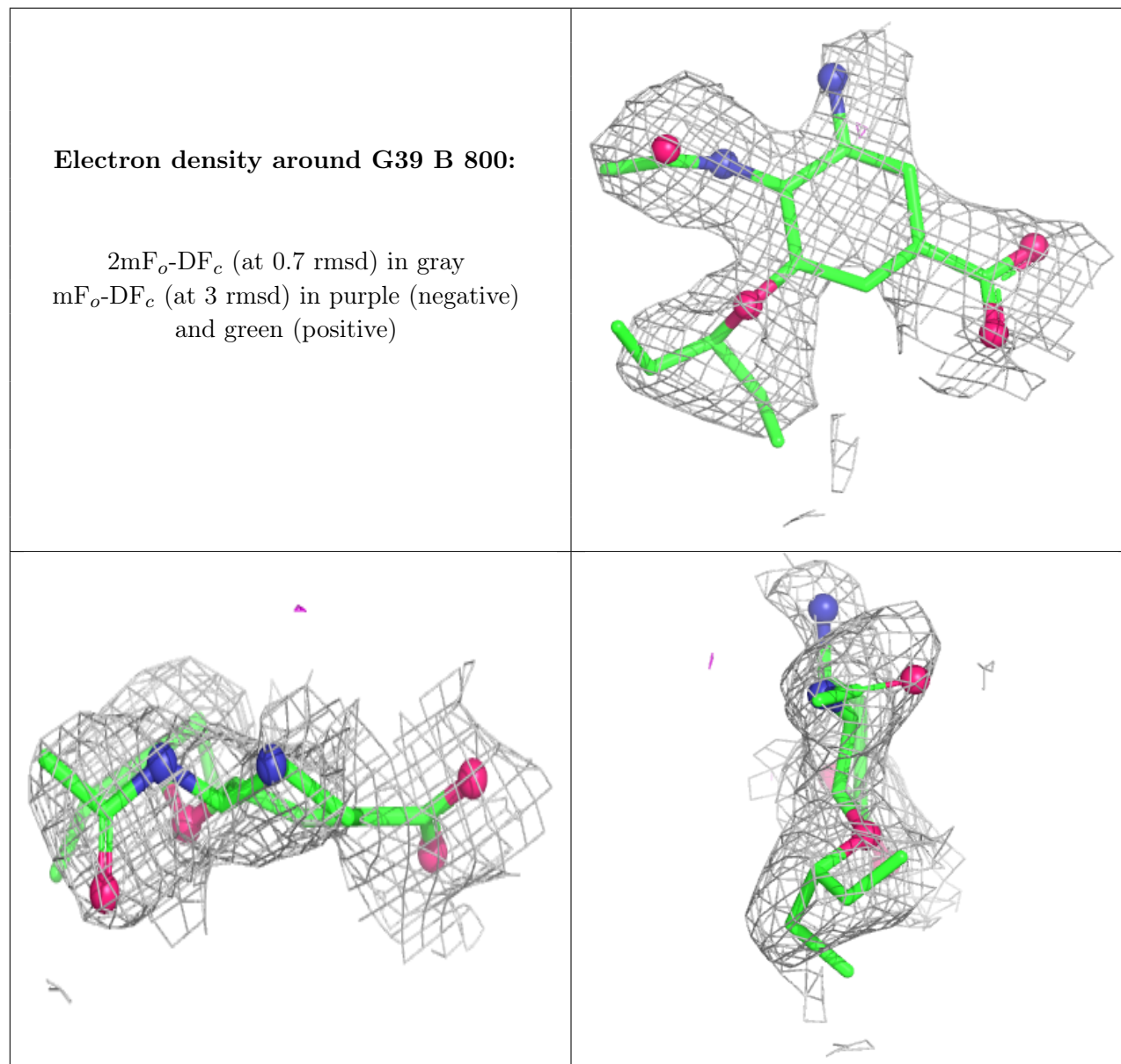
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G39	B	800	20/20	0.99	0.04	47,55,58,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.