



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:06 PM UTC

PDB ID : 2HU4 / pdb_00002hu4
Title : N1 neuraminidase in complex with oseltamivir 2
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 : 2.50 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

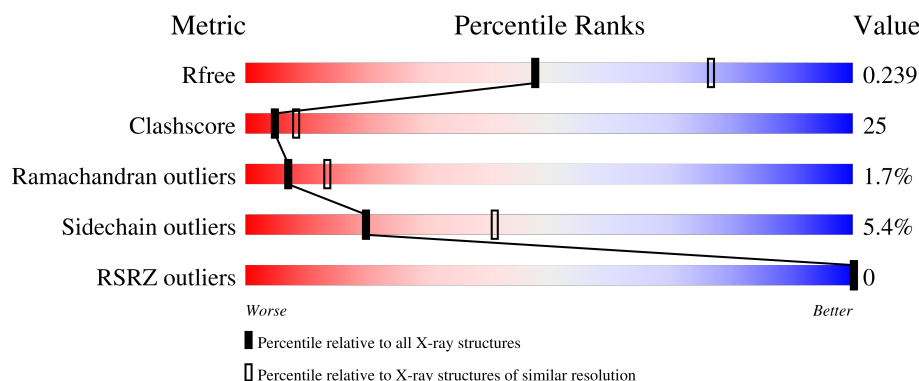
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	 59% 35% 6% ..
1	B	387	 60% 33% 6% ..
1	C	387	 58% 35% 6% ..
1	D	387	 55% 37% 6% ..
1	E	387	 60% 33% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	387	 61%33%5% ..
1	G	387	 58%36%5% ..
1	H	387	 59%34%6% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23856 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.

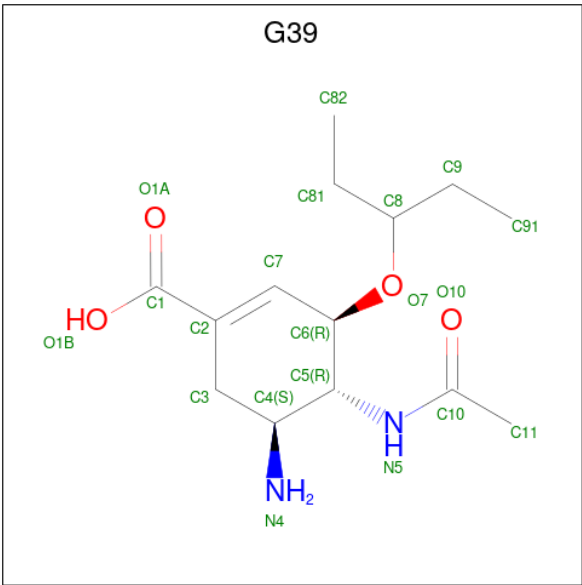
- Molecule 1 is a protein called Neuraminidase.

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	252	TYR	HIS	engineered mutation	UNP Q6DPL2
B	252	TYR	HIS	engineered mutation	UNP Q6DPL2
C	252	TYR	HIS	engineered mutation	UNP Q6DPL2
D	252	TYR	HIS	engineered mutation	UNP Q6DPL2
E	252	TYR	HIS	engineered mutation	UNP Q6DPL2
F	252	TYR	HIS	engineered mutation	UNP Q6DPL2
G	252	TYR	HIS	engineered mutation	UNP Q6DPL2
H	252	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).

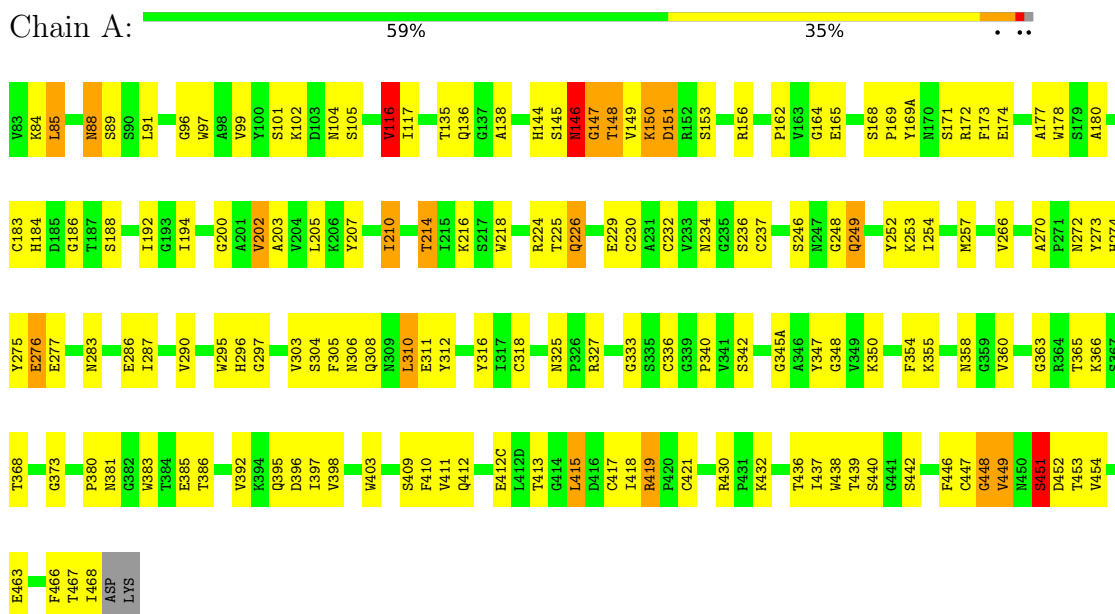


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	14	2	4		
2	B	1	Total	C	N	O	0	0
			20	14	2	4		
2	C	1	Total	C	N	O	0	0
			20	14	2	4		
2	D	1	Total	C	N	O	0	0
			20	14	2	4		
2	E	1	Total	C	N	O	0	0
			20	14	2	4		
2	F	1	Total	C	N	O	0	0
			20	14	2	4		
2	G	1	Total	C	N	O	0	0
			20	14	2	4		
2	H	1	Total	C	N	O	0	0
			20	14	2	4		

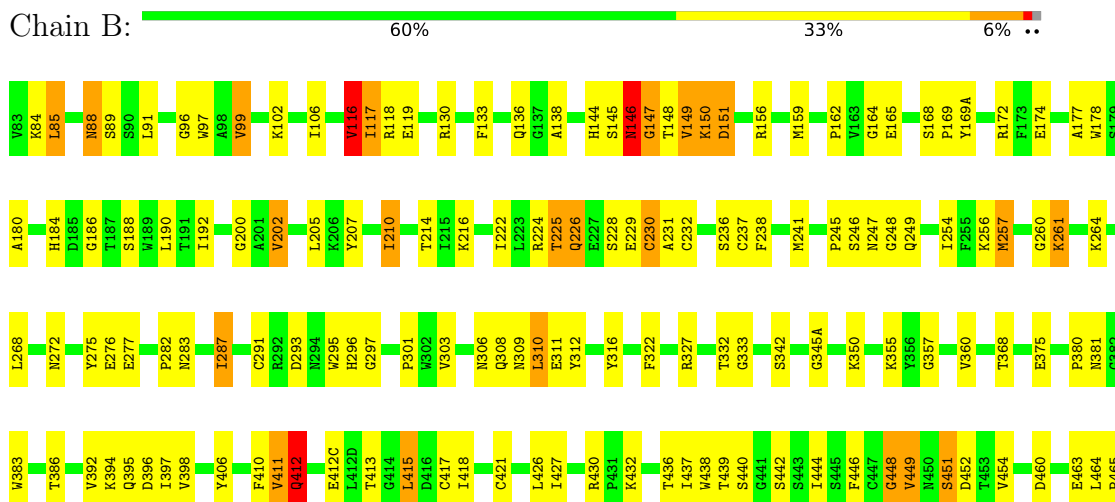
3 Residue-property plots

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



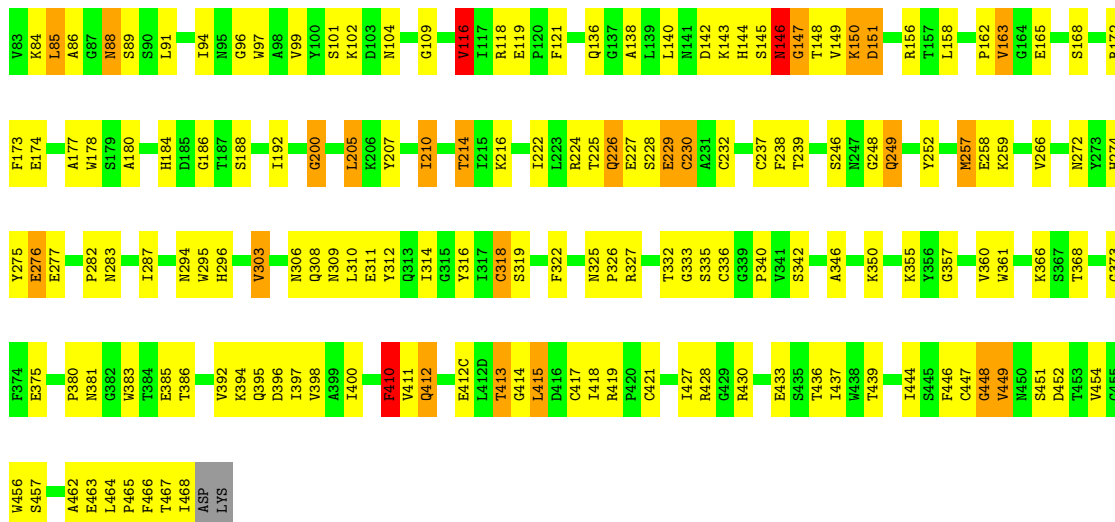
• Molecule 1: Neuraminidase



F466
T467
I468
ASP
LYS

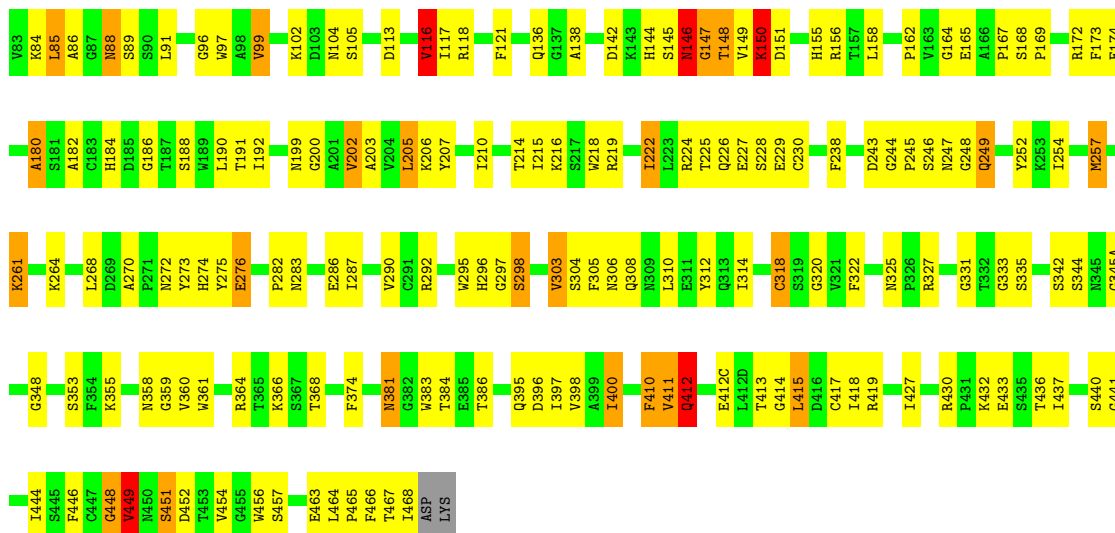
• Molecule 1: Neuraminidase

Chain C: 58% 35% 6% ..



• Molecule 1: Neuraminidase

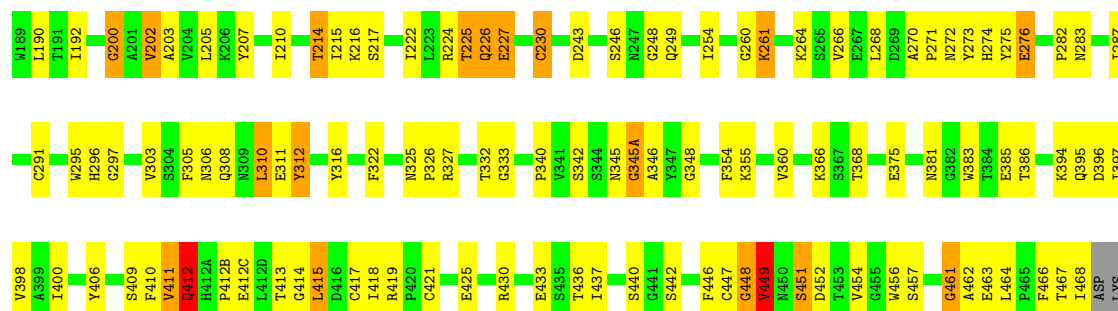
Chain D: 55% 37% 6% ..



• Molecule 1: Neuraminidase

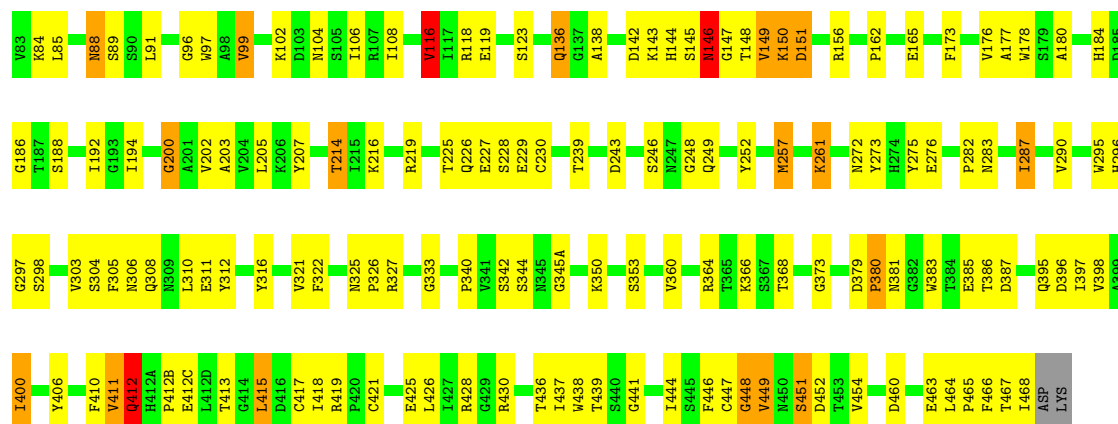
Chain E: 60% 33% 6% ..





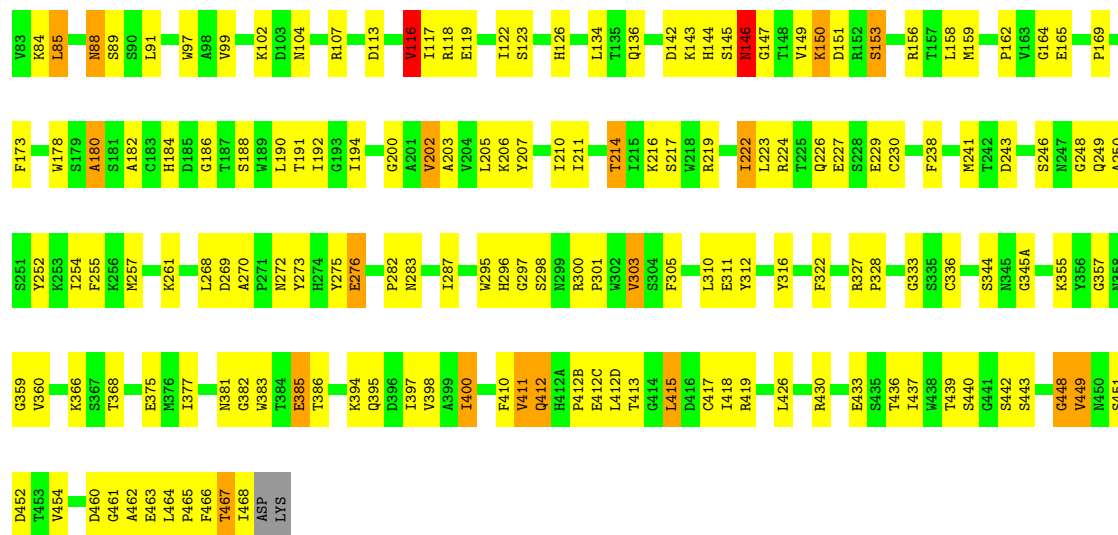
• Molecule 1: Neuraminidase

Chain F: 61% 33% 5% ..



• Molecule 1: Neuraminidase

Chain G: 58% 36% 5% ..



• Molecule 1: Neuraminidase

Chain H: 59% 34% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	201.06Å 201.24Å 211.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 93.0 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.273 0.240 , 0.239	Depositor DCC
R_{free} test set	6823 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 0.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.079 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23856	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.04% 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	0.48	0/3045	1.06	19/4141 (0.5%)
1	B	0.53	1/3045 (0.0%)	1.11	19/4141 (0.5%)
1	C	0.51	1/3045 (0.0%)	1.09	24/4141 (0.6%)
1	D	0.56	2/3045 (0.1%)	1.11	25/4141 (0.6%)
1	E	0.53	2/3045 (0.1%)	1.06	18/4141 (0.4%)
1	F	0.53	1/3045 (0.0%)	1.08	16/4141 (0.4%)
1	G	0.47	0/3045	1.08	18/4141 (0.4%)
1	H	0.47	0/3045	1.08	20/4141 (0.5%)
All	All	0.51	7/24360 (0.0%)	1.08	159/33128 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	412	GLN	C-N	-11.84	1.06	1.34
1	D	412	GLN	C-N	-10.38	1.10	1.34
1	E	412	GLN	C-N	-9.68	1.11	1.34
1	B	412	GLN	C-N	-9.25	1.12	1.34
1	D	410	PHE	C-N	-9.12	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	410	PHE	C-N	-8.32	1.24	1.33
1	C	410	PHE	C-N	-6.30	1.25	1.33

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	226	GLN	N-CA-C	11.67	125.12	111.11
1	D	246	SER	N-CA-C	-11.54	98.73	112.92
1	B	226	GLN	N-CA-C	11.16	124.50	111.11
1	D	226	GLN	N-CA-C	10.58	123.80	111.11
1	F	246	SER	N-CA-C	-10.43	99.43	112.88
1	G	226	GLN	N-CA-C	10.39	123.58	111.11
1	A	246	SER	N-CA-C	-10.13	100.60	113.16
1	A	226	GLN	N-CA-C	10.02	123.13	111.11
1	E	246	SER	N-CA-C	-9.81	100.22	112.88
1	B	246	SER	N-CA-C	-9.75	101.32	113.02
1	D	412	GLN	O-C-N	-9.63	107.29	122.70
1	C	246	SER	N-CA-C	-9.33	101.59	113.16
1	G	246	SER	N-CA-C	-9.27	101.52	112.92
1	E	226	GLN	N-CA-C	8.95	121.85	111.11
1	H	246	SER	N-CA-C	-8.85	102.02	113.17
1	D	312	TYR	N-CA-C	8.57	122.44	109.41
1	D	342	SER	N-CA-C	8.12	121.04	111.71
1	F	150	LYS	N-CA-C	7.81	122.50	112.34
1	B	311	GLU	N-CA-C	-7.81	97.34	109.76
1	F	226	GLN	N-CA-C	7.77	124.11	111.37
1	E	116	VAL	N-CA-C	-7.74	98.68	108.89
1	G	312	TYR	N-CA-C	7.56	119.91	109.18
1	H	180	ALA	N-CA-C	7.55	117.96	108.45
1	G	300	ARG	N-CA-C	7.53	119.13	109.72
1	F	180	ALA	N-CA-C	7.45	117.84	108.45
1	E	180	ALA	N-CA-C	7.39	119.39	108.60
1	H	312	TYR	N-CA-C	7.34	120.57	109.41
1	G	180	ALA	N-CA-C	7.34	117.95	108.34
1	A	311	GLU	N-CA-C	-7.31	98.14	109.76
1	A	312	TYR	N-CA-C	7.30	119.55	109.18
1	H	116	VAL	N-CA-C	-7.23	99.38	109.21
1	G	311	GLU	N-CA-C	-7.22	98.28	109.76
1	E	150	LYS	N-CA-C	7.16	121.65	112.34
1	A	180	ALA	N-CA-C	7.09	118.53	108.74
1	F	412	GLN	CB-CA-C	7.04	121.25	110.62
1	C	412	GLN	CB-CA-C	7.04	121.22	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	LYS	N-CA-C	7.01	120.93	112.38
1	B	412	GLN	CB-CA-C	6.96	121.28	110.14
1	D	412	GLN	CB-CA-C	6.95	121.16	109.48
1	D	116	VAL	N-CA-C	-6.93	98.60	108.58
1	E	412	GLN	CB-CA-C	6.93	121.22	110.14
1	E	414	GLY	N-CA-C	-6.81	105.92	115.32
1	C	342	SER	N-CA-C	6.80	118.70	111.28
1	C	413	THR	N-CA-C	6.77	120.02	111.69
1	G	153	SER	CA-C-N	6.75	126.38	119.56
1	G	153	SER	C-N-CA	6.75	126.38	119.56
1	H	149	VAL	N-CA-C	-6.75	106.07	113.43
1	F	116	VAL	N-CA-C	-6.73	100.00	108.89
1	B	312	TYR	N-CA-C	6.73	118.74	109.18
1	E	461	GLY	N-CA-C	6.67	124.20	115.40
1	H	438	TRP	N-CA-C	6.67	118.65	109.18
1	B	427	ILE	N-CA-C	6.59	118.30	108.54
1	H	311	GLU	N-CA-C	-6.58	98.53	109.46
1	H	427	ILE	N-CA-C	6.57	118.28	108.23
1	E	311	GLU	N-CA-C	-6.55	99.23	109.25
1	G	150	LYS	N-CA-C	6.47	120.27	112.38
1	A	116	VAL	N-CA-C	-6.38	99.20	108.71
1	H	411	VAL	O-C-N	6.38	129.79	122.97
1	B	150	LYS	N-CA-C	6.37	120.61	112.34
1	E	312	TYR	N-CA-C	6.35	118.84	109.69
1	G	116	VAL	N-CA-C	-6.35	99.44	108.58
1	C	226	GLN	N-CA-C	6.32	124.26	110.80
1	D	427	ILE	N-CA-C	6.31	117.88	108.54
1	E	342	SER	N-CA-C	6.30	120.07	112.38
1	B	117	ILE	N-CA-C	6.29	116.20	108.53
1	C	427	ILE	N-CA-C	6.28	117.83	108.54
1	F	136	GLN	N-CA-C	-6.17	103.83	113.02
1	H	320	GLY	N-CA-C	-6.16	107.25	115.32
1	G	411	VAL	O-C-N	6.15	129.86	123.04
1	H	150	LYS	N-CA-C	6.14	119.87	112.38
1	C	410	PHE	O-C-N	-6.13	116.26	123.25
1	C	225	THR	N-CA-C	6.05	116.08	108.45
1	A	177	ALA	N-CA-C	6.04	117.70	108.52
1	B	180	ALA	N-CA-C	6.04	117.08	108.74
1	A	171	SER	N-CA-C	6.04	119.08	109.24
1	C	163	VAL	N-CA-C	6.02	117.19	109.30
1	A	150	LYS	N-CA-C	6.00	120.14	112.34
1	D	227	GLU	N-CA-C	-6.00	105.27	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	225	THR	N-CA-C	6.00	116.19	108.34
1	F	311	GLU	N-CA-C	-5.99	99.43	108.96
1	C	319	SER	N-CA-C	5.96	118.00	110.24
1	D	244	GLY	CA-C-N	5.92	125.86	119.76
1	D	244	GLY	C-N-CA	5.92	125.86	119.76
1	E	411	VAL	CA-C-O	-5.92	116.03	121.72
1	H	225	THR	N-CA-C	5.91	116.23	108.07
1	C	414	GLY	N-CA-C	-5.90	107.67	114.69
1	D	441	GLY	N-CA-C	5.89	119.94	110.87
1	E	449	VAL	N-CA-C	5.89	121.60	109.34
1	C	229	GLU	N-CA-C	5.89	118.77	110.23
1	D	414	GLY	N-CA-C	-5.88	107.20	115.32
1	B	116	VAL	N-CA-C	-5.86	100.14	108.58
1	D	411	VAL	O-C-N	5.86	129.54	123.04
1	D	432	LYS	N-CA-C	5.86	118.61	111.82
1	D	412	GLN	CA-C-N	5.84	130.06	117.20
1	D	361	TRP	N-CA-C	-5.84	99.21	108.73
1	G	227	GLU	N-CA-C	-5.84	104.82	113.40
1	G	336	CYS	N-CA-C	-5.83	105.75	112.92
1	C	361	TRP	N-CA-C	-5.80	99.27	108.73
1	A	101	SER	N-CA-C	5.79	117.05	108.60
1	G	136	GLN	N-CA-C	-5.77	103.73	111.87
1	F	342	SER	N-CA-C	5.75	119.55	112.54
1	E	411	VAL	O-C-N	5.74	128.03	122.69
1	C	227	GLU	N-CA-C	-5.72	105.60	112.58
1	D	180	ALA	N-CA-C	5.71	116.61	108.74
1	A	225	THR	N-CA-C	5.66	115.88	108.07
1	A	438	TRP	N-CA-C	5.64	117.19	109.18
1	H	300	ARG	N-CA-C	5.64	117.79	109.62
1	H	361	TRP	N-CA-C	-5.63	100.06	109.24
1	A	105	SER	N-CA-C	5.60	118.11	111.33
1	B	149	VAL	N-CA-C	-5.58	106.89	113.42
1	C	180	ALA	N-CA-C	5.57	116.43	108.74
1	D	449	VAL	N-CA-C	5.57	120.93	109.34
1	A	363	GLY	N-CA-C	-5.56	102.20	110.71
1	G	412	GLN	CB-CA-C	5.55	119.68	110.74
1	H	412	GLN	CB-CA-C	5.55	119.67	110.74
1	C	177	ALA	N-CA-C	5.54	116.94	108.52
1	B	432	LYS	N-CA-C	5.52	118.23	111.82
1	D	150	LYS	N-CA-C	5.49	122.50	110.80
1	C	311	GLU	N-CA-C	-5.49	100.35	109.46
1	D	225	THR	N-CA-C	5.49	115.65	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	THR	N-CA-C	5.49	115.64	108.07
1	H	449	VAL	N-CA-C	5.49	120.75	109.34
1	C	101	SER	N-CA-C	5.47	116.59	108.60
1	D	410	PHE	O-C-N	-5.46	117.16	123.33
1	E	227	GLU	N-CA-C	-5.46	105.38	113.40
1	B	467	THR	N-CA-C	-5.44	106.34	112.87
1	A	342	SER	N-CA-C	5.42	119.00	112.38
1	A	419	ARG	N-CA-C	5.42	116.48	109.65
1	F	380	PRO	N-CA-C	-5.39	103.33	111.41
1	D	298	SER	N-CA-C	-5.37	106.90	113.50
1	B	411	VAL	CA-C-O	-5.36	115.98	121.67
1	C	86	ALA	N-CA-C	-5.36	101.81	110.32
1	H	177	ALA	N-CA-C	5.34	116.64	108.42
1	F	411	VAL	CA-C-O	-5.30	116.06	121.67
1	C	312	TYR	N-CA-C	5.27	117.42	109.41
1	H	227	GLU	N-CA-C	-5.26	106.81	113.23
1	D	427	ILE	CB-CA-C	-5.26	104.93	111.08
1	A	290	VAL	N-CA-C	-5.23	100.11	107.75
1	B	438	TRP	N-CA-C	5.22	117.34	109.41
1	B	177	ALA	N-CA-C	5.21	116.45	108.52
1	C	116	VAL	N-CA-C	-5.20	100.93	108.36
1	E	143	LYS	N-CA-C	5.18	116.93	111.28
1	D	86	ALA	N-CA-C	-5.16	102.64	110.28
1	F	441	GLY	N-CA-C	5.15	118.63	110.96
1	F	379	ASP	CA-C-N	-5.13	114.95	120.03
1	F	379	ASP	C-N-CA	-5.13	114.95	120.03
1	E	291	CYS	N-CA-C	5.12	117.26	109.63
1	C	318	CYS	N-CA-C	5.11	118.78	112.54
1	G	443	SER	N-CA-C	5.11	116.96	109.24
1	B	342	SER	N-CA-C	5.11	116.66	111.14
1	F	438	TRP	N-CA-C	5.10	117.62	109.81
1	A	392	VAL	N-CA-C	5.08	116.67	108.85
1	C	94	ILE	N-CA-C	5.06	116.29	108.44
1	B	291	CYS	N-CA-C	5.06	118.02	108.65
1	G	305	PHE	N-CA-C	5.06	116.49	108.96
1	H	270	ALA	N-CA-C	5.04	118.15	108.97
1	G	269	ASP	N-CA-C	-5.03	102.61	109.71
1	A	318	CYS	N-CA-C	5.02	119.11	112.89
1	E	225	THR	N-CA-C	5.00	114.98	108.07

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	412	GLN	Mainchain
1	C	410	PHE	Mainchain
1	D	412	GLN	Mainchain
1	E	412	GLN	Mainchain
1	F	412	GLN	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	158	0
1	B	2962	0	2782	164	0
1	C	2962	0	2783	158	0
1	D	2962	0	2782	179	0
1	E	2962	0	2782	174	0
1	F	2962	0	2782	144	0
1	G	2962	0	2783	164	0
1	H	2962	0	2783	152	0
2	A	20	0	23	0	0
2	B	20	0	23	1	0
2	C	20	0	23	0	0
2	D	20	0	23	0	0
2	E	20	0	23	0	0
2	F	20	0	23	0	0
2	G	20	0	23	0	0
2	H	20	0	23	0	0
All	All	23856	0	22444	1177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1177) 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:G:327:ARG:O	1:G:368:THR:CG2	1.67	1.42
1:F:327:ARG:O	1:F:368:THR:CG2	1.73	1.37
1:H:327:ARG:O	1:H:368:THR:CG2	1.74	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:O	1:A:368:THR:CG2	1.71	1.35
1:B:327:ARG:O	1:B:368:THR:CG2	1.82	1.28
1:E:327:ARG:O	1:E:368:THR:CG2	1.88	1.21
1:C:327:ARG:O	1:C:368:THR:CG2	1.90	1.20
1:D:412:GLN:OE1	1:D:419:ARG:HD2	1.45	1.14
1:F:327:ARG:O	1:F:368:THR:HG22	1.46	1.14
1:H:327:ARG:O	1:H:368:THR:HG22	1.41	1.11
1:D:327:ARG:O	1:D:368:THR:CG2	2.02	1.07
1:D:411:VAL:HG12	1:D:412:GLN:O	1.55	1.06
1:G:327:ARG:O	1:G:368:THR:HG23	1.52	1.06
1:H:412:GLN:OE1	1:H:419:ARG:HD2	1.54	1.06
1:C:413:THR:HG21	1:C:415:LEU:HD22	1.36	1.06
1:D:358:ASN:O	1:D:381:ASN:HA	1.57	1.05
1:B:413:THR:HG21	1:B:415:LEU:HD22	1.37	1.04
1:F:412:GLN:OE1	1:F:419:ARG:HD2	1.56	1.03
1:A:413:THR:HG21	1:A:415:LEU:HD22	1.38	1.03
1:E:413:THR:HG21	1:E:415:LEU:HD22	1.39	1.03
1:D:359:GLY:HA2	1:D:381:ASN:H	1.23	1.03
1:H:327:ARG:HG3	1:H:368:THR:HG23	1.40	1.03
1:G:327:ARG:O	1:G:368:THR:HG22	1.55	1.01
1:A:411:VAL:HG11	1:A:418:ILE:HG23	1.40	1.01
1:C:327:ARG:O	1:C:368:THR:HG22	1.57	1.00
1:A:327:ARG:O	1:A:368:THR:HG23	1.59	1.00
1:E:452:ASP:HB2	1:G:216:LYS:NZ	1.77	1.00
1:B:327:ARG:O	1:B:368:THR:HG22	1.63	0.98
1:F:91:LEU:HG	1:F:283:ASN:HD22	1.29	0.98
1:E:327:ARG:O	1:E:368:THR:HG22	1.61	0.97
1:G:413:THR:HG21	1:G:415:LEU:HD22	1.46	0.96
1:G:85:LEU:HD12	1:G:412(C):GLU:HG3	1.47	0.95
1:A:216:LYS:HZ1	1:D:452:ASP:HB2	1.32	0.94
1:A:216:LYS:NZ	1:D:452:ASP:HB2	1.82	0.94
1:D:413:THR:HG21	1:D:415:LEU:HD22	1.49	0.93
1:A:327:ARG:O	1:A:368:THR:HG22	1.65	0.93
1:B:451:SER:HB2	1:D:214:THR:HB	1.49	0.92
1:A:452:ASP:HB2	1:C:216:LYS:NZ	1.85	0.92
1:B:452:ASP:HB2	1:D:216:LYS:HZ1	1.34	0.91
1:B:452:ASP:HB2	1:D:216:LYS:NZ	1.84	0.91
1:H:397:ILE:HG22	1:H:398:VAL:HG23	1.53	0.91
1:B:188:SER:OG	1:B:207:TYR:CZ	2.24	0.91
1:D:359:GLY:CA	1:D:381:ASN:H	1.84	0.90
1:H:89:SER:OG	1:H:417:CYS:HA	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:HE21	1:B:272:ASN:H	1.14	0.90
1:E:249:GLN:NE2	1:E:272:ASN:H	1.70	0.89
1:F:327:ARG:O	1:F:368:THR:HG23	1.69	0.89
1:B:91:LEU:HG	1:B:283:ASN:HD22	1.35	0.88
1:D:381:ASN:N	1:D:381:ASN:HD22	1.69	0.88
1:G:397:ILE:HG22	1:G:398:VAL:HG23	1.56	0.87
1:A:452:ASP:HB2	1:C:216:LYS:HZ1	1.38	0.87
1:B:192:ILE:HD11	1:B:257:MET:HE1	1.55	0.87
1:A:91:LEU:HG	1:A:283:ASN:HD22	1.38	0.87
1:H:413:THR:HG21	1:H:415:LEU:HD22	1.55	0.87
1:B:200:GLY:O	1:C:454:VAL:HG11	1.74	0.87
1:C:91:LEU:HG	1:C:283:ASN:HD22	1.40	0.87
1:E:192:ILE:HG12	1:E:205:LEU:HD22	1.55	0.86
1:A:327:ARG:O	1:A:368:THR:HG21	1.75	0.86
1:E:214:THR:HG21	1:H:452:ASP:O	1.76	0.86
1:A:85:LEU:HD12	1:A:412(C):GLU:HG3	1.55	0.86
1:A:150:LYS:O	1:A:151:ASP:HB2	1.76	0.86
1:B:327:ARG:HG3	1:B:368:THR:HG23	1.58	0.86
1:F:214:THR:HB	1:G:451:SER:OG	1.76	0.86
1:D:327:ARG:O	1:D:368:THR:HG22	1.75	0.85
1:E:452:ASP:O	1:G:214:THR:HG21	1.75	0.85
1:A:192:ILE:HG12	1:A:205:LEU:HD22	1.58	0.85
1:C:188:SER:OG	1:C:207:TYR:CZ	2.29	0.85
1:A:413:THR:HG22	1:A:415:LEU:HD13	1.58	0.85
1:B:249:GLN:NE2	1:B:272:ASN:H	1.75	0.84
1:A:411:VAL:HG11	1:A:418:ILE:CG2	2.06	0.84
1:G:91:LEU:HG	1:G:283:ASN:HD22	1.42	0.84
1:G:413:THR:HG22	1:G:415:LEU:HD13	1.59	0.84
1:H:327:ARG:O	1:H:368:THR:HG21	1.76	0.83
1:B:452:ASP:O	1:D:214:THR:HG21	1.77	0.83
1:F:452:ASP:O	1:H:214:THR:HG21	1.78	0.83
1:B:327:ARG:O	1:B:368:THR:HG23	1.78	0.82
1:D:359:GLY:HA2	1:D:381:ASN:N	1.94	0.82
1:E:200:GLY:O	1:H:454:VAL:HG11	1.79	0.82
1:A:144:HIS:HE1	1:D:463:GLU:H	1.25	0.82
1:A:188:SER:OG	1:A:207:TYR:CZ	2.32	0.82
1:A:452:ASP:O	1:C:214:THR:HG21	1.78	0.81
1:F:413:THR:HG21	1:F:415:LEU:HD22	1.62	0.81
1:B:85:LEU:HD12	1:B:412(C):GLU:HG3	1.63	0.81
1:B:144:HIS:HE1	1:C:463:GLU:H	1.29	0.81
1:B:454:VAL:HG11	1:D:200:GLY:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:ARG:O	1:D:368:THR:HG23	1.80	0.81
1:A:327:ARG:HG3	1:A:368:THR:HG23	1.64	0.80
1:C:327:ARG:HG3	1:C:368:THR:HG23	1.63	0.80
1:E:327:ARG:O	1:E:368:THR:HG23	1.80	0.80
1:D:85:LEU:HD12	1:D:412(C):GLU:HG3	1.62	0.80
1:E:144:HIS:HE1	1:H:463:GLU:H	1.27	0.80
1:F:282:PRO:HD2	1:F:411:VAL:HG21	1.62	0.79
1:F:452:ASP:HB2	1:H:216:LYS:HZ1	1.45	0.79
1:F:466:PHE:C	1:F:468:ILE:H	1.91	0.79
1:E:97:TRP:H	1:E:395:GLN:HE22	1.29	0.79
1:A:89:SER:OG	1:A:417:CYS:HA	1.82	0.79
1:G:327:ARG:O	1:G:368:THR:HG21	1.81	0.79
1:D:89:SER:OG	1:D:417:CYS:HA	1.83	0.79
1:C:413:THR:HG22	1:C:415:LEU:HD13	1.64	0.79
1:G:381:ASN:HB3	1:G:385:GLU:HG3	1.65	0.79
1:A:452:ASP:HB3	1:C:216:LYS:HD3	1.64	0.78
1:H:333:GLY:N	1:H:386:THR:HG23	1.99	0.78
1:A:147:GLY:HA2	1:A:430:ARG:HH12	1.48	0.78
1:D:411:VAL:CG1	1:D:412:GLN:O	2.31	0.78
1:E:89:SER:OG	1:E:417:CYS:HA	1.83	0.78
1:A:411:VAL:HG12	1:A:412:GLN:N	1.98	0.78
1:C:448:GLY:O	1:C:449:VAL:HB	1.84	0.78
1:G:381:ASN:O	1:G:385:GLU:HG3	1.83	0.78
1:C:150:LYS:O	1:C:151:ASP:HB2	1.84	0.78
1:E:452:ASP:HB2	1:G:216:LYS:HZ1	1.49	0.78
1:E:454:VAL:HG11	1:G:200:GLY:O	1.84	0.77
1:A:214:THR:HG21	1:D:452:ASP:O	1.84	0.77
1:B:463:GLU:H	1:D:144:HIS:HE1	1.32	0.77
1:F:327:ARG:HG3	1:F:368:THR:HG23	1.66	0.77
1:F:412:GLN:NE2	1:F:447:CYS:SG	2.58	0.77
1:B:397:ILE:HG22	1:B:398:VAL:HG23	1.67	0.77
1:E:216:LYS:HZ1	1:H:452:ASP:HB2	1.50	0.77
1:H:188:SER:OG	1:H:207:TYR:CZ	2.37	0.76
1:F:150:LYS:O	1:F:151:ASP:HB2	1.86	0.76
1:F:412:GLN:OE1	1:F:419:ARG:CD	2.33	0.76
1:F:452:ASP:HB3	1:H:216:LYS:HD3	1.66	0.76
1:F:463:GLU:H	1:H:144:HIS:HE1	1.33	0.76
1:E:184:HIS:HD2	1:E:186:GLY:H	1.33	0.76
1:E:397:ILE:HG22	1:E:398:VAL:HG23	1.66	0.76
1:C:89:SER:OG	1:C:417:CYS:HA	1.86	0.76
1:E:249:GLN:HE21	1:E:272:ASN:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LEU:HD21	1:B:257:MET:HE3	1.68	0.75
1:F:214:THR:HG21	1:G:452:ASP:O	1.86	0.75
1:E:85:LEU:HD12	1:E:412(C):GLU:HG3	1.67	0.75
1:G:147:GLY:HA2	1:G:430:ARG:HH12	1.50	0.75
1:C:97:TRP:H	1:C:395:GLN:HE22	1.33	0.75
1:F:97:TRP:H	1:F:395:GLN:HE22	1.34	0.75
1:B:327:ARG:O	1:B:368:THR:HG21	1.86	0.75
1:E:412:GLN:NE2	1:E:447:CYS:SG	2.59	0.75
1:H:327:ARG:CG	1:H:368:THR:HG23	2.17	0.75
1:C:188:SER:OG	1:C:207:TYR:CE1	2.38	0.75
1:E:327:ARG:HG3	1:E:368:THR:HG23	1.69	0.74
1:G:188:SER:OG	1:G:207:TYR:CZ	2.40	0.74
1:D:360:VAL:HG13	1:D:383:TRP:HB2	1.68	0.74
1:A:397:ILE:HG22	1:A:398:VAL:HG23	1.69	0.74
1:E:463:GLU:H	1:G:144:HIS:HE1	1.34	0.74
1:A:162:PRO:HG2	1:A:165:GLU:CD	2.13	0.74
1:H:412:GLN:NE2	1:H:447:CYS:SG	2.60	0.74
1:A:411:VAL:HG13	1:A:419:ARG:O	1.88	0.74
1:C:327:ARG:O	1:C:368:THR:HG23	1.86	0.73
1:A:216:LYS:HD3	1:D:452:ASP:HB3	1.68	0.73
1:D:188:SER:OG	1:D:207:TYR:CZ	2.42	0.73
1:H:147:GLY:HA2	1:H:430:ARG:HH12	1.54	0.73
1:E:282:PRO:HD2	1:E:411:VAL:HG21	1.68	0.73
1:H:412:GLN:OE1	1:H:419:ARG:CD	2.35	0.73
1:F:216:LYS:NZ	1:G:452:ASP:HB2	2.02	0.73
1:B:413:THR:CG2	1:B:415:LEU:HD22	2.16	0.73
1:G:85:LEU:CD1	1:G:412(C):GLU:HG3	2.19	0.73
1:B:150:LYS:O	1:B:151:ASP:HB2	1.86	0.72
1:F:411:VAL:CG1	1:F:418:ILE:HG23	2.19	0.72
1:E:91:LEU:H	1:E:283:ASN:ND2	1.87	0.72
1:E:249:GLN:NE2	1:E:272:ASN:N	2.37	0.72
1:B:360:VAL:HG13	1:B:383:TRP:HB2	1.71	0.72
1:B:287:ILE:N	1:B:287:ILE:HD12	2.04	0.72
1:B:214:THR:HG21	1:C:452:ASP:O	1.88	0.72
1:D:412:GLN:CD	1:D:419:ARG:HD2	2.15	0.72
1:G:448:GLY:O	1:G:449:VAL:HB	1.88	0.72
1:B:188:SER:OG	1:B:207:TYR:CE1	2.43	0.72
1:D:192:ILE:HG12	1:D:205:LEU:HD22	1.72	0.71
1:E:91:LEU:H	1:E:283:ASN:HD21	1.39	0.71
1:B:162:PRO:HG2	1:B:165:GLU:CD	2.15	0.71
1:H:333:GLY:H	1:H:386:THR:HG23	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:LYS:HZ1	1:G:452:ASP:HB2	1.54	0.71
1:B:411:VAL:HG12	1:B:412:GLN:N	2.05	0.71
1:F:452:ASP:HB2	1:H:216:LYS:NZ	2.05	0.70
1:E:150:LYS:O	1:E:151:ASP:HB2	1.90	0.70
1:F:200:GLY:O	1:G:454:VAL:HG11	1.91	0.70
1:E:188:SER:OG	1:E:207:TYR:CZ	2.43	0.70
1:E:411:VAL:HG12	1:E:412:GLN:N	2.05	0.70
1:F:142:ASP:O	1:F:145:SER:HB3	1.91	0.70
1:A:411:VAL:CG1	1:A:418:ILE:HG23	2.18	0.70
1:G:366:LYS:HD3	1:G:400:ILE:HG12	1.73	0.70
1:B:333:GLY:N	1:B:386:THR:HG23	2.07	0.70
1:F:411:VAL:HG12	1:F:412:GLN:N	2.05	0.70
1:A:116:VAL:HG13	1:A:136:GLN:HB2	1.72	0.70
1:B:192:ILE:HG12	1:B:205:LEU:HD22	1.72	0.70
1:D:145:SER:O	1:D:146:ASN:O	2.10	0.70
1:C:149:VAL:HG23	1:C:430:ARG:NH1	2.07	0.69
1:E:116:VAL:HG12	1:E:138:ALA:O	1.92	0.69
1:B:91:LEU:HG	1:B:283:ASN:ND2	2.05	0.69
1:C:192:ILE:HG12	1:C:205:LEU:HD22	1.74	0.69
1:E:214:THR:HB	1:H:451:SER:OG	1.90	0.69
1:D:261:LYS:HB2	1:D:261:LYS:NZ	2.07	0.69
1:D:381:ASN:N	1:D:381:ASN:ND2	2.40	0.69
1:E:261:LYS:HB2	1:E:261:LYS:NZ	2.08	0.69
1:A:216:LYS:NZ	1:D:452:ASP:CB	2.55	0.69
1:B:216:LYS:NZ	1:C:452:ASP:HB2	2.07	0.69
1:E:452:ASP:HB2	1:G:216:LYS:HZ2	1.53	0.69
1:F:413:THR:HG22	1:F:415:LEU:HD13	1.74	0.69
1:A:188:SER:OG	1:A:207:TYR:CE1	2.45	0.69
1:A:214:THR:HB	1:D:451:SER:OG	1.93	0.69
1:F:396:ASP:O	1:F:397:ILE:HD12	1.93	0.68
1:F:466:PHE:C	1:F:468:ILE:N	2.49	0.68
1:H:150:LYS:O	1:H:151:ASP:HB2	1.93	0.68
1:E:275:TYR:CE2	1:E:303:VAL:HG23	2.29	0.68
1:B:214:THR:HB	1:C:451:SER:OG	1.94	0.68
1:E:184:HIS:CD2	1:E:186:GLY:H	2.11	0.68
1:C:91:LEU:HG	1:C:283:ASN:ND2	2.07	0.68
1:A:360:VAL:HG13	1:A:383:TRP:HB2	1.73	0.68
1:B:411:VAL:CG1	1:B:418:ILE:HG23	2.24	0.68
1:G:91:LEU:HG	1:G:283:ASN:ND2	2.07	0.68
1:B:89:SER:OG	1:B:417:CYS:HA	1.94	0.68
1:D:97:TRP:HD1	1:D:395:GLN:NE2	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:360:VAL:HG11	1:H:383:TRP:HE3	1.59	0.68
1:A:184:HIS:HD2	1:A:186:GLY:H	1.40	0.68
1:D:413:THR:HG22	1:D:415:LEU:HD13	1.75	0.68
1:F:91:LEU:HG	1:F:283:ASN:ND2	2.06	0.68
1:F:192:ILE:HG12	1:F:205:LEU:HD22	1.74	0.67
1:C:184:HIS:HD2	1:C:186:GLY:H	1.42	0.67
1:E:386:THR:HG22	1:E:386:THR:O	1.94	0.67
1:G:333:GLY:H	1:G:386:THR:HG23	1.60	0.67
1:C:413:THR:CG2	1:C:415:LEU:HD13	2.23	0.67
1:E:216:LYS:NZ	1:H:452:ASP:HB2	2.08	0.67
1:A:452:ASP:CB	1:C:216:LYS:NZ	2.58	0.67
1:F:406:TYR:HB2	1:F:425:GLU:OE1	1.94	0.67
1:C:147:GLY:HA2	1:C:430:ARG:HH12	1.59	0.67
1:D:358:ASN:C	1:D:381:ASN:HA	2.20	0.67
1:F:448:GLY:O	1:F:449:VAL:HB	1.95	0.67
1:A:463:GLU:H	1:C:144:HIS:HE1	1.43	0.67
1:D:85:LEU:CD1	1:D:412(C):GLU:HG3	2.24	0.67
1:F:249:GLN:NE2	1:F:272:ASN:H	1.93	0.67
1:D:147:GLY:HA2	1:D:430:ARG:HH12	1.59	0.67
1:F:249:GLN:HE21	1:F:272:ASN:H	1.43	0.67
1:F:454:VAL:HG11	1:H:200:GLY:O	1.95	0.67
1:A:88:ASN:H	1:A:88:ASN:HD22	1.44	0.66
1:A:413:THR:CG2	1:A:415:LEU:HD22	2.20	0.66
1:C:145:SER:O	1:C:146:ASN:O	2.13	0.66
1:E:452:ASP:CB	1:G:216:LYS:NZ	2.58	0.66
1:H:88:ASN:N	1:H:88:ASN:HD22	1.93	0.66
1:H:249:GLN:HE21	1:H:272:ASN:H	1.42	0.66
1:A:91:LEU:HG	1:A:283:ASN:ND2	2.08	0.66
1:B:145:SER:O	1:B:146:ASN:O	2.14	0.66
1:B:451:SER:CB	1:D:214:THR:HB	2.25	0.66
1:H:386:THR:HG22	1:H:386:THR:O	1.95	0.66
1:C:360:VAL:HG11	1:C:383:TRP:HE3	1.60	0.66
1:E:360:VAL:HG11	1:E:383:TRP:HE3	1.59	0.66
1:H:88:ASN:ND2	1:H:88:ASN:H	1.92	0.66
1:D:275:TYR:CE2	1:D:303:VAL:HG22	2.31	0.66
1:C:142:ASP:O	1:C:145:SER:HB3	1.96	0.66
1:E:452:ASP:CB	1:G:216:LYS:HZ2	2.09	0.66
1:F:464:LEU:HB3	1:F:465:PRO:HA	1.78	0.66
1:D:190:LEU:HD21	1:D:257:MET:HE3	1.78	0.66
1:G:287:ILE:HD12	1:G:287:ILE:N	2.12	0.65
1:H:184:HIS:HD2	1:H:186:GLY:H	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:NZ	1:C:452:ASP:CB	2.60	0.65
1:C:360:VAL:CG1	1:C:383:TRP:HE3	2.10	0.65
1:D:397:ILE:HG22	1:D:398:VAL:HG23	1.78	0.65
1:E:451:SER:OG	1:G:214:THR:HB	1.96	0.65
1:F:396:ASP:C	1:F:397:ILE:HD12	2.22	0.65
1:H:239:THR:HG22	1:H:257:MET:HE1	1.78	0.65
1:C:116:VAL:HG12	1:C:138:ALA:O	1.96	0.65
1:C:162:PRO:HG2	1:C:165:GLU:CD	2.22	0.65
1:G:184:HIS:HD2	1:G:186:GLY:H	1.45	0.65
1:H:327:ARG:C	1:H:368:THR:CG2	2.66	0.64
1:B:216:LYS:HZ1	1:C:452:ASP:HB2	1.61	0.64
1:B:261:LYS:HB2	1:B:261:LYS:NZ	2.12	0.64
1:F:85:LEU:HD13	1:F:186:GLY:HA2	1.79	0.64
1:G:89:SER:OG	1:G:417:CYS:HA	1.98	0.64
1:H:413:THR:HG22	1:H:415:LEU:HD13	1.79	0.64
1:E:270:ALA:HB1	1:E:273:TYR:HB2	1.80	0.64
1:F:84:LYS:H	1:F:84:LYS:HD2	1.62	0.64
1:G:411:VAL:HG12	1:G:412:GLN:N	2.12	0.64
1:B:85:LEU:CD1	1:B:412(C):GLU:HG3	2.28	0.64
1:E:451:SER:CB	1:G:214:THR:HB	2.27	0.64
1:C:102:LYS:HZ2	1:C:104:ASN:HD21	1.45	0.64
1:A:448:GLY:O	1:A:449:VAL:HB	1.96	0.64
1:C:412:GLN:NE2	1:C:447:CYS:SG	2.71	0.64
1:D:146:ASN:O	1:D:148:THR:N	2.28	0.64
1:F:162:PRO:HG2	1:F:165:GLU:CD	2.22	0.64
1:F:451:SER:CB	1:H:214:THR:HB	2.27	0.64
1:B:360:VAL:CG1	1:B:383:TRP:HE3	2.11	0.64
1:H:411:VAL:HG12	1:H:412:GLN:N	2.12	0.64
1:D:360:VAL:CG1	1:D:383:TRP:HE3	2.09	0.64
1:A:145:SER:O	1:A:146:ASN:O	2.16	0.63
1:B:144:HIS:CE1	1:C:463:GLU:H	2.15	0.63
1:D:202:VAL:HG23	1:D:214:THR:HG23	1.80	0.63
1:D:162:PRO:HG2	1:D:165:GLU:CD	2.22	0.63
1:C:360:VAL:HG13	1:C:383:TRP:HB2	1.79	0.63
1:E:413:THR:HG22	1:E:415:LEU:HD13	1.80	0.63
1:F:116:VAL:HG13	1:F:136:GLN:HB2	1.79	0.63
1:A:88:ASN:HD22	1:A:88:ASN:N	1.96	0.63
1:E:463:GLU:HG3	1:G:143:LYS:NZ	2.14	0.63
1:E:466:PHE:C	1:E:468:ILE:H	2.07	0.63
1:C:85:LEU:HD12	1:C:412(C):GLU:HG3	1.80	0.63
1:G:184:HIS:CD2	1:G:186:GLY:H	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:375:GLU:OE1	1:G:394:LYS:HE3	1.98	0.63
1:D:366:LYS:HD3	1:D:400:ILE:HG12	1.81	0.62
1:E:142:ASP:O	1:E:145:SER:HB3	1.99	0.62
1:F:147:GLY:HA2	1:F:430:ARG:HH12	1.63	0.62
1:B:452:ASP:CB	1:D:216:LYS:NZ	2.62	0.62
1:F:327:ARG:C	1:F:368:THR:HG23	2.23	0.62
1:F:451:SER:OG	1:H:214:THR:HB	1.99	0.62
1:E:452:ASP:HB3	1:G:216:LYS:HD3	1.80	0.62
1:G:150:LYS:O	1:G:151:ASP:HB2	1.98	0.62
1:B:249:GLN:NE2	1:B:272:ASN:N	2.47	0.62
1:E:172:ARG:HD2	1:E:174:GLU:OE1	2.00	0.62
1:G:463:GLU:O	1:G:463:GLU:HG3	1.97	0.62
1:H:239:THR:CG2	1:H:257:MET:HE1	2.29	0.62
1:E:360:VAL:HG13	1:E:383:TRP:HB2	1.82	0.62
1:G:360:VAL:HG11	1:G:383:TRP:HE3	1.63	0.62
1:C:184:HIS:CD2	1:C:186:GLY:H	2.17	0.62
1:F:327:ARG:O	1:F:368:THR:HG21	1.90	0.62
1:G:466:PHE:C	1:G:468:ILE:H	2.06	0.62
1:B:214:THR:HB	1:C:451:SER:CB	2.30	0.62
1:C:412:GLN:NE2	1:C:421:CYS:SG	2.73	0.62
1:H:327:ARG:O	1:H:368:THR:HG23	1.89	0.62
1:D:411:VAL:CG1	1:D:418:ILE:HG23	2.30	0.62
1:F:306:ASN:CG	1:F:308:GLN:N	2.58	0.62
1:H:184:HIS:CD2	1:H:186:GLY:H	2.18	0.62
1:H:322:PHE:CD1	1:H:328:PRO:HG2	2.35	0.62
1:A:454:VAL:HG11	1:C:200:GLY:O	2.00	0.61
1:G:229:GLU:OE1	1:G:410:PHE:HA	2.00	0.61
1:A:411:VAL:CG1	1:A:412:GLN:N	2.63	0.61
1:C:396:ASP:O	1:C:397:ILE:HD12	2.00	0.61
1:E:411:VAL:HG13	1:E:418:ILE:HG23	1.81	0.61
1:F:412:GLN:NE2	1:F:421:CYS:SG	2.72	0.61
1:G:466:PHE:C	1:G:468:ILE:N	2.57	0.61
1:B:91:LEU:H	1:B:283:ASN:ND2	1.99	0.61
1:C:397:ILE:HG22	1:C:398:VAL:HG23	1.82	0.61
1:C:411:VAL:HG12	1:C:412:GLN:N	2.15	0.61
1:E:202:VAL:HG23	1:E:214:THR:HG23	1.82	0.61
1:H:360:VAL:HG13	1:H:383:TRP:HB2	1.81	0.61
1:B:97:TRP:H	1:B:395:GLN:HE22	1.48	0.61
1:F:360:VAL:CG1	1:F:383:TRP:HE3	2.12	0.61
1:G:118:ARG:HB3	1:G:119:GLU:CD	2.25	0.61
1:B:249:GLN:HE21	1:B:272:ASN:N	1.94	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ILE:N	1:D:287:ILE:HD12	2.16	0.61
1:G:411:VAL:CG1	1:G:412:GLN:N	2.64	0.61
1:F:397:ILE:HG22	1:F:398:VAL:HG23	1.82	0.61
1:A:97:TRP:H	1:A:395:GLN:HE22	1.48	0.61
1:A:286:GLU:C	1:A:287:ILE:HD12	2.26	0.61
1:A:287:ILE:HD12	1:A:287:ILE:N	2.15	0.61
1:B:452:ASP:HB3	1:D:216:LYS:HD3	1.83	0.61
1:H:89:SER:HG	1:H:417:CYS:HA	1.65	0.61
1:H:162:PRO:HG2	1:H:165:GLU:CD	2.26	0.61
1:B:216:LYS:HZ2	1:C:452:ASP:CB	2.14	0.61
1:E:413:THR:CG2	1:E:415:LEU:HD22	2.25	0.61
1:E:466:PHE:C	1:E:468:ILE:N	2.56	0.61
1:E:266:VAL:HG23	1:E:310:LEU:HD23	1.81	0.60
1:G:360:VAL:CG1	1:G:383:TRP:HE3	2.13	0.60
1:H:316:TYR:HB2	1:H:336:CYS:O	2.01	0.60
1:A:102:LYS:HZ2	1:A:104:ASN:HD21	1.48	0.60
1:H:411:VAL:CG1	1:H:412:GLN:N	2.64	0.60
1:B:136:GLN:HG3	1:B:148:THR:HB	1.83	0.60
1:B:156:ARG:HG2	1:B:178:TRP:HA	1.82	0.60
1:B:216:LYS:HZ2	1:C:452:ASP:HB3	1.64	0.60
1:E:97:TRP:N	1:E:395:GLN:HE22	1.97	0.60
1:F:287:ILE:N	1:F:287:ILE:HD12	2.16	0.60
1:F:373:GLY:HA2	1:F:398:VAL:HG12	1.84	0.60
1:C:102:LYS:HZ2	1:C:104:ASN:ND2	1.98	0.60
1:E:360:VAL:CG1	1:E:383:TRP:HE3	2.14	0.60
1:F:306:ASN:CG	1:F:308:GLN:H	2.08	0.60
1:G:327:ARG:C	1:G:368:THR:HG23	2.26	0.60
1:H:360:VAL:CG1	1:H:383:TRP:HE3	2.15	0.60
1:D:102:LYS:HG3	1:D:444:ILE:HG22	1.84	0.60
1:A:360:VAL:HG11	1:A:383:TRP:HE3	1.65	0.60
1:C:277:GLU:HB3	1:C:350:LYS:HD2	1.84	0.60
1:E:88:ASN:HD22	1:E:88:ASN:H	1.50	0.60
1:F:102:LYS:HG3	1:F:444:ILE:HG22	1.82	0.60
1:H:88:ASN:HD22	1:H:88:ASN:H	1.45	0.60
1:H:229:GLU:OE1	1:H:410:PHE:HA	2.01	0.60
1:H:366:LYS:HD3	1:H:400:ILE:HG12	1.83	0.60
1:B:466:PHE:C	1:B:468:ILE:H	2.10	0.59
1:B:466:PHE:C	1:B:468:ILE:N	2.59	0.59
1:E:249:GLN:HG2	1:E:295:TRP:CH2	2.37	0.59
1:F:451:SER:HB2	1:H:214:THR:HB	1.83	0.59
1:B:411:VAL:HG11	1:B:418:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LEU:HD22	1:D:180:ALA:HB1	1.83	0.59
1:D:306:ASN:CG	1:D:308:GLN:H	2.10	0.59
1:E:463:GLU:H	1:G:144:HIS:CE1	2.18	0.59
1:A:164:GLY:HA3	1:C:173:PHE:CG	2.37	0.59
1:E:188:SER:OG	1:E:207:TYR:CE1	2.54	0.59
1:H:88:ASN:O	1:H:284:ALA:HA	2.02	0.59
1:H:322:PHE:HB2	1:H:327:ARG:HD2	1.84	0.59
1:A:149:VAL:HG22	1:A:439:THR:OG1	2.02	0.59
1:H:109:GLY:HA3	1:H:140:LEU:HD12	1.84	0.59
1:B:411:VAL:CG1	1:B:412:GLN:N	2.65	0.59
1:H:97:TRP:HD1	1:H:395:GLN:NE2	2.00	0.59
1:A:229:GLU:OE1	1:A:410:PHE:HA	2.03	0.59
1:E:88:ASN:H	1:E:88:ASN:ND2	2.01	0.59
1:A:207:TYR:O	1:A:210:ILE:HG12	2.03	0.59
1:G:411:VAL:CG1	1:G:418:ILE:HG23	2.31	0.59
1:F:466:PHE:O	1:F:468:ILE:N	2.36	0.59
1:A:366:LYS:HD2	1:A:398:VAL:O	2.03	0.59
1:F:411:VAL:CG1	1:F:412:GLN:N	2.65	0.59
1:G:145:SER:O	1:G:146:ASN:O	2.21	0.59
1:A:249:GLN:HE21	1:A:272:ASN:H	1.51	0.58
1:B:430:ARG:HD2	1:B:436:THR:O	2.02	0.58
1:E:412:GLN:OE1	1:E:419:ARG:HD2	2.03	0.58
1:A:411:VAL:HG12	1:A:412:GLN:H	1.67	0.58
1:E:411:VAL:CG1	1:E:418:ILE:HG23	2.33	0.58
1:F:188:SER:OG	1:F:207:TYR:CZ	2.56	0.58
1:G:149:VAL:HG22	1:G:439:THR:OG1	2.03	0.58
1:G:327:ARG:HG3	1:G:368:THR:HG23	1.84	0.58
1:H:145:SER:O	1:H:146:ASN:O	2.22	0.58
1:G:107:ARG:HD2	1:G:461:GLY:HA3	1.85	0.58
1:H:102:LYS:HG3	1:H:444:ILE:HG22	1.86	0.58
1:E:146:ASN:ND2	1:E:437:ILE:HB	2.19	0.58
1:G:413:THR:CG2	1:G:415:LEU:HD22	2.29	0.58
1:A:200:GLY:O	1:D:454:VAL:HG11	2.03	0.58
1:B:130:ARG:HH21	1:B:130:ARG:HG2	1.69	0.58
1:D:91:LEU:HG	1:D:283:ASN:HD22	1.69	0.58
1:E:207:TYR:O	1:E:210:ILE:HG12	2.04	0.58
1:E:162:PRO:HG2	1:E:165:GLU:CD	2.28	0.58
1:E:411:VAL:CG1	1:E:412:GLN:N	2.65	0.58
1:E:451:SER:HB2	1:G:214:THR:HB	1.86	0.58
1:A:368:THR:HG22	1:A:368:THR:O	2.02	0.58
1:C:467:THR:O	1:C:468:ILE:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:GLN:HE21	1:E:272:ASN:N	1.95	0.58
1:G:249:GLN:HE21	1:G:272:ASN:H	1.48	0.58
1:C:316:TYR:CZ	1:C:340:PRO:HG3	2.39	0.58
1:A:116:VAL:HG23	1:A:440:SER:HB2	1.86	0.58
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.84	0.57
1:B:228:SER:HB3	1:B:350:LYS:CE	2.33	0.57
1:C:316:TYR:HB2	1:C:336:CYS:O	2.04	0.57
1:D:466:PHE:C	1:D:468:ILE:N	2.61	0.57
1:E:226:GLN:HE22	1:E:230:CYS:HA	1.68	0.57
1:D:147:GLY:C	1:D:149:VAL:H	2.11	0.57
1:E:332:THR:HG23	1:E:386:THR:HG22	1.87	0.57
1:F:228:SER:HB3	1:F:350:LYS:CE	2.34	0.57
1:G:322:PHE:HB2	1:G:327:ARG:HD2	1.86	0.57
1:H:188:SER:OG	1:H:207:TYR:CE2	2.57	0.57
1:A:116:VAL:HG12	1:A:138:ALA:O	2.05	0.57
1:E:381:ASN:O	1:E:385:GLU:HB2	2.04	0.57
1:H:146:ASN:ND2	1:H:437:ILE:HB	2.19	0.57
1:H:290:VAL:HG21	1:H:353:SER:HB2	1.87	0.57
1:D:396:ASP:C	1:D:397:ILE:HD12	2.29	0.57
1:G:91:LEU:H	1:G:283:ASN:ND2	2.02	0.57
1:H:84:LYS:HD2	1:H:84:LYS:N	2.20	0.57
1:D:249:GLN:HE21	1:D:272:ASN:H	1.50	0.57
1:F:463:GLU:HG3	1:F:463:GLU:O	2.03	0.57
1:F:151:ASP:O	1:F:156:ARG:NH2	2.38	0.57
1:B:282:PRO:HD2	1:B:411:VAL:HG21	1.87	0.57
1:E:84:LYS:H	1:E:84:LYS:HD2	1.70	0.57
1:A:146:ASN:O	1:A:148:THR:N	2.32	0.56
1:H:84:LYS:HD2	1:H:84:LYS:H	1.69	0.56
1:C:266:VAL:HG23	1:C:310:LEU:HD23	1.87	0.56
1:C:411:VAL:CG1	1:C:418:ILE:HG23	2.36	0.56
1:D:184:HIS:CD2	1:D:186:GLY:H	2.24	0.56
1:H:224:ARG:NE	1:H:276:GLU:OE1	2.34	0.56
1:C:146:ASN:O	1:C:148:THR:N	2.37	0.56
1:C:282:PRO:HD2	1:C:411:VAL:HG21	1.87	0.56
1:E:88:ASN:HD22	1:E:88:ASN:N	2.01	0.56
1:E:248:GLY:HA2	1:E:295:TRP:CD1	2.40	0.56
1:F:123:SER:HB2	1:F:229:GLU:HB3	1.87	0.56
1:B:467:THR:O	1:B:468:ILE:HB	2.05	0.56
1:G:467:THR:O	1:G:468:ILE:HB	2.04	0.56
1:H:142:ASP:O	1:H:145:SER:HB3	2.04	0.56
1:H:466:PHE:C	1:H:468:ILE:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:TYR:CE2	1:F:303:VAL:HG23	2.41	0.56
1:H:249:GLN:HE21	1:H:272:ASN:N	2.03	0.56
1:D:192:ILE:HD11	1:D:257:MET:HE1	1.86	0.56
1:F:216:LYS:NZ	1:G:452:ASP:CB	2.69	0.56
1:A:333:GLY:N	1:A:386:THR:HG23	2.20	0.56
1:F:89:SER:OG	1:F:417:CYS:HA	2.05	0.56
1:G:102:LYS:HZ2	1:G:104:ASN:HD21	1.53	0.56
1:H:301:PRO:HB3	1:H:316:TYR:CZ	2.41	0.56
1:C:333:GLY:N	1:C:386:THR:HG23	2.21	0.56
1:D:118:ARG:HB2	1:D:156:ARG:HH12	1.71	0.56
1:F:85:LEU:HD13	1:F:186:GLY:CA	2.35	0.56
1:G:188:SER:OG	1:G:207:TYR:CE1	2.59	0.56
1:A:360:VAL:CG1	1:A:383:TRP:HB2	2.36	0.56
1:G:275:TYR:CE2	1:G:303:VAL:HG22	2.41	0.56
1:E:146:ASN:O	1:E:148:THR:N	2.33	0.55
1:G:116:VAL:HG23	1:G:440:SER:HB2	1.88	0.55
1:G:191:THR:OG1	1:G:206:LYS:HB2	2.06	0.55
1:H:322:PHE:CE1	1:H:328:PRO:HG2	2.41	0.55
1:H:85:LEU:HD12	1:H:412(C):GLU:HG3	1.88	0.55
1:H:282:PRO:HD2	1:H:411:VAL:HG21	1.88	0.55
1:B:254:ILE:HD11	1:B:268:LEU:HD21	1.86	0.55
1:B:333:GLY:H	1:B:386:THR:HG23	1.70	0.55
1:D:116:VAL:HG13	1:D:136:GLN:HB2	1.87	0.55
1:H:218:TRP:CD1	1:H:219:ARG:HG2	2.41	0.55
1:H:466:PHE:C	1:H:468:ILE:H	2.13	0.55
1:E:216:LYS:NZ	1:H:452:ASP:CB	2.69	0.55
1:A:102:LYS:HZ2	1:A:104:ASN:ND2	2.03	0.55
1:B:360:VAL:CG1	1:B:383:TRP:HB2	2.36	0.55
1:C:149:VAL:CG2	1:C:430:ARG:NH1	2.69	0.55
1:C:412:GLN:OE1	1:C:419:ARG:HD2	2.06	0.55
1:F:452:ASP:CB	1:H:216:LYS:NZ	2.69	0.55
1:B:146:ASN:ND2	1:B:437:ILE:HB	2.22	0.55
1:E:306:ASN:CG	1:E:308:GLN:N	2.65	0.55
1:E:144:HIS:CE1	1:H:463:GLU:H	2.16	0.55
1:B:147:GLY:HA2	1:B:430:ARG:HH12	1.71	0.55
1:B:248:GLY:O	1:B:249:GLN:C	2.48	0.55
1:B:360:VAL:HG11	1:B:383:TRP:HE3	1.70	0.55
1:E:396:ASP:O	1:E:397:ILE:HD12	2.06	0.55
1:F:146:ASN:O	1:F:437:ILE:O	2.25	0.55
1:B:229:GLU:OE1	1:B:410:PHE:HA	2.07	0.55
1:E:145:SER:O	1:E:146:ASN:O	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:SER:OG	1:F:207:TYR:CE1	2.60	0.55
1:D:464:LEU:HB3	1:D:465:PRO:HA	1.88	0.55
1:H:430:ARG:HD2	1:H:436:THR:O	2.06	0.55
1:H:406:TYR:HB2	1:H:425:GLU:OE1	2.06	0.54
1:C:381:ASN:O	1:C:385:GLU:HB2	2.07	0.54
1:F:194:ILE:HG12	1:F:203:ALA:HB2	1.89	0.54
1:G:84:LYS:N	1:G:84:LYS:HD2	2.23	0.54
1:G:381:ASN:HB3	1:G:385:GLU:CG	2.36	0.54
1:H:91:LEU:HG	1:H:283:ASN:HD22	1.71	0.54
1:A:411:VAL:CG1	1:A:412:GLN:H	2.21	0.54
1:D:116:VAL:HG12	1:D:138:ALA:O	2.08	0.54
1:E:412:GLN:NE2	1:E:421:CYS:SG	2.80	0.54
1:H:275:TYR:CE2	1:H:303:VAL:CG2	2.89	0.54
1:B:464:LEU:HB3	1:B:465:PRO:HA	1.88	0.54
1:D:172:ARG:HD2	1:D:174:GLU:OE1	2.08	0.54
1:D:466:PHE:C	1:D:468:ILE:H	2.13	0.54
1:F:380:PRO:O	1:F:381:ASN:C	2.49	0.54
1:G:333:GLY:N	1:G:386:THR:HG23	2.22	0.54
1:H:202:VAL:HG23	1:H:214:THR:HG23	1.90	0.54
1:D:191:THR:OG1	1:D:206:LYS:HB2	2.08	0.54
1:C:355:LYS:NZ	1:C:357:GLY:O	2.38	0.54
1:C:375:GLU:OE1	1:C:394:LYS:HE3	2.06	0.54
1:D:84:LYS:HD2	1:D:84:LYS:N	2.22	0.54
1:D:254:ILE:HD13	1:D:305:PHE:CD2	2.43	0.54
1:E:254:ILE:HD11	1:E:268:LEU:HD21	1.88	0.54
1:F:261:LYS:HB2	1:F:261:LYS:NZ	2.23	0.54
1:G:84:LYS:HD2	1:G:84:LYS:H	1.73	0.54
1:G:355:LYS:HD2	1:G:383:TRP:CE2	2.42	0.54
1:H:261:LYS:NZ	1:H:261:LYS:HB2	2.23	0.54
1:A:358:ASN:O	1:A:381:ASN:HA	2.07	0.54
1:B:164:GLY:HA3	1:D:173:PHE:CG	2.43	0.54
1:C:274:HIS:HB2	1:C:295:TRP:HE3	1.73	0.54
1:C:332:THR:HG23	1:C:386:THR:CG2	2.36	0.54
1:F:144:HIS:HE1	1:G:463:GLU:H	1.55	0.54
1:H:411:VAL:CG1	1:H:418:ILE:HG23	2.38	0.54
1:B:248:GLY:HA2	1:B:295:TRP:CD2	2.42	0.54
1:A:430:ARG:HD2	1:A:436:THR:O	2.08	0.54
1:B:91:LEU:H	1:B:283:ASN:HD21	1.53	0.54
1:H:421:CYS:HB3	1:H:446:PHE:O	2.08	0.54
1:A:96:GLY:O	1:A:448:GLY:O	2.26	0.53
1:A:360:VAL:CG1	1:A:383:TRP:HE3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:GLU:C	1:D:287:ILE:HD12	2.33	0.53
1:E:118:ARG:HB2	1:E:156:ARG:NH1	2.23	0.53
1:F:360:VAL:HG13	1:F:383:TRP:HB2	1.90	0.53
1:B:275:TYR:CE2	1:B:303:VAL:HG23	2.44	0.53
1:F:411:VAL:HG11	1:F:418:ILE:HG23	1.90	0.53
1:G:156:ARG:HG2	1:G:178:TRP:HA	1.88	0.53
1:B:413:THR:HG22	1:B:415:LEU:HD13	1.90	0.53
1:C:84:LYS:HD2	1:C:84:LYS:N	2.24	0.53
1:C:156:ARG:HG2	1:C:178:TRP:HA	1.91	0.53
1:F:360:VAL:HG11	1:F:383:TRP:HE3	1.73	0.53
1:A:88:ASN:H	1:A:88:ASN:ND2	2.05	0.53
1:H:464:LEU:HB3	1:H:465:PRO:HA	1.89	0.53
1:G:102:LYS:HZ2	1:G:104:ASN:ND2	2.07	0.53
1:G:411:VAL:HG13	1:G:418:ILE:HG23	1.88	0.53
1:A:202:VAL:HG12	1:D:454:VAL:HG22	1.90	0.53
1:D:142:ASP:O	1:D:145:SER:HB3	2.08	0.53
1:D:202:VAL:CG2	1:D:214:THR:HG23	2.39	0.53
1:C:248:GLY:HA2	1:C:295:TRP:CG	2.44	0.53
1:D:355:LYS:HD2	1:D:383:TRP:CE2	2.44	0.53
1:F:96:GLY:O	1:F:448:GLY:O	2.27	0.53
1:F:275:TYR:CE2	1:F:303:VAL:CG2	2.92	0.53
1:G:282:PRO:HD2	1:G:411:VAL:HG21	1.91	0.53
1:C:226:GLN:HE22	1:C:230:CYS:HA	1.74	0.53
1:C:239:THR:CG2	1:C:257:MET:HE1	2.39	0.53
1:C:248:GLY:HA2	1:C:295:TRP:CD1	2.44	0.53
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.90	0.53
1:G:151:ASP:O	1:G:156:ARG:NH2	2.41	0.53
1:A:452:ASP:CB	1:C:216:LYS:HZ2	2.22	0.53
1:H:224:ARG:NH1	1:H:276:GLU:OE1	2.39	0.53
1:C:88:ASN:N	1:C:88:ASN:HD22	2.05	0.52
1:E:214:THR:HB	1:H:451:SER:CB	2.39	0.52
1:G:466:PHE:O	1:G:468:ILE:N	2.42	0.52
1:A:85:LEU:HD13	1:A:186:GLY:HA2	1.91	0.52
1:A:266:VAL:HG23	1:A:310:LEU:HD23	1.90	0.52
1:A:413:THR:HG21	1:A:415:LEU:CD2	2.23	0.52
1:B:297:GLY:C	1:B:345(A):GLY:HA3	2.34	0.52
1:D:282:PRO:HD2	1:D:411:VAL:HG21	1.91	0.52
1:E:462:ALA:HA	1:G:144:HIS:CE1	2.44	0.52
1:F:411:VAL:HG13	1:F:418:ILE:HG23	1.92	0.52
1:H:366:LYS:HD2	1:H:398:VAL:O	2.10	0.52
1:A:216:LYS:HD3	1:D:452:ASP:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HG22	1:B:439:THR:OG1	2.09	0.52
1:D:102:LYS:HZ2	1:D:104:ASN:ND2	2.06	0.52
1:H:143:LYS:C	1:H:145:SER:H	2.17	0.52
1:A:466:PHE:C	1:A:468:ILE:N	2.66	0.52
1:C:116:VAL:HG13	1:C:136:GLN:HB2	1.92	0.52
1:C:303:VAL:HG13	1:C:314:ILE:HG22	1.91	0.52
1:D:218:TRP:CD1	1:D:219:ARG:HG2	2.45	0.52
1:A:380:PRO:O	1:A:381:ASN:C	2.53	0.52
1:B:216:LYS:HD3	1:C:452:ASP:HB3	1.91	0.52
1:E:118:ARG:HB2	1:E:156:ARG:HH12	1.73	0.52
1:A:146:ASN:ND2	1:A:437:ILE:HB	2.24	0.52
1:B:96:GLY:O	1:B:448:GLY:O	2.28	0.52
1:C:96:GLY:O	1:C:448:GLY:O	2.28	0.52
1:C:97:TRP:N	1:C:395:GLN:HE22	2.06	0.52
1:D:158:LEU:HD22	1:D:180:ALA:CB	2.40	0.52
1:D:162:PRO:HG2	1:D:165:GLU:OE2	2.10	0.52
1:D:261:LYS:HB2	1:D:261:LYS:HZ2	1.72	0.52
1:D:411:VAL:HG12	1:D:412:GLN:N	2.24	0.52
1:D:463:GLU:HG3	1:D:463:GLU:O	2.09	0.52
1:F:162:PRO:HG2	1:F:165:GLU:OE2	2.10	0.52
1:F:430:ARG:HD2	1:F:436:THR:O	2.09	0.52
1:H:88:ASN:HD22	1:H:89:SER:H	1.58	0.52
1:H:156:ARG:HG2	1:H:178:TRP:HA	1.92	0.52
1:A:216:LYS:HZ2	1:D:452:ASP:CB	2.23	0.52
1:B:99:VAL:HG13	1:B:446:PHE:CE2	2.45	0.52
1:F:227:GLU:O	1:F:350:LYS:HE2	2.09	0.52
1:C:318:CYS:HA	1:C:335:SER:O	2.09	0.52
1:C:368:THR:HG22	1:C:368:THR:O	2.10	0.52
1:F:327:ARG:C	1:F:368:THR:CG2	2.70	0.52
1:B:116:VAL:HG13	1:B:136:GLN:HB2	1.92	0.51
1:C:355:LYS:HD2	1:C:383:TRP:CE2	2.45	0.51
1:E:368:THR:HG22	1:E:368:THR:O	2.09	0.51
1:G:97:TRP:H	1:G:395:GLN:HE22	1.58	0.51
1:A:234:ASN:O	1:A:234:ASN:CG	2.53	0.51
1:A:467:THR:O	1:A:468:ILE:HB	2.09	0.51
1:F:239:THR:CG2	1:F:257:MET:HE1	2.41	0.51
1:G:333:GLY:H	1:G:386:THR:CG2	2.22	0.51
1:A:252:TYR:OH	1:A:274:HIS:HA	2.10	0.51
1:C:84:LYS:HD2	1:C:84:LYS:H	1.75	0.51
1:C:411:VAL:CG1	1:C:412:GLN:N	2.73	0.51
1:D:333:GLY:N	1:D:386:THR:HG23	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ASP:O	1:D:397:ILE:HD12	2.10	0.51
1:H:96:GLY:O	1:H:448:GLY:O	2.28	0.51
1:H:227:GLU:HA	1:H:227:GLU:OE1	2.09	0.51
1:B:355:LYS:NZ	1:B:357:GLY:O	2.41	0.51
1:F:91:LEU:HA	1:F:418:ILE:O	2.10	0.51
1:C:466:PHE:C	1:C:468:ILE:N	2.67	0.51
1:D:306:ASN:CG	1:D:308:GLN:N	2.67	0.51
1:E:214:THR:CG2	1:E:215:ILE:N	2.74	0.51
1:H:226:GLN:NE2	1:H:239:THR:OG1	2.44	0.51
1:H:466:PHE:O	1:H:468:ILE:HG13	2.11	0.51
1:C:322:PHE:HB2	1:C:327:ARG:HD2	1.93	0.51
1:F:216:LYS:HZ2	1:G:452:ASP:CB	2.24	0.51
1:G:97:TRP:HD1	1:G:395:GLN:NE2	2.09	0.51
1:G:126:HIS:HA	1:G:412(D):LEU:HB2	1.92	0.51
1:H:305:PHE:HB3	1:H:312:TYR:HB3	1.93	0.51
1:B:463:GLU:H	1:D:144:HIS:CE1	2.21	0.51
1:D:150:LYS:O	1:D:151:ASP:HB2	2.10	0.51
1:D:318:CYS:HA	1:D:335:SER:O	2.10	0.51
1:H:194:ILE:HG12	1:H:203:ALA:HB2	1.91	0.51
1:H:306:ASN:CG	1:H:308:GLN:H	2.17	0.51
1:F:228:SER:HB3	1:F:350:LYS:HE2	1.92	0.51
1:H:113:ASP:O	1:H:169:PRO:HD2	2.11	0.51
1:A:306:ASN:CG	1:A:308:GLN:N	2.69	0.51
1:A:306:ASN:CG	1:A:308:GLN:H	2.19	0.51
1:E:306:ASN:CG	1:E:308:GLN:H	2.19	0.51
1:F:411:VAL:CG1	1:F:412:GLN:H	2.24	0.51
1:B:224:ARG:NE	1:B:276:GLU:OE1	2.41	0.50
1:B:144:HIS:HE1	1:C:463:GLU:N	2.03	0.50
1:B:287:ILE:N	1:B:287:ILE:CD1	2.73	0.50
1:B:411:VAL:CG1	1:B:412:GLN:H	2.24	0.50
1:D:433:GLU:CD	1:D:464:LEU:HD12	2.36	0.50
1:D:467:THR:O	1:D:468:ILE:HB	2.12	0.50
1:B:214:THR:HB	1:C:451:SER:HB2	1.94	0.50
1:E:411:VAL:CG1	1:E:412:GLN:H	2.24	0.50
1:E:452:ASP:CB	1:G:216:LYS:HD3	2.41	0.50
1:F:298:SER:OG	1:F:344:SER:O	2.29	0.50
1:H:306:ASN:CG	1:H:308:GLN:N	2.69	0.50
1:B:228:SER:HB3	1:B:350:LYS:NZ	2.26	0.50
1:C:121:PHE:CG	1:C:228:SER:HA	2.47	0.50
1:G:381:ASN:O	1:G:385:GLU:CG	2.57	0.50
1:H:355:LYS:HD2	1:H:383:TRP:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:CG	1:A:368:THR:HG23	2.40	0.50
1:A:355:LYS:HD2	1:A:383:TRP:CE2	2.47	0.50
1:D:245:PRO:C	1:D:247:ASN:H	2.17	0.50
1:A:97:TRP:N	1:A:395:GLN:HE22	2.09	0.50
1:E:261:LYS:HB2	1:E:261:LYS:HZ2	1.76	0.50
1:D:117:ILE:O	1:D:440:SER:HA	2.11	0.50
1:D:297:GLY:C	1:D:345(A):GLY:HA3	2.36	0.50
1:D:411:VAL:HG11	1:D:418:ILE:HG23	1.93	0.50
1:G:355:LYS:NZ	1:G:357:GLY:O	2.42	0.50
1:B:355:LYS:HB2	1:B:383:TRP:CE3	2.47	0.50
1:H:228:SER:HB3	1:H:350:LYS:CE	2.42	0.50
1:A:365:THR:HA	1:A:373:GLY:O	2.11	0.49
1:G:238:PHE:CD1	1:G:238:PHE:N	2.80	0.49
1:H:433:GLU:CD	1:H:464:LEU:HD12	2.36	0.49
1:A:452:ASP:CG	1:A:453:THR:H	2.20	0.49
1:E:297:GLY:C	1:E:345(A):GLY:HA3	2.37	0.49
1:F:176:VAL:O	1:F:177:ALA:HB2	2.11	0.49
1:F:411:VAL:CG1	1:F:418:ILE:CG2	2.89	0.49
1:G:224:ARG:NE	1:G:276:GLU:OE1	2.42	0.49
1:G:464:LEU:HB3	1:G:465:PRO:HA	1.94	0.49
1:H:146:ASN:O	1:H:437:ILE:O	2.30	0.49
1:F:144:HIS:CE1	1:G:462:ALA:HA	2.47	0.49
1:F:273:TYR:CD2	1:F:316:TYR:HE1	2.29	0.49
1:H:188:SER:OG	1:H:207:TYR:CE1	2.63	0.49
1:D:184:HIS:HD2	1:D:186:GLY:H	1.60	0.49
1:D:290:VAL:HG11	1:D:353:SER:HB2	1.94	0.49
1:G:322:PHE:CE1	1:G:328:PRO:HG2	2.47	0.49
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.93	0.49
1:B:84:LYS:H	1:B:84:LYS:HD2	1.76	0.49
1:E:184:HIS:HD2	1:E:186:GLY:N	2.06	0.49
1:H:248:GLY:HA2	1:H:295:TRP:CG	2.47	0.49
1:D:360:VAL:HG11	1:D:383:TRP:HE3	1.76	0.49
1:B:355:LYS:HD2	1:B:383:TRP:CE2	2.48	0.49
1:C:102:LYS:NZ	1:C:104:ASN:ND2	2.60	0.49
1:C:147:GLY:HA2	1:C:430:ARG:NH1	2.27	0.49
1:E:316:TYR:CZ	1:E:340:PRO:HG3	2.47	0.49
1:A:147:GLY:C	1:A:149:VAL:H	2.20	0.49
1:B:88:ASN:N	1:B:88:ASN:HD22	2.10	0.49
1:C:366:LYS:HD2	1:C:398:VAL:O	2.13	0.49
1:D:102:LYS:HZ2	1:D:104:ASN:HD21	1.61	0.49
1:A:333:GLY:CA	1:A:386:THR:HG23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASN:HD22	1:B:437:ILE:HB	1.78	0.49
1:D:188:SER:OG	1:D:207:TYR:CE2	2.65	0.49
1:D:327:ARG:HG3	1:D:368:THR:HG23	1.94	0.49
1:E:287:ILE:HD12	1:E:287:ILE:N	2.28	0.49
1:F:413:THR:CG2	1:F:415:LEU:HD22	2.39	0.49
1:D:121:PHE:CG	1:D:228:SER:HA	2.48	0.48
1:F:366:LYS:HD3	1:F:400:ILE:HG12	1.95	0.48
1:B:130:ARG:HG2	1:B:130:ARG:NH2	2.27	0.48
1:B:309:ASN:O	1:B:310:LEU:HB2	2.12	0.48
1:D:88:ASN:HD22	1:D:88:ASN:H	1.61	0.48
1:D:386:THR:O	1:D:386:THR:HG22	2.14	0.48
1:E:261:LYS:HB2	1:E:261:LYS:HZ3	1.78	0.48
1:D:203:ALA:HB3	1:D:215:ILE:HB	1.95	0.48
1:C:386:THR:HG22	1:C:386:THR:O	2.12	0.48
1:A:84:LYS:H	1:A:84:LYS:HD2	1.79	0.48
1:B:106:ILE:HD12	1:B:460:ASP:OD2	2.14	0.48
1:B:375:GLU:OE1	1:B:394:LYS:HE3	2.14	0.48
1:C:430:ARG:HD2	1:C:436:THR:O	2.13	0.48
1:D:229:GLU:OE1	1:D:410:PHE:HA	2.12	0.48
1:E:147:GLY:C	1:E:149:VAL:H	2.21	0.48
1:G:97:TRP:N	1:G:395:GLN:HE22	2.11	0.48
1:G:430:ARG:HD2	1:G:436:THR:O	2.13	0.48
1:H:325:ASN:O	1:H:348:GLY:HA2	2.13	0.48
1:C:207:TYR:O	1:C:210:ILE:HG12	2.14	0.48
1:C:224:ARG:NE	1:C:276:GLU:OE1	2.42	0.48
1:E:366:LYS:HD2	1:E:398:VAL:O	2.13	0.48
1:F:97:TRP:N	1:F:395:GLN:HE22	2.07	0.48
1:G:88:ASN:N	1:G:88:ASN:HD22	2.11	0.48
1:G:413:THR:CG2	1:G:415:LEU:HD13	2.37	0.48
1:A:183:CYS:HB3	1:A:230:CYS:O	2.14	0.48
1:E:248:GLY:HA2	1:E:295:TRP:CG	2.49	0.48
1:F:322:PHE:HB2	1:F:327:ARG:HD2	1.94	0.48
1:G:222:ILE:O	1:G:224:ARG:NH2	2.44	0.48
1:G:254:ILE:HD11	1:G:268:LEU:HD21	1.94	0.48
1:H:327:ARG:C	1:H:368:THR:HG23	2.38	0.48
1:A:89:SER:HG	1:A:417:CYS:HA	1.74	0.48
1:D:97:TRP:HD1	1:D:395:GLN:HE22	1.58	0.48
1:D:147:GLY:O	1:D:149:VAL:N	2.42	0.48
1:E:305:PHE:HB3	1:E:312:TYR:HB3	1.96	0.48
1:E:396:ASP:C	1:E:397:ILE:HD12	2.39	0.48
1:H:375:GLU:OE1	1:H:394:LYS:HE3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:VAL:HG12	1:B:394:LYS:N	2.28	0.48
1:B:421:CYS:HB3	1:B:446:PHE:O	2.13	0.48
1:D:84:LYS:HD2	1:D:84:LYS:H	1.79	0.48
1:D:91:LEU:HA	1:D:418:ILE:O	2.14	0.48
1:F:249:GLN:HE21	1:F:272:ASN:N	2.09	0.48
1:B:301:PRO:HB3	1:B:316:TYR:CZ	2.49	0.47
1:B:426:LEU:HD13	1:B:460:ASP:N	2.29	0.47
1:E:327:ARG:O	1:E:368:THR:HG21	2.01	0.47
1:G:158:LEU:HD22	1:G:180:ALA:HB1	1.95	0.47
1:A:224:ARG:NH1	1:A:276:GLU:OE1	2.45	0.47
1:D:287:ILE:O	1:D:304:SER:HA	2.14	0.47
1:D:411:VAL:CG1	1:D:412:GLN:N	2.76	0.47
1:A:224:ARG:NE	1:A:276:GLU:OE1	2.44	0.47
1:E:203:ALA:HB3	1:E:215:ILE:HB	1.96	0.47
1:E:333:GLY:C	1:E:386:THR:HG23	2.39	0.47
1:E:345:ASN:C	1:E:346:ALA:H	2.21	0.47
1:A:149:VAL:HG23	1:A:430:ARG:NH1	2.28	0.47
1:B:448:GLY:O	1:B:449:VAL:HB	2.13	0.47
1:D:99:VAL:HG13	1:D:446:PHE:CE2	2.50	0.47
1:E:91:LEU:N	1:E:283:ASN:ND2	2.60	0.47
1:A:466:PHE:C	1:A:468:ILE:H	2.22	0.47
1:B:116:VAL:HG12	1:B:138:ALA:O	2.15	0.47
1:E:158:LEU:O	1:E:174:GLU:HB2	2.15	0.47
1:G:118:ARG:HB2	1:G:156:ARG:NH1	2.29	0.47
1:D:254:ILE:CD1	1:D:268:LEU:HD21	2.45	0.47
1:F:136:GLN:O	1:G:107:ARG:NH1	2.43	0.47
1:F:316:TYR:CZ	1:F:340:PRO:HG3	2.50	0.47
1:A:316:TYR:CZ	1:A:340:PRO:HG3	2.50	0.47
1:B:225:THR:HB	1:B:241:MET:HE2	1.97	0.47
1:C:332:THR:HG23	1:C:386:THR:HG22	1.97	0.47
1:D:96:GLY:O	1:D:448:GLY:O	2.33	0.47
1:D:320:GLY:HA3	1:D:331:GLY:O	2.15	0.47
1:D:412:GLN:HB2	1:D:419:ARG:HB3	1.97	0.47
1:E:327:ARG:C	1:E:368:THR:HG23	2.40	0.47
1:E:448:GLY:O	1:E:449:VAL:HB	2.15	0.47
1:G:301:PRO:HB3	1:G:316:TYR:CZ	2.50	0.47
1:G:381:ASN:CB	1:G:385:GLU:HG3	2.38	0.47
1:H:411:VAL:HG13	1:H:418:ILE:HG23	1.96	0.47
1:A:147:GLY:HA2	1:A:430:ARG:NH1	2.24	0.47
1:B:275:TYR:CE2	1:B:303:VAL:CG2	2.98	0.47
1:C:88:ASN:HD22	1:C:88:ASN:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLU:OE1	1:C:350:LYS:HB2	2.14	0.47
1:E:264:LYS:HG2	1:E:310:LEU:HD22	1.96	0.47
1:E:345:ASN:O	1:E:346:ALA:N	2.44	0.47
1:G:249:GLN:HE21	1:G:272:ASN:N	2.13	0.47
1:G:412(B):PRO:HB3	1:G:415:LEU:O	2.15	0.47
1:C:433:GLU:CD	1:C:464:LEU:HD12	2.40	0.47
1:D:355:LYS:HB2	1:D:383:TRP:CZ3	2.50	0.47
1:E:102:LYS:HZ2	1:E:104:ASN:ND2	2.13	0.47
1:F:249:GLN:NE2	1:F:272:ASN:N	2.60	0.47
1:F:411:VAL:HG13	1:F:418:ILE:CG2	2.45	0.47
1:A:421:CYS:HB3	1:A:446:PHE:O	2.15	0.47
1:C:239:THR:HG22	1:C:257:MET:CE	2.45	0.47
1:E:102:LYS:HZ2	1:E:104:ASN:HD21	1.63	0.47
1:E:226:GLN:O	1:E:227:GLU:HB2	2.14	0.47
1:G:275:TYR:CE2	1:G:303:VAL:CG2	2.97	0.47
1:H:295:TRP:O	1:H:346:ALA:HA	2.14	0.47
1:A:327:ARG:C	1:A:368:THR:HG23	2.34	0.46
1:B:248:GLY:HA2	1:B:295:TRP:CG	2.49	0.46
1:C:238:PHE:N	1:C:238:PHE:CD1	2.83	0.46
1:E:91:LEU:HG	1:E:283:ASN:ND2	2.31	0.46
1:E:102:LYS:NZ	1:E:104:ASN:ND2	2.63	0.46
1:H:117:ILE:O	1:H:440:SER:HA	2.14	0.46
1:A:403:TRP:CZ3	1:A:432:LYS:HG3	2.50	0.46
1:B:149:VAL:HG23	1:B:430:ARG:NH1	2.30	0.46
1:B:190:LEU:HD13	1:B:260:GLY:HA2	1.97	0.46
1:B:238:PHE:N	1:B:238:PHE:CD1	2.83	0.46
1:B:332:THR:HG23	1:B:386:THR:CG2	2.46	0.46
1:C:109:GLY:HA3	1:C:140:LEU:HD12	1.97	0.46
1:E:146:ASN:HA	1:E:437:ILE:CD1	2.45	0.46
1:E:147:GLY:HA2	1:E:430:ARG:HH12	1.80	0.46
1:E:333:GLY:N	1:E:386:THR:HG23	2.30	0.46
1:F:156:ARG:HG2	1:F:178:TRP:HA	1.97	0.46
1:G:202:VAL:HG23	1:G:214:THR:HG23	1.97	0.46
1:C:118:ARG:HB3	1:C:119:GLU:CD	2.41	0.46
1:C:466:PHE:C	1:C:468:ILE:H	2.23	0.46
1:E:406:TYR:HB2	1:E:425:GLU:OE1	2.15	0.46
1:E:413:THR:HA	1:G:210:ILE:HD12	1.97	0.46
1:F:85:LEU:HD12	1:F:412(C):GLU:HG3	1.97	0.46
1:G:359:GLY:HA2	1:G:382:GLY:H	1.81	0.46
1:D:248:GLY:HA2	1:D:295:TRP:CG	2.50	0.46
1:E:117:ILE:O	1:E:440:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:HG12	1:A:203:ALA:HB2	1.97	0.46
1:C:143:LYS:C	1:C:145:SER:H	2.22	0.46
1:C:249:GLN:NE2	1:C:272:ASN:H	2.14	0.46
1:D:85:LEU:HD13	1:D:186:GLY:HA2	1.98	0.46
1:E:274:HIS:HB2	1:E:295:TRP:HE3	1.81	0.46
1:E:421:CYS:HB3	1:E:446:PHE:O	2.16	0.46
1:G:270:ALA:HB1	1:G:273:TYR:HB2	1.98	0.46
1:H:275:TYR:CE2	1:H:303:VAL:HG23	2.51	0.46
1:H:412:GLN:HB2	1:H:419:ARG:HB3	1.98	0.46
1:H:448:GLY:O	1:H:449:VAL:HB	2.14	0.46
1:A:173:PHE:CG	1:D:164:GLY:HA3	2.51	0.46
1:A:452:ASP:CB	1:C:216:LYS:HD3	2.41	0.46
1:C:396:ASP:C	1:C:397:ILE:HD12	2.41	0.46
1:D:97:TRP:H	1:D:395:GLN:HE22	1.64	0.46
1:D:430:ARG:HD2	1:D:436:THR:O	2.15	0.46
1:E:96:GLY:O	1:E:448:GLY:O	2.33	0.46
1:F:149:VAL:HG22	1:F:439:THR:OG1	2.16	0.46
1:G:224:ARG:NH1	1:G:276:GLU:OE1	2.45	0.46
1:A:117:ILE:HG22	1:A:135:THR:HA	1.97	0.46
1:C:258:GLU:O	1:C:259:LYS:C	2.59	0.46
1:D:146:ASN:ND2	1:D:437:ILE:HB	2.31	0.46
1:E:88:ASN:ND2	1:E:88:ASN:N	2.61	0.46
1:E:146:ASN:HA	1:E:437:ILE:HD12	1.97	0.46
1:E:375:GLU:OE1	1:E:394:LYS:HE3	2.15	0.46
1:G:102:LYS:NZ	1:G:104:ASN:ND2	2.64	0.46
1:H:202:VAL:CG2	1:H:214:THR:HG23	2.46	0.46
1:H:381:ASN:O	1:H:385:GLU:HB2	2.16	0.46
1:A:84:LYS:HD2	1:A:84:LYS:N	2.31	0.46
1:B:118:ARG:HB3	1:B:119:GLU:CD	2.41	0.46
1:C:239:THR:HG22	1:C:257:MET:HE1	1.98	0.46
1:C:327:ARG:O	1:C:368:THR:HG21	2.05	0.46
1:D:88:ASN:HD22	1:D:88:ASN:N	2.12	0.46
1:H:85:LEU:HD13	1:H:186:GLY:CA	2.46	0.46
1:H:118:ARG:NE	1:H:425:GLU:OE2	2.35	0.46
1:H:248:GLY:HA2	1:H:295:TRP:CD1	2.51	0.46
1:H:332:THR:HG23	1:H:386:THR:HG21	1.98	0.46
1:A:202:VAL:CG1	1:D:454:VAL:HG22	2.45	0.46
1:B:88:ASN:H	1:B:88:ASN:ND2	2.14	0.46
1:B:146:ASN:O	1:B:437:ILE:O	2.34	0.46
1:B:327:ARG:C	1:B:368:THR:HG23	2.40	0.46
1:E:466:PHE:O	1:E:468:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:ALA:HA	1:G:190:LEU:O	2.16	0.46
1:A:453:THR:O	1:A:454:VAL:HG13	2.16	0.46
1:B:184:HIS:CD2	1:B:186:GLY:H	2.34	0.46
1:G:248:GLY:HA2	1:G:295:TRP:CD1	2.51	0.46
1:H:156:ARG:HB3	1:H:177:ALA:O	2.15	0.46
1:H:270:ALA:HB1	1:H:273:TYR:HB2	1.98	0.46
1:A:172:ARG:HD2	1:A:174:GLU:OE1	2.15	0.45
1:C:88:ASN:H	1:C:88:ASN:ND2	2.14	0.45
1:D:381:ASN:H	1:D:381:ASN:HD22	1.58	0.45
1:F:147:GLY:C	1:F:149:VAL:H	2.24	0.45
1:A:226:GLN:HE22	1:A:230:CYS:HA	1.82	0.45
1:D:333:GLY:H	1:D:386:THR:HG23	1.82	0.45
1:F:118:ARG:HB3	1:F:119:GLU:CD	2.41	0.45
1:H:102:LYS:HZ2	1:H:104:ASN:HD21	1.65	0.45
1:A:333:GLY:C	1:A:386:THR:HG23	2.41	0.45
1:D:249:GLN:NE2	1:D:272:ASN:H	2.14	0.45
1:H:85:LEU:HD13	1:H:186:GLY:HA2	1.98	0.45
1:B:192:ILE:CD1	1:B:257:MET:HE1	2.37	0.45
1:B:226:GLN:HE22	1:B:230:CYS:HA	1.81	0.45
1:C:421:CYS:HB3	1:C:446:PHE:O	2.17	0.45
1:F:184:HIS:CD2	1:F:186:GLY:H	2.34	0.45
1:G:91:LEU:HA	1:G:418:ILE:O	2.17	0.45
1:E:225:THR:OG1	1:E:226:GLN:N	2.49	0.45
1:A:297:GLY:C	1:A:345(A):GLY:HA3	2.41	0.45
1:B:232:CYS:HA	1:B:237:CYS:HA	1.99	0.45
1:C:275:TYR:CE2	1:C:303:VAL:HG22	2.51	0.45
1:D:290:VAL:HG21	1:D:353:SER:HB2	1.97	0.45
1:F:297:GLY:C	1:F:345(A):GLY:HA3	2.42	0.45
1:G:322:PHE:CD1	1:G:328:PRO:HG2	2.52	0.45
1:A:413:THR:HA	1:C:210:ILE:HD12	1.99	0.45
1:B:102:LYS:HG3	1:B:444:ILE:HG22	1.99	0.45
1:D:276:GLU:O	1:D:292:ARG:HB3	2.17	0.45
1:E:430:ARG:HD2	1:E:436:THR:O	2.17	0.45
1:G:150:LYS:HE3	1:G:153:SER:HB3	1.98	0.45
1:A:248:GLY:HA2	1:A:295:TRP:CD1	2.51	0.45
1:F:145:SER:O	1:F:146:ASN:O	2.34	0.45
1:B:277:GLU:OE2	1:B:406:TYR:OH	2.34	0.45
1:B:452:ASP:CB	1:D:216:LYS:HZ2	2.29	0.45
1:D:199:ASN:C	1:D:199:ASN:OD1	2.60	0.45
1:E:467:THR:O	1:E:468:ILE:HB	2.16	0.45
1:F:143:LYS:C	1:F:145:SER:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:GLY:C	1:G:149:VAL:H	2.24	0.45
1:A:97:TRP:N	1:A:453:THR:HG21	2.32	0.45
1:A:218:TRP:CE2	1:A:253:LYS:HE3	2.52	0.45
1:B:411:VAL:HG13	1:B:418:ILE:HG23	1.96	0.45
1:C:327:ARG:C	1:C:368:THR:HG23	2.42	0.45
1:A:102:LYS:NZ	1:A:104:ASN:ND2	2.65	0.44
1:A:254:ILE:HD13	1:A:305:PHE:CD2	2.52	0.44
1:B:261:LYS:HB2	1:B:261:LYS:HZ2	1.80	0.44
1:C:85:LEU:HD13	1:C:186:GLY:HA2	2.00	0.44
1:C:428:ARG:HB3	1:C:464:LEU:HD11	1.97	0.44
1:H:248:GLY:HA2	1:H:295:TRP:CD2	2.52	0.44
1:A:232:CYS:HA	1:A:237:CYS:HA	1.99	0.44
1:B:202:VAL:HG23	1:B:214:THR:HG23	1.98	0.44
1:G:147:GLY:HA2	1:G:430:ARG:NH1	2.26	0.44
1:H:91:LEU:HG	1:H:283:ASN:ND2	2.32	0.44
1:B:99:VAL:HA	1:B:446:PHE:CD2	2.52	0.44
1:C:306:ASN:CG	1:C:308:GLN:N	2.74	0.44
1:C:325:ASN:HA	1:C:326:PRO:C	2.42	0.44
1:D:102:LYS:NZ	1:D:104:ASN:ND2	2.65	0.44
1:D:261:LYS:HB2	1:D:261:LYS:HZ3	1.80	0.44
1:E:466:PHE:O	1:E:468:ILE:HG13	2.17	0.44
1:A:287:ILE:O	1:A:304:SER:HA	2.17	0.44
1:C:380:PRO:O	1:C:381:ASN:C	2.60	0.44
1:D:355:LYS:HB2	1:D:383:TRP:CE3	2.52	0.44
1:E:214:THR:HB	1:H:451:SER:HG	1.79	0.44
1:E:217:SER:OG	1:E:243:ASP:OD1	2.35	0.44
1:G:333:GLY:N	1:G:386:THR:CG2	2.81	0.44
1:G:411:VAL:HG12	1:G:412:GLN:C	2.42	0.44
1:H:412:GLN:NE2	1:H:421:CYS:SG	2.90	0.44
1:D:298:SER:OG	1:D:344:SER:O	2.33	0.44
1:E:216:LYS:HZ2	1:H:452:ASP:CB	2.30	0.44
1:F:88:ASN:N	1:F:88:ASN:HD22	2.14	0.44
1:F:333:GLY:C	1:F:386:THR:HG23	2.43	0.44
1:G:248:GLY:HA2	1:G:295:TRP:CG	2.52	0.44
1:H:411:VAL:HG12	1:H:412:GLN:C	2.42	0.44
1:B:168:SER:OG	1:B:169:PRO:HD2	2.18	0.44
1:C:162:PRO:HG2	1:C:165:GLU:OE2	2.16	0.44
1:D:146:ASN:HD22	1:D:437:ILE:HB	1.82	0.44
1:E:254:ILE:HD13	1:E:305:PHE:CD2	2.53	0.44
1:B:264:LYS:HG2	1:B:310:LEU:HD22	1.99	0.44
1:C:147:GLY:C	1:C:149:VAL:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ILE:HG23	1:D:205:LEU:CD2	2.48	0.44
1:E:447:CYS:HB2	1:G:211:ILE:HD12	1.99	0.44
1:G:122:ILE:HG22	1:G:123:SER:N	2.31	0.44
1:G:192:ILE:HG23	1:G:205:LEU:CD2	2.48	0.44
1:G:368:THR:HG22	1:G:368:THR:O	2.17	0.44
1:F:321:VAL:HG13	1:F:364:ARG:NH2	2.33	0.44
1:G:375:GLU:OE2	1:G:377:ILE:HD11	2.17	0.44
1:G:119:GLU:HB2	1:G:134:LEU:HD12	2.00	0.44
1:B:144:HIS:CE1	1:C:462:ALA:HA	2.53	0.43
1:C:316:TYR:CE1	1:C:340:PRO:HG3	2.53	0.43
1:E:456:TRP:CG	1:E:457:SER:H	2.36	0.43
1:G:118:ARG:HB3	1:G:119:GLU:OE2	2.18	0.43
1:A:325:ASN:O	1:A:348:GLY:HA2	2.18	0.43
1:B:88:ASN:HD22	1:B:88:ASN:H	1.64	0.43
1:B:355:LYS:HB2	1:B:383:TRP:CZ3	2.53	0.43
1:C:373:GLY:HA2	1:C:398:VAL:HG12	2.00	0.43
1:E:97:TRP:HD1	1:E:395:GLN:NE2	2.16	0.43
1:A:156:ARG:HG2	1:A:178:TRP:HA	1.99	0.43
1:A:287:ILE:N	1:A:287:ILE:CD1	2.82	0.43
1:B:380:PRO:O	1:B:381:ASN:C	2.59	0.43
1:D:264:LYS:HG2	1:D:310:LEU:HD22	1.99	0.43
1:F:99:VAL:HG13	1:F:446:PHE:CE2	2.53	0.43
1:F:116:VAL:CG1	1:F:136:GLN:HB2	2.46	0.43
1:G:113:ASP:O	1:G:169:PRO:HD2	2.18	0.43
1:G:297:GLY:C	1:G:345(A):GLY:HA3	2.43	0.43
1:H:219:ARG:HB2	1:H:243:ASP:CG	2.43	0.43
1:C:248:GLY:HA2	1:C:295:TRP:CD2	2.54	0.43
1:D:97:TRP:CD1	1:D:395:GLN:HE22	2.36	0.43
1:F:173:PHE:CG	1:G:164:GLY:HA3	2.53	0.43
1:F:381:ASN:O	1:F:385:GLU:HB2	2.19	0.43
1:A:232:CYS:HA	1:A:236:SER:O	2.19	0.43
1:C:102:LYS:HG3	1:C:444:ILE:HG22	2.01	0.43
1:E:84:LYS:HD2	1:E:84:LYS:N	2.33	0.43
1:E:143:LYS:C	1:E:145:SER:H	2.26	0.43
1:E:433:GLU:CD	1:E:464:LEU:HD12	2.43	0.43
1:H:364:ARG:HG3	1:H:365:THR:O	2.17	0.43
1:A:421:CYS:HA	1:A:447:CYS:HA	2.00	0.43
1:B:133:PHE:CE1	1:B:159:MET:HB2	2.54	0.43
1:C:222:ILE:O	1:C:224:ARG:NH2	2.50	0.43
1:E:325:ASN:O	1:E:348:GLY:HA2	2.18	0.43
1:E:412(B):PRO:HB3	1:E:415:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:ILE:HG23	1:F:205:LEU:CD2	2.49	0.43
1:B:396:ASP:C	1:B:397:ILE:HD12	2.44	0.43
1:F:143:LYS:C	1:F:145:SER:N	2.76	0.43
1:F:386:THR:O	1:F:387:ASP:HB3	2.18	0.43
1:G:355:LYS:HD2	1:G:383:TRP:CD2	2.54	0.43
1:A:169:PRO:HG2	1:A:169(A):TYR:CE2	2.53	0.43
1:A:451:SER:OG	1:C:214:THR:HB	2.19	0.43
1:B:396:ASP:O	1:B:397:ILE:HD12	2.18	0.43
1:C:146:ASN:O	1:C:437:ILE:O	2.36	0.43
1:E:446:PHE:CD1	1:E:446:PHE:N	2.86	0.43
1:E:463:GLU:N	1:G:144:HIS:HE1	2.07	0.43
1:F:426:LEU:HD13	1:F:460:ASP:N	2.34	0.43
1:F:437:ILE:HD13	1:F:468:ILE:HG23	2.00	0.43
1:G:250:ALA:HB3	1:G:252:TYR:CE2	2.52	0.43
1:A:91:LEU:HA	1:A:418:ILE:O	2.19	0.43
1:D:411:VAL:HG13	1:D:418:ILE:HG23	2.00	0.43
1:F:287:ILE:O	1:F:304:SER:HA	2.18	0.43
1:F:366:LYS:NZ	1:F:396:ASP:OD1	2.46	0.43
1:G:411:VAL:HG11	1:G:418:ILE:HG23	1.99	0.43
1:B:332:THR:HG23	1:B:386:THR:HG22	2.00	0.43
1:E:463:GLU:HG3	1:G:143:LYS:HZ1	1.84	0.43
1:G:249:GLN:HG2	1:G:295:TRP:CH2	2.54	0.43
1:H:332:THR:HG23	1:H:386:THR:CG2	2.48	0.43
1:A:162:PRO:HG2	1:A:165:GLU:OE2	2.17	0.42
1:B:276:GLU:CD	2:B:801:G39:H92	2.44	0.42
1:C:287:ILE:HD12	1:C:287:ILE:N	2.34	0.42
1:D:364:ARG:O	1:D:374:PHE:HA	2.19	0.42
1:F:106:ILE:HD13	1:F:428:ARG:HB2	2.01	0.42
1:F:116:VAL:HG12	1:F:138:ALA:O	2.19	0.42
1:F:219:ARG:HB2	1:F:243:ASP:CG	2.44	0.42
1:H:266:VAL:HG23	1:H:310:LEU:HD23	2.00	0.42
1:D:222:ILE:O	1:D:224:ARG:NH2	2.51	0.42
1:G:217:SER:HB2	1:G:223:LEU:HB2	2.01	0.42
1:H:168:SER:OG	1:H:169:PRO:HD2	2.19	0.42
1:H:298:SER:OG	1:H:344:SER:O	2.35	0.42
1:A:368:THR:CG2	1:A:368:THR:O	2.66	0.42
1:E:85:LEU:CD1	1:E:412(C):GLU:HG3	2.44	0.42
1:E:116:VAL:HG12	1:E:138:ALA:C	2.45	0.42
1:F:248:GLY:HA2	1:F:295:TRP:CG	2.54	0.42
1:F:261:LYS:HB2	1:F:261:LYS:HZ3	1.84	0.42
1:G:287:ILE:N	1:G:287:ILE:CD1	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASN:O	1:C:346:ALA:O	2.37	0.42
1:C:332:THR:HG23	1:C:386:THR:HG21	2.01	0.42
1:D:88:ASN:H	1:D:88:ASN:ND2	2.17	0.42
1:F:146:ASN:HB3	1:F:147:GLY:H	1.69	0.42
1:G:249:GLN:NE2	1:G:272:ASN:H	2.16	0.42
1:H:90:SER:O	1:H:417:CYS:HB2	2.19	0.42
1:B:216:LYS:NZ	1:C:452:ASP:HB3	2.28	0.42
1:B:306:ASN:CG	1:B:308:GLN:N	2.77	0.42
1:C:88:ASN:N	1:C:88:ASN:ND2	2.67	0.42
1:C:412(C):GLU:CD	1:C:412(C):GLU:H	2.27	0.42
1:E:325:ASN:HA	1:E:326:PRO:C	2.43	0.42
1:E:355:LYS:HD2	1:E:383:TRP:CE2	2.54	0.42
1:F:325:ASN:HA	1:F:326:PRO:C	2.44	0.42
1:G:162:PRO:HG2	1:G:165:GLU:CD	2.44	0.42
1:G:412:GLN:OE1	1:G:419:ARG:HD2	2.19	0.42
1:G:426:LEU:HD13	1:G:460:ASP:N	2.35	0.42
1:H:368:THR:HG22	1:H:368:THR:O	2.18	0.42
1:A:210:ILE:HD12	1:D:413:THR:HA	2.01	0.42
1:B:232:CYS:HA	1:B:236:SER:O	2.20	0.42
1:D:147:GLY:C	1:D:149:VAL:N	2.78	0.42
1:D:303:VAL:HG13	1:D:314:ILE:HG22	2.01	0.42
1:D:325:ASN:O	1:D:348:GLY:HA2	2.20	0.42
1:E:107:ARG:HD2	1:E:461:GLY:HA3	2.02	0.42
1:E:149:VAL:HG21	1:E:430:ARG:CZ	2.50	0.42
1:E:154:PRO:HG3	1:H:456:TRP:CH2	2.55	0.42
1:E:190:LEU:HD13	1:E:260:GLY:HA2	2.02	0.42
1:G:194:ILE:HG12	1:G:203:ALA:HB2	2.00	0.42
1:G:360:VAL:HG13	1:G:383:TRP:HB2	2.00	0.42
1:B:102:LYS:HZ2	1:D:155:HIS:HD2	1.66	0.42
1:C:456:TRP:CG	1:C:457:SER:H	2.38	0.42
1:D:238:PHE:CD1	1:D:238:PHE:N	2.88	0.42
1:H:453:THR:C	1:H:454:VAL:HG13	2.45	0.42
1:C:91:LEU:HA	1:C:418:ILE:O	2.20	0.42
1:D:383:TRP:HD1	1:D:384:THR:HG23	1.84	0.42
1:E:164:GLY:HA3	1:G:173:PHE:CG	2.55	0.42
1:A:85:LEU:HD13	1:A:186:GLY:CA	2.50	0.42
1:A:347:TYR:CG	1:A:348:GLY:N	2.87	0.42
1:B:368:THR:HG22	1:B:368:THR:O	2.19	0.42
1:C:88:ASN:HD22	1:C:89:SER:N	2.17	0.42
1:C:309:ASN:O	1:C:310:LEU:HB2	2.19	0.42
1:D:188:SER:OG	1:D:207:TYR:CE1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:SER:HA	1:G:173:PHE:CZ	2.55	0.42
1:F:84:LYS:HD2	1:F:84:LYS:N	2.33	0.42
1:F:412(B):PRO:HB3	1:F:415:LEU:O	2.20	0.42
1:A:354:PHE:CZ	1:A:409:SER:HB2	2.55	0.41
1:B:245:PRO:C	1:B:247:ASN:H	2.23	0.41
1:B:322:PHE:HB2	1:B:327:ARG:HD2	2.02	0.41
1:C:229:GLU:OE1	1:C:410:PHE:HA	2.20	0.41
1:C:392:VAL:HG12	1:C:394:LYS:N	2.34	0.41
1:D:448:GLY:O	1:D:449:VAL:HB	2.20	0.41
1:D:456:TRP:CG	1:D:457:SER:H	2.38	0.41
1:F:305:PHE:HB3	1:F:312:TYR:HB3	2.02	0.41
1:G:433:GLU:CD	1:G:464:LEU:HD12	2.45	0.41
1:H:396:ASP:C	1:H:397:ILE:HD12	2.45	0.41
1:A:275:TYR:CE2	1:A:303:VAL:HG23	2.55	0.41
1:D:287:ILE:N	1:D:287:ILE:CD1	2.83	0.41
1:D:466:PHE:O	1:D:468:ILE:N	2.53	0.41
1:F:229:GLU:OE1	1:F:410:PHE:HA	2.20	0.41
1:C:158:LEU:O	1:C:174:GLU:HB2	2.20	0.41
1:C:172:ARG:HD2	1:C:174:GLU:OE1	2.20	0.41
1:C:232:CYS:HA	1:C:237:CYS:HA	2.02	0.41
1:D:433:GLU:OE1	1:D:464:LEU:HD12	2.21	0.41
1:E:150:LYS:O	1:E:151:ASP:CB	2.65	0.41
1:F:290:VAL:HG21	1:F:353:SER:HB2	2.02	0.41
1:F:412:GLN:HB2	1:F:419:ARG:HB3	2.02	0.41
1:H:238:PHE:CD1	1:H:238:PHE:N	2.88	0.41
1:A:116:VAL:CG1	1:A:136:GLN:HB2	2.44	0.41
1:B:463:GLU:O	1:B:463:GLU:HG3	2.19	0.41
1:D:105:SER:HB3	1:D:167:PRO:HD2	2.02	0.41
1:D:252:TYR:OH	1:D:274:HIS:HA	2.19	0.41
1:E:322:PHE:HB2	1:E:327:ARG:HD2	2.03	0.41
1:F:287:ILE:N	1:F:287:ILE:CD1	2.83	0.41
1:A:249:GLN:HE21	1:A:272:ASN:N	2.17	0.41
1:B:149:VAL:CG2	1:B:430:ARG:NH1	2.83	0.41
1:B:256:LYS:C	1:B:257:MET:HG2	2.41	0.41
1:D:360:VAL:CG1	1:D:383:TRP:HB2	2.45	0.41
1:A:316:TYR:HB2	1:A:336:CYS:O	2.21	0.41
1:B:169:PRO:HG2	1:B:169(A):TYR:CE2	2.56	0.41
1:D:366:LYS:HD2	1:D:398:VAL:O	2.19	0.41
1:D:412:GLN:CD	1:D:419:ARG:CD	2.92	0.41
1:E:354:PHE:CZ	1:E:409:SER:HB2	2.56	0.41
1:F:104:ASN:O	1:F:108:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:O	1:B:440:SER:HA	2.21	0.41
1:B:360:VAL:HG12	1:B:383:TRP:HE3	1.84	0.41
1:C:464:LEU:HB3	1:C:465:PRO:HA	2.02	0.41
1:F:219:ARG:HD3	1:F:219:ARG:HA	1.92	0.41
1:G:219:ARG:HB2	1:G:243:ASP:CG	2.46	0.41
1:A:216:LYS:CD	1:D:452:ASP:HB3	2.44	0.41
1:A:333:GLY:N	1:A:386:THR:CG2	2.84	0.41
1:A:466:PHE:O	1:A:468:ILE:HG13	2.21	0.41
1:B:162:PRO:HG2	1:B:165:GLU:OE2	2.19	0.41
1:C:411:VAL:HG13	1:C:418:ILE:CG2	2.51	0.41
1:D:270:ALA:HB1	1:D:273:TYR:HB2	2.03	0.41
1:E:146:ASN:HA	1:E:437:ILE:HG13	2.03	0.41
1:E:224:ARG:NH1	1:E:276:GLU:OE1	2.52	0.41
1:G:84:LYS:H	1:G:84:LYS:CD	2.33	0.41
1:G:146:ASN:O	1:G:437:ILE:O	2.39	0.41
1:A:396:ASP:C	1:A:397:ILE:HD12	2.46	0.41
1:C:118:ARG:HB2	1:C:156:ARG:NH1	2.35	0.41
1:C:149:VAL:HG22	1:C:439:THR:OG1	2.21	0.41
1:C:275:TYR:CE2	1:C:303:VAL:CG2	3.03	0.41
1:D:146:ASN:HD22	1:D:146:ASN:HA	1.64	0.41
1:D:219:ARG:HB2	1:D:243:ASP:CG	2.46	0.41
1:D:248:GLY:HA2	1:D:295:TRP:CD2	2.55	0.41
1:E:162:PRO:HG2	1:E:165:GLU:OE2	2.21	0.41
1:E:275:TYR:CZ	1:E:303:VAL:CG2	3.04	0.41
1:E:333:GLY:O	1:E:386:THR:HG23	2.20	0.41
1:E:411:VAL:HG12	1:E:412:GLN:H	1.80	0.41
1:G:248:GLY:HA2	1:G:295:TRP:CD2	2.56	0.41
1:H:91:LEU:H	1:H:283:ASN:ND2	2.19	0.41
1:A:144:HIS:CE1	1:D:463:GLU:H	2.18	0.41
1:E:271:PRO:O	1:E:272:ASN:HB3	2.21	0.41
1:H:105:SER:HB3	1:H:167:PRO:HD2	2.02	0.41
1:A:274:HIS:CE1	1:A:276:GLU:OE2	2.73	0.40
1:A:277:GLU:OE1	1:A:350:LYS:HB2	2.21	0.40
1:A:333:GLY:H	1:A:386:THR:HG23	1.86	0.40
1:A:413:THR:CG2	1:A:415:LEU:HD13	2.41	0.40
1:B:147:GLY:C	1:B:149:VAL:H	2.29	0.40
1:B:172:ARG:HD2	1:B:174:GLU:OE1	2.22	0.40
1:B:293:ASP:OD2	1:B:293:ASP:C	2.64	0.40
1:D:162:PRO:CG	1:D:165:GLU:OE2	2.68	0.40
1:D:182:ALA:O	1:D:229:GLU:HA	2.21	0.40
1:G:117:ILE:O	1:G:440:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:MET:HG2	1:G:173:PHE:HA	2.02	0.40
1:G:241:MET:HB2	1:G:255:PHE:HE1	1.86	0.40
1:G:298:SER:OG	1:G:344:SER:O	2.36	0.40
1:B:231:ALA:O	1:B:237:CYS:HA	2.20	0.40
1:B:248:GLY:HA2	1:B:295:TRP:CE2	2.55	0.40
1:G:142:ASP:OD2	1:G:144:HIS:HD2	2.04	0.40
1:G:146:ASN:HB3	1:G:147:GLY:H	1.67	0.40
1:G:433:GLU:OE2	1:G:464:LEU:HD12	2.20	0.40
1:A:169:PRO:HG2	1:A:169(A):TYR:CD2	2.57	0.40
1:A:184:HIS:CD2	1:A:186:GLY:H	2.28	0.40
1:A:381:ASN:O	1:A:385:GLU:HB2	2.20	0.40
1:B:207:TYR:O	1:B:210:ILE:HG12	2.19	0.40
1:C:252:TYR:OH	1:C:274:HIS:HA	2.21	0.40
1:D:113:ASP:O	1:D:169:PRO:HD2	2.21	0.40
1:F:214:THR:HG22	1:G:451:SER:HB2	2.02	0.40
1:A:452:ASP:HB3	1:C:216:LYS:CD	2.42	0.40
1:B:84:LYS:HD2	1:B:84:LYS:N	2.36	0.40
1:E:271:PRO:O	1:E:272:ASN:CB	2.70	0.40
1:H:143:LYS:C	1:H:145:SER:N	2.74	0.40
1:A:295:TRP:CD1	1:A:295:TRP:C	2.99	0.40
1:B:386:THR:HG22	1:B:386:THR:O	2.21	0.40
1:D:116:VAL:HG23	1:D:440:SER:HB2	2.03	0.40
1:E:216:LYS:HZ2	1:H:452:ASP:HB3	1.85	0.40
1:F:452:ASP:HB3	1:H:216:LYS:CD	2.45	0.40
1:H:287:ILE:O	1:H:304:SER:HA	2.22	0.40
1:H:297:GLY:C	1:H:345(A):GLY:HA3	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/387 (99%)	350 (91%)	26 (7%)	7 (2%)	6	12
1	B	383/387 (99%)	347 (91%)	30 (8%)	6 (2%)	7	14
1	C	383/387 (99%)	348 (91%)	29 (8%)	6 (2%)	7	14
1	D	383/387 (99%)	347 (91%)	29 (8%)	7 (2%)	6	12
1	E	383/387 (99%)	338 (88%)	37 (10%)	8 (2%)	5	9
1	F	383/387 (99%)	344 (90%)	32 (8%)	7 (2%)	6	12
1	G	383/387 (99%)	348 (91%)	30 (8%)	5 (1%)	9	18
1	H	383/387 (99%)	345 (90%)	33 (9%)	5 (1%)	9	18
All	All	3064/3096 (99%)	2767 (90%)	246 (8%)	51 (2%)	7	13

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	B	146	ASN
1	C	146	ASN
1	C	448	GLY
1	D	146	ASN
1	E	146	ASN
1	F	146	ASN
1	F	448	GLY
1	G	146	ASN
1	H	146	ASN
1	A	147	GLY
1	A	151	ASP
1	A	448	GLY
1	A	449	VAL
1	B	448	GLY
1	B	449	VAL
1	C	147	GLY
1	C	449	VAL
1	D	147	GLY
1	D	148	THR
1	D	448	GLY
1	D	449	VAL
1	E	147	GLY
1	E	448	GLY
1	E	449	VAL
1	F	449	VAL
1	G	448	GLY

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Mol	Chain	Res	Type
1	G	449	VAL
1	H	448	GLY
1	H	449	VAL
1	B	151	ASP
1	D	150	LYS
1	E	148	THR
1	F	467	THR
1	G	467	THR
1	H	151	ASP
1	A	148	THR
1	C	151	ASP
1	C	200	GLY
1	F	148	THR
1	F	151	ASP
1	F	200	GLY
1	A	451	SER
1	E	345(A)	GLY
1	E	200	GLY
1	H	147	GLY
1	B	147	GLY
1	G	222	ILE
1	D	222	ILE
1	B	222	ILE
1	E	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%)	311 (94%)	18 (6%)	19	40
1	B	329/331 (99%)	313 (95%)	16 (5%)	22	45
1	C	329/331 (99%)	311 (94%)	18 (6%)	19	40
1	D	329/331 (99%)	308 (94%)	21 (6%)	16	33
1	E	329/331 (99%)	313 (95%)	16 (5%)	22	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	329/331 (99%)	311 (94%)	18 (6%)	19	40
1	G	329/331 (99%)	311 (94%)	18 (6%)	19	40
1	H	329/331 (99%)	312 (95%)	17 (5%)	21	42
All	All	2632/2648 (99%)	2490 (95%)	142 (5%)	20	41

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	88	ASN
1	A	99	VAL
1	A	116	VAL
1	A	146	ASN
1	A	153	SER
1	A	168	SER
1	A	202	VAL
1	A	210	ILE
1	A	214	THR
1	A	249	GLN
1	A	257	MET
1	A	276	GLU
1	A	296	HIS
1	A	310	LEU
1	A	415	LEU
1	A	442	SER
1	A	451	SER
1	B	85	LEU
1	B	88	ASN
1	B	99	VAL
1	B	116	VAL
1	B	146	ASN
1	B	202	VAL
1	B	210	ILE
1	B	230	CYS
1	B	257	MET
1	B	261	LYS
1	B	287	ILE
1	B	296	HIS
1	B	310	LEU
1	B	415	LEU
1	B	442	SER

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Mol	Chain	Res	Type
1	B	451	SER
1	C	85	LEU
1	C	88	ASN
1	C	99	VAL
1	C	116	VAL
1	C	146	ASN
1	C	163	VAL
1	C	168	SER
1	C	205	LEU
1	C	210	ILE
1	C	214	THR
1	C	230	CYS
1	C	249	GLN
1	C	257	MET
1	C	276	GLU
1	C	296	HIS
1	C	303	VAL
1	C	400	ILE
1	C	415	LEU
1	D	85	LEU
1	D	88	ASN
1	D	99	VAL
1	D	116	VAL
1	D	146	ASN
1	D	168	SER
1	D	202	VAL
1	D	205	LEU
1	D	210	ILE
1	D	230	CYS
1	D	249	GLN
1	D	257	MET
1	D	261	LYS
1	D	276	GLU
1	D	296	HIS
1	D	303	VAL
1	D	318	CYS
1	D	381	ASN
1	D	400	ILE
1	D	415	LEU
1	D	451	SER
1	E	85	LEU
1	E	88	ASN

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Mol	Chain	Res	Type
1	E	99	VAL
1	E	116	VAL
1	E	146	ASN
1	E	202	VAL
1	E	214	THR
1	E	230	CYS
1	E	261	LYS
1	E	276	GLU
1	E	296	HIS
1	E	310	LEU
1	E	400	ILE
1	E	415	LEU
1	E	442	SER
1	E	451	SER
1	F	88	ASN
1	F	99	VAL
1	F	116	VAL
1	F	146	ASN
1	F	149	VAL
1	F	202	VAL
1	F	214	THR
1	F	230	CYS
1	F	252	TYR
1	F	257	MET
1	F	261	LYS
1	F	276	GLU
1	F	287	ILE
1	F	296	HIS
1	F	310	LEU
1	F	400	ILE
1	F	415	LEU
1	F	451	SER
1	G	85	LEU
1	G	88	ASN
1	G	99	VAL
1	G	116	VAL
1	G	146	ASN
1	G	202	VAL
1	G	214	THR
1	G	230	CYS
1	G	257	MET
1	G	261	LYS

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Mol	Chain	Res	Type
1	G	276	GLU
1	G	296	HIS
1	G	303	VAL
1	G	310	LEU
1	G	385	GLU
1	G	400	ILE
1	G	415	LEU
1	G	442	SER
1	H	85	LEU
1	H	88	ASN
1	H	99	VAL
1	H	116	VAL
1	H	146	ASN
1	H	156	ARG
1	H	202	VAL
1	H	230	CYS
1	H	257	MET
1	H	261	LYS
1	H	276	GLU
1	H	296	HIS
1	H	298	SER
1	H	310	LEU
1	H	400	ILE
1	H	415	LEU
1	H	442	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	104	ASN
1	A	144	HIS
1	A	146	ASN
1	A	184	HIS
1	A	208	ASN
1	A	226	GLN
1	A	249	GLN
1	A	283	ASN
1	A	313	GLN
1	A	395	GLN
1	B	88	ASN
1	B	104	ASN

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Mol	Chain	Res	Type
1	B	144	HIS
1	B	146	ASN
1	B	155	HIS
1	B	184	HIS
1	B	226	GLN
1	B	249	GLN
1	B	283	ASN
1	B	296	HIS
1	B	313	GLN
1	B	395	GLN
1	B	412(A)	HIS
1	B	450	ASN
1	C	88	ASN
1	C	104	ASN
1	C	144	HIS
1	C	146	ASN
1	C	155	HIS
1	C	184	HIS
1	C	226	GLN
1	C	283	ASN
1	C	313	GLN
1	C	381	ASN
1	C	395	GLN
1	D	88	ASN
1	D	104	ASN
1	D	144	HIS
1	D	146	ASN
1	D	155	HIS
1	D	184	HIS
1	D	208	ASN
1	D	226	GLN
1	D	249	GLN
1	D	283	ASN
1	D	296	HIS
1	D	313	GLN
1	D	358	ASN
1	D	381	ASN
1	D	395	GLN
1	D	412(A)	HIS
1	D	450	ASN
1	E	88	ASN
1	E	104	ASN

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Mol	Chain	Res	Type
1	E	144	HIS
1	E	146	ASN
1	E	155	HIS
1	E	184	HIS
1	E	226	GLN
1	E	249	GLN
1	E	283	ASN
1	E	296	HIS
1	E	313	GLN
1	E	345	ASN
1	E	381	ASN
1	E	395	GLN
1	E	412(A)	HIS
1	F	88	ASN
1	F	104	ASN
1	F	144	HIS
1	F	146	ASN
1	F	155	HIS
1	F	184	HIS
1	F	226	GLN
1	F	249	GLN
1	F	283	ASN
1	F	296	HIS
1	F	313	GLN
1	F	325	ASN
1	F	395	GLN
1	F	450	ASN
1	G	88	ASN
1	G	104	ASN
1	G	144	HIS
1	G	146	ASN
1	G	184	HIS
1	G	226	GLN
1	G	249	GLN
1	G	283	ASN
1	G	313	GLN
1	G	395	GLN
1	G	412(A)	HIS
1	G	450	ASN
1	H	88	ASN
1	H	104	ASN
1	H	144	HIS

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Mol	Chain	Res	Type
1	H	146	ASN
1	H	184	HIS
1	H	226	GLN
1	H	249	GLN
1	H	272	ASN
1	H	283	ASN
1	H	308	GLN
1	H	313	GLN
1	H	345	ASN
1	H	358	ASN
1	H	381	ASN
1	H	395	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	G39	A	800	-	19,20,20	2.69	6 (31%)	20,27,27	2.10	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G39	G	806	-	19,20,20	2.70	6 (31%)	20,27,27	2.06	5 (25%)
2	G39	F	805	-	19,20,20	2.66	7 (36%)	20,27,27	2.06	5 (25%)
2	G39	D	803	-	19,20,20	2.75	7 (36%)	20,27,27	2.11	7 (35%)
2	G39	B	801	-	19,20,20	2.65	7 (36%)	20,27,27	2.11	5 (25%)
2	G39	C	802	-	19,20,20	2.63	7 (36%)	20,27,27	2.09	6 (30%)
2	G39	H	807	-	19,20,20	2.81	7 (36%)	20,27,27	2.11	5 (25%)
2	G39	E	804	-	19,20,20	2.67	8 (42%)	20,27,27	2.06	5 (25%)

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	A	800	-	-	1/16/32/32	0/1/1/1
2	G39	G	806	-	-	4/16/32/32	0/1/1/1
2	G39	F	805	-	-	2/16/32/32	0/1/1/1
2	G39	D	803	-	-	2/16/32/32	0/1/1/1
2	G39	B	801	-	-	3/16/32/32	0/1/1/1
2	G39	C	802	-	-	2/16/32/32	0/1/1/1
2	G39	H	807	-	-	1/16/32/32	0/1/1/1
2	G39	E	804	-	-	2/16/32/32	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	807	G39	C3-C2	7.82	1.64	1.51
2	A	800	G39	C3-C2	7.68	1.64	1.51
2	D	803	G39	C3-C2	7.58	1.63	1.51
2	G	806	G39	C3-C2	7.49	1.63	1.51
2	B	801	G39	C3-C2	7.43	1.63	1.51
2	F	805	G39	C3-C2	7.34	1.63	1.51
2	C	802	G39	C3-C2	7.33	1.63	1.51
2	E	804	G39	C3-C2	7.27	1.63	1.51
2	H	807	G39	C7-C2	4.87	1.44	1.33
2	D	803	G39	C7-C2	4.80	1.44	1.33
2	G	806	G39	C7-C2	4.61	1.43	1.33
2	E	804	G39	C7-C2	4.58	1.43	1.33
2	C	802	G39	C7-C2	4.56	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	G39	C7-C2	4.44	1.43	1.33
2	F	805	G39	C7-C2	4.38	1.43	1.33
2	A	800	G39	C7-C2	4.32	1.43	1.33
2	D	803	G39	O7-C8	4.05	1.50	1.44
2	F	805	G39	C5-N5	3.96	1.52	1.45
2	G	806	G39	O7-C8	3.91	1.50	1.44
2	E	804	G39	O7-C8	3.90	1.50	1.44
2	H	807	G39	O7-C8	3.87	1.50	1.44
2	H	807	G39	C3-C4	3.85	1.60	1.54
2	A	800	G39	C5-N5	3.79	1.51	1.45
2	B	801	G39	C5-N5	3.74	1.51	1.45
2	C	802	G39	O7-C8	3.64	1.49	1.44
2	A	800	G39	C3-C4	3.61	1.59	1.54
2	C	802	G39	C5-N5	3.53	1.51	1.45
2	G	806	G39	C5-N5	3.49	1.51	1.45
2	D	803	G39	C3-C4	3.46	1.59	1.54
2	H	807	G39	C5-N5	3.42	1.51	1.45
2	B	801	G39	O7-C8	3.41	1.49	1.44
2	G	806	G39	O7-C6	3.39	1.51	1.44
2	F	805	G39	C3-C4	3.39	1.59	1.54
2	E	804	G39	C3-C4	3.36	1.59	1.54
2	B	801	G39	C3-C4	3.26	1.59	1.54
2	A	800	G39	O7-C8	3.25	1.49	1.44
2	F	805	G39	O7-C8	3.22	1.49	1.44
2	E	804	G39	C5-N5	3.21	1.50	1.45
2	D	803	G39	C5-N5	3.20	1.50	1.45
2	D	803	G39	O7-C6	3.13	1.50	1.44
2	E	804	G39	O7-C6	3.00	1.50	1.44
2	A	800	G39	O7-C6	2.99	1.50	1.44
2	C	802	G39	C3-C4	2.97	1.58	1.54
2	F	805	G39	O7-C6	2.96	1.50	1.44
2	H	807	G39	O7-C6	2.94	1.50	1.44
2	C	802	G39	O7-C6	2.90	1.50	1.44
2	G	806	G39	C3-C4	2.82	1.58	1.54
2	B	801	G39	O7-C6	2.73	1.49	1.44
2	H	807	G39	O1A-C1	2.28	1.28	1.22
2	E	804	G39	C1-C2	-2.19	1.44	1.49
2	B	801	G39	O1A-C1	2.17	1.27	1.22
2	E	804	G39	O1A-C1	2.15	1.27	1.22
2	C	802	G39	C1-C2	-2.11	1.44	1.49
2	F	805	G39	C1-C2	-2.03	1.44	1.49
2	D	803	G39	C1-C2	-2.00	1.44	1.49

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	G39	C4-C3-C2	6.33	116.89	109.72
2	H	807	G39	C4-C3-C2	6.18	116.72	109.72
2	A	800	G39	C4-C3-C2	6.04	116.56	109.72
2	D	803	G39	C4-C3-C2	5.98	116.49	109.72
2	C	802	G39	C4-C3-C2	5.88	116.37	109.72
2	G	806	G39	C4-C3-C2	5.87	116.37	109.72
2	F	805	G39	C4-C3-C2	5.77	116.25	109.72
2	E	804	G39	C4-C3-C2	5.64	116.11	109.72
2	H	807	G39	C3-C2-C7	-3.44	118.01	122.25
2	B	801	G39	C3-C2-C7	-3.42	118.03	122.25
2	F	805	G39	C3-C2-C7	-3.39	118.06	122.25
2	G	806	G39	C3-C2-C7	-3.36	118.11	122.25
2	E	804	G39	C3-C2-C7	-3.32	118.15	122.25
2	A	800	G39	C3-C2-C7	-3.32	118.15	122.25
2	D	803	G39	C3-C2-C7	-3.24	118.25	122.25
2	C	802	G39	C3-C2-C7	-3.19	118.31	122.25
2	A	800	G39	C3-C2-C1	2.87	122.26	116.99
2	A	800	G39	O1B-C1-C2	2.85	121.45	115.43
2	E	804	G39	C3-C2-C1	2.84	122.20	116.99
2	D	803	G39	O1B-C1-C2	2.79	121.32	115.43
2	D	803	G39	C3-C2-C1	2.76	122.05	116.99
2	F	805	G39	O1B-C1-C2	2.71	121.17	115.43
2	H	807	G39	C3-C2-C1	2.69	121.92	116.99
2	F	805	G39	C3-C2-C1	2.65	121.84	116.99
2	E	804	G39	O1B-C1-C2	2.62	120.97	115.43
2	C	802	G39	O1B-C1-C2	2.57	120.87	115.43
2	H	807	G39	O1B-C1-C2	2.57	120.87	115.43
2	B	801	G39	O1B-C1-C2	2.50	120.70	115.43
2	G	806	G39	O1B-C1-C2	2.48	120.67	115.43
2	C	802	G39	C3-C2-C1	2.46	121.50	116.99
2	B	801	G39	C3-C2-C1	2.44	121.47	116.99
2	G	806	G39	C3-C2-C1	2.35	121.30	116.99
2	G	806	G39	O7-C8-C9	2.26	118.25	108.87
2	C	802	G39	O10-C10-C11	-2.21	118.11	122.05
2	E	804	G39	O7-C8-C9	2.12	117.67	108.87
2	C	802	G39	O7-C8-C9	2.11	117.60	108.87
2	A	800	G39	O7-C8-C9	2.10	117.57	108.87
2	D	803	G39	O1A-C1-C2	-2.09	117.97	121.64
2	H	807	G39	O10-C10-C11	-2.09	118.34	122.05
2	D	803	G39	O7-C8-C9	2.08	117.51	108.87
2	B	801	G39	O10-C10-C11	-2.07	118.38	122.05
2	D	803	G39	O10-C10-C11	-2.05	118.40	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	805	G39	O10-C10-C11	-2.01	118.47	122.05
2	A	800	G39	O10-C10-C11	-2.01	118.48	122.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	G39	C9-C8-C81-C82
2	D	803	G39	C9-C8-C81-C82
2	F	805	G39	C9-C8-C81-C82
2	A	800	G39	C9-C8-O7-C6
2	B	801	G39	C9-C8-O7-C6
2	C	802	G39	C9-C8-O7-C6
2	D	803	G39	C9-C8-O7-C6
2	E	804	G39	C9-C8-O7-C6
2	F	805	G39	C9-C8-O7-C6
2	G	806	G39	C9-C8-O7-C6
2	H	807	G39	C9-C8-O7-C6
2	G	806	G39	O7-C8-C9-C91
2	B	801	G39	C5-C6-O7-C8
2	G	806	G39	C5-C6-O7-C8
2	C	802	G39	C9-C8-C81-C82
2	G	806	G39	C9-C8-C81-C82
2	E	804	G39	C9-C8-C81-C82

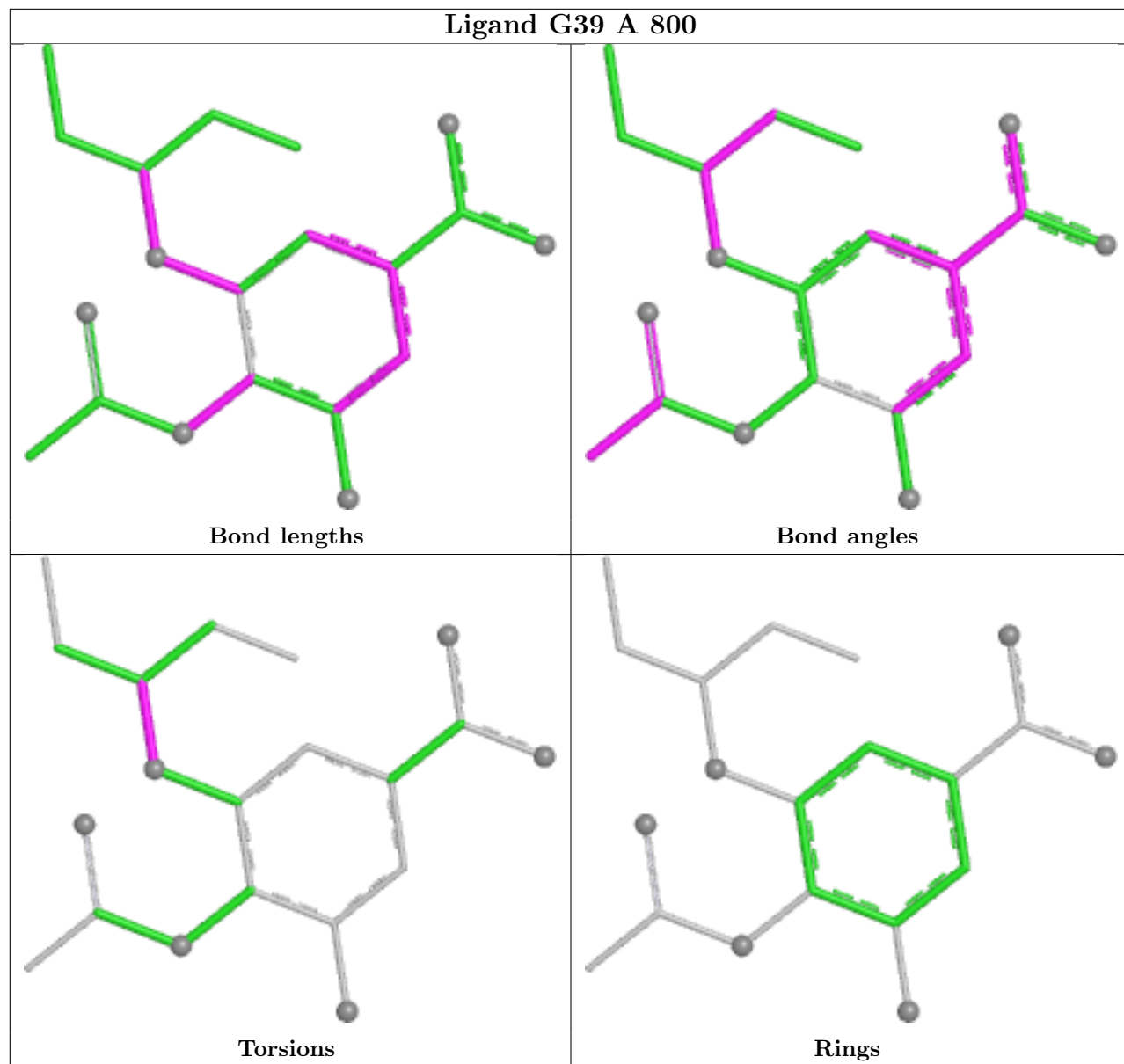
There are no ring outliers.

1 monomer is involved in 1 short contact:

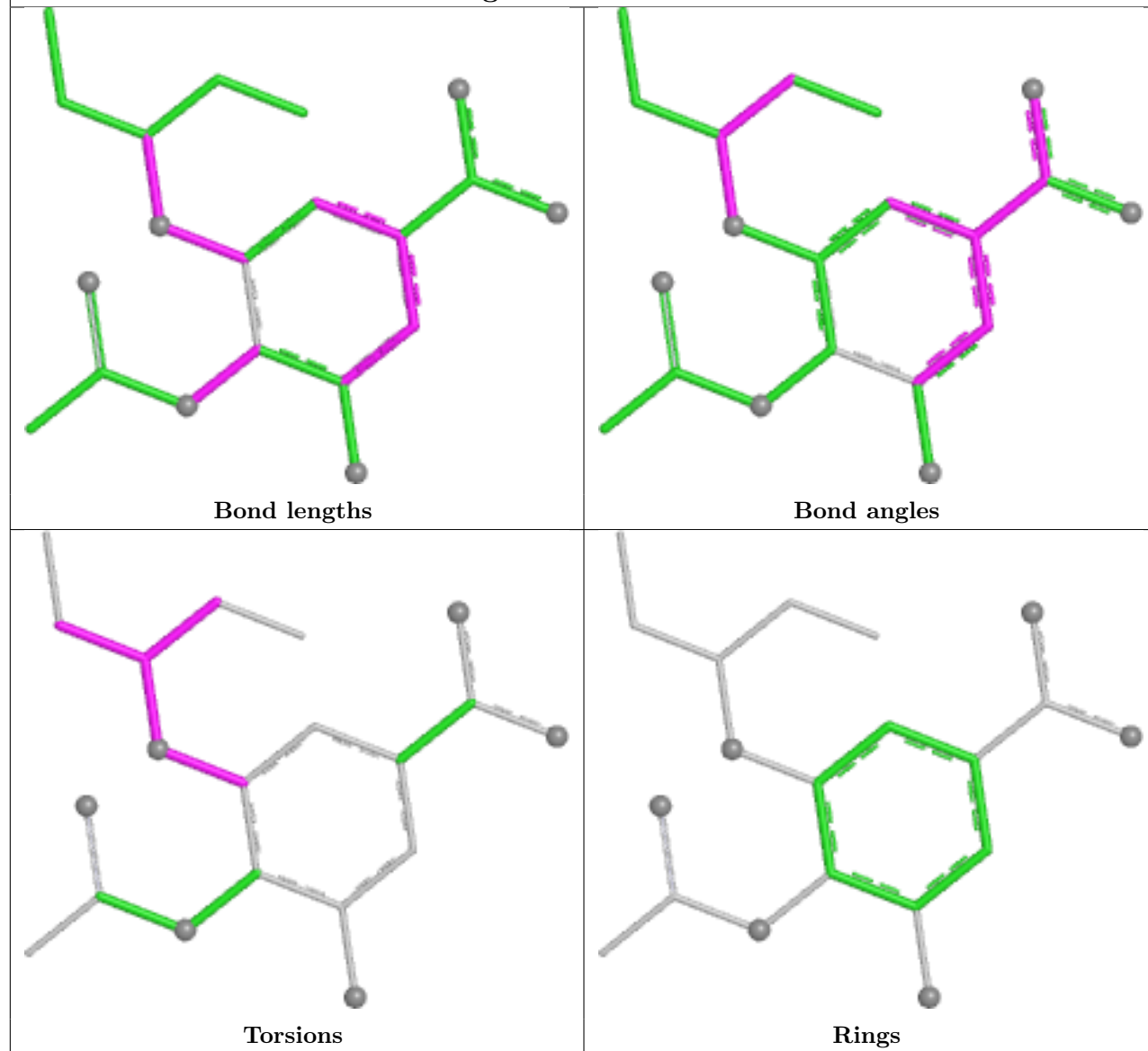
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	G39	1	0

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

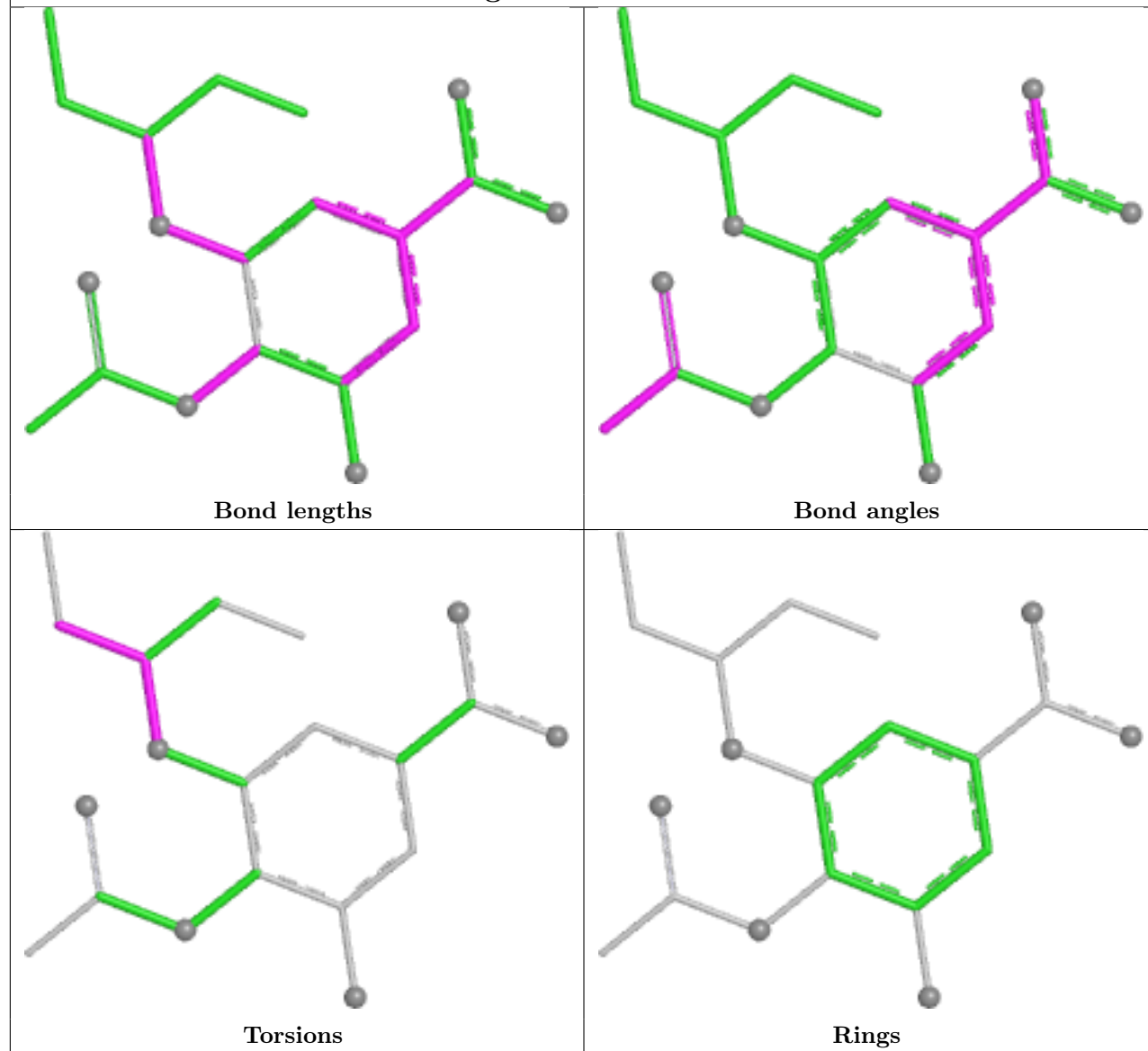
equivalents in the CSD to analyse the geometry.



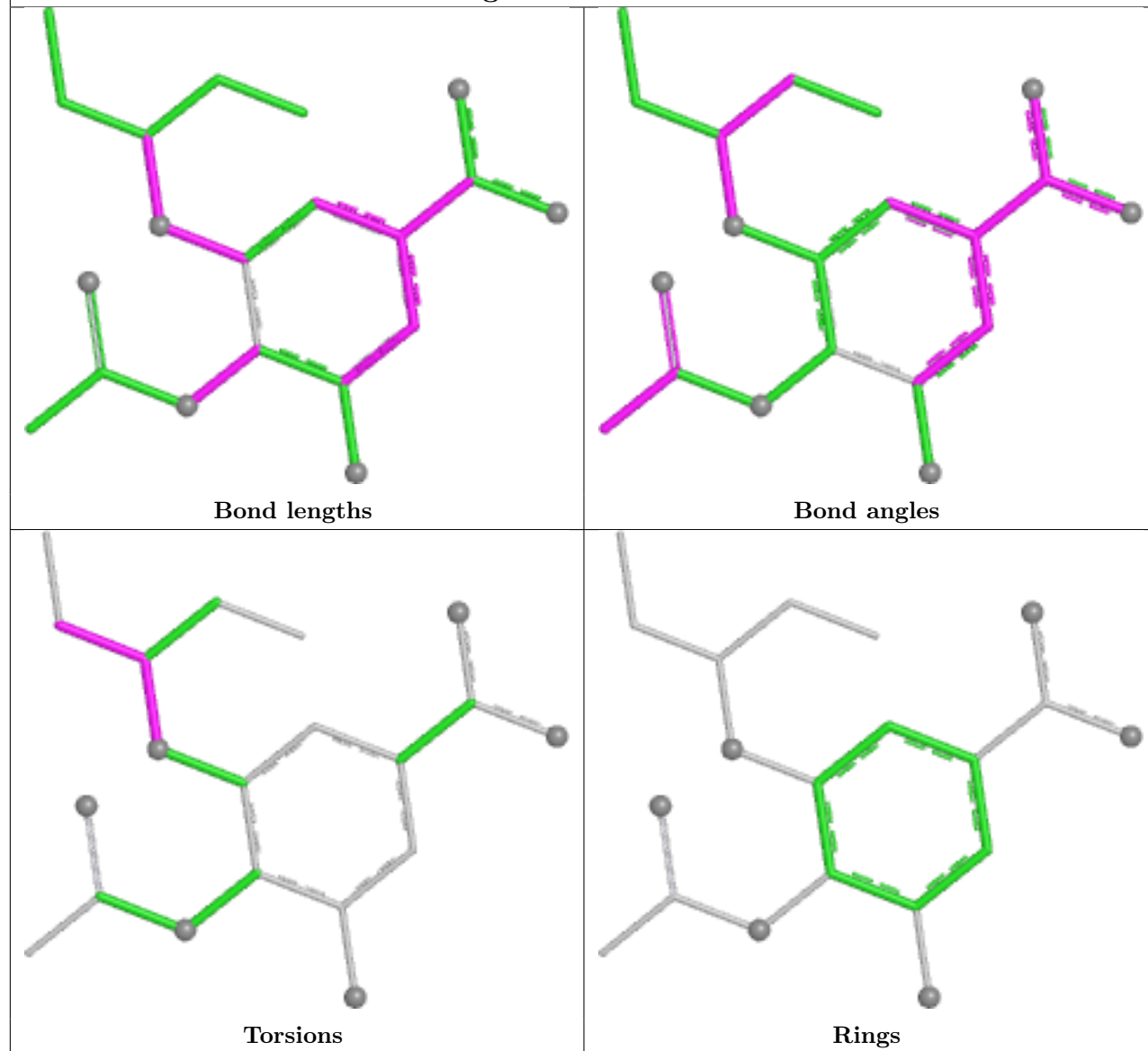
Ligand G39 G 806



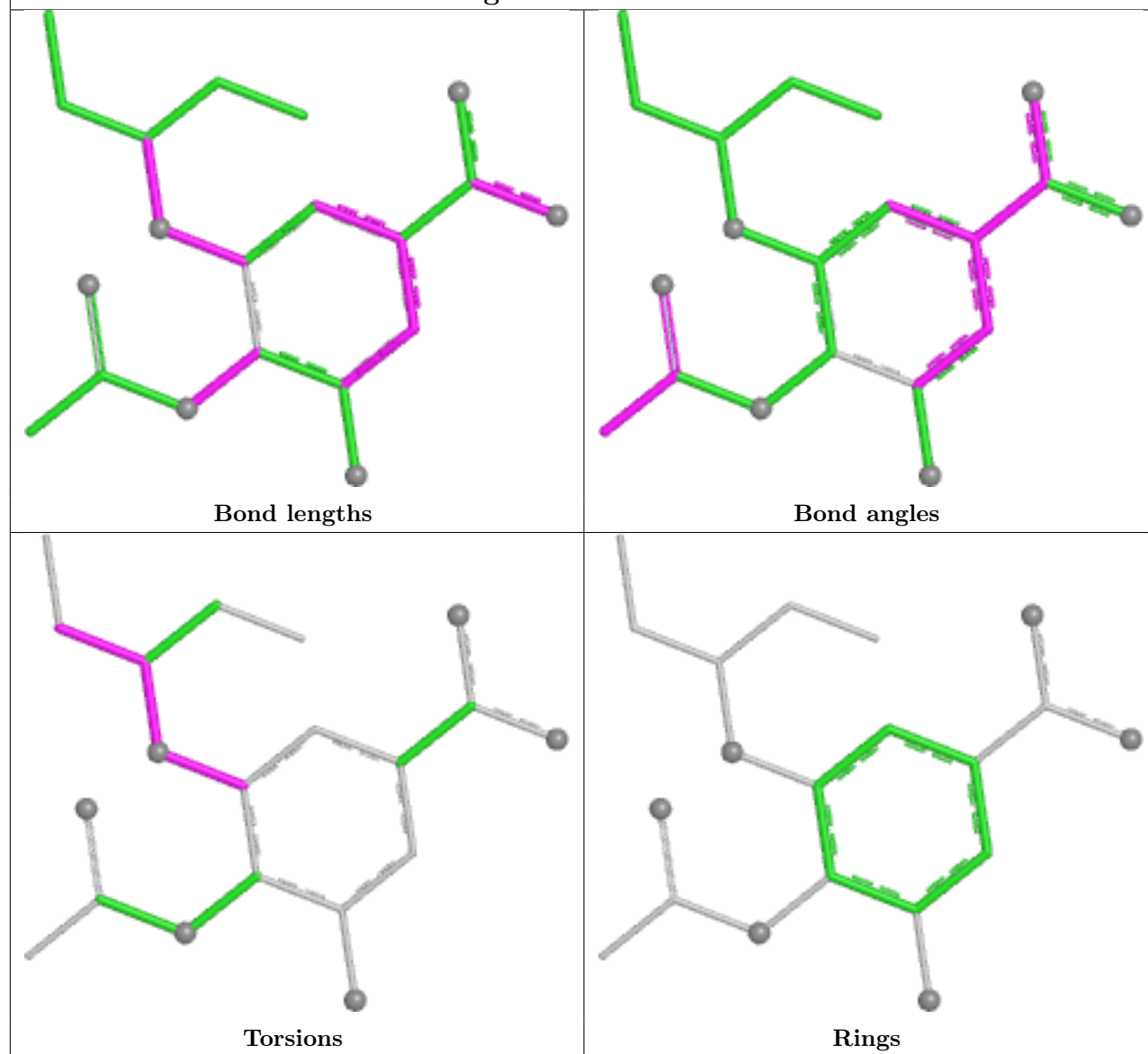
Ligand G39 F 805



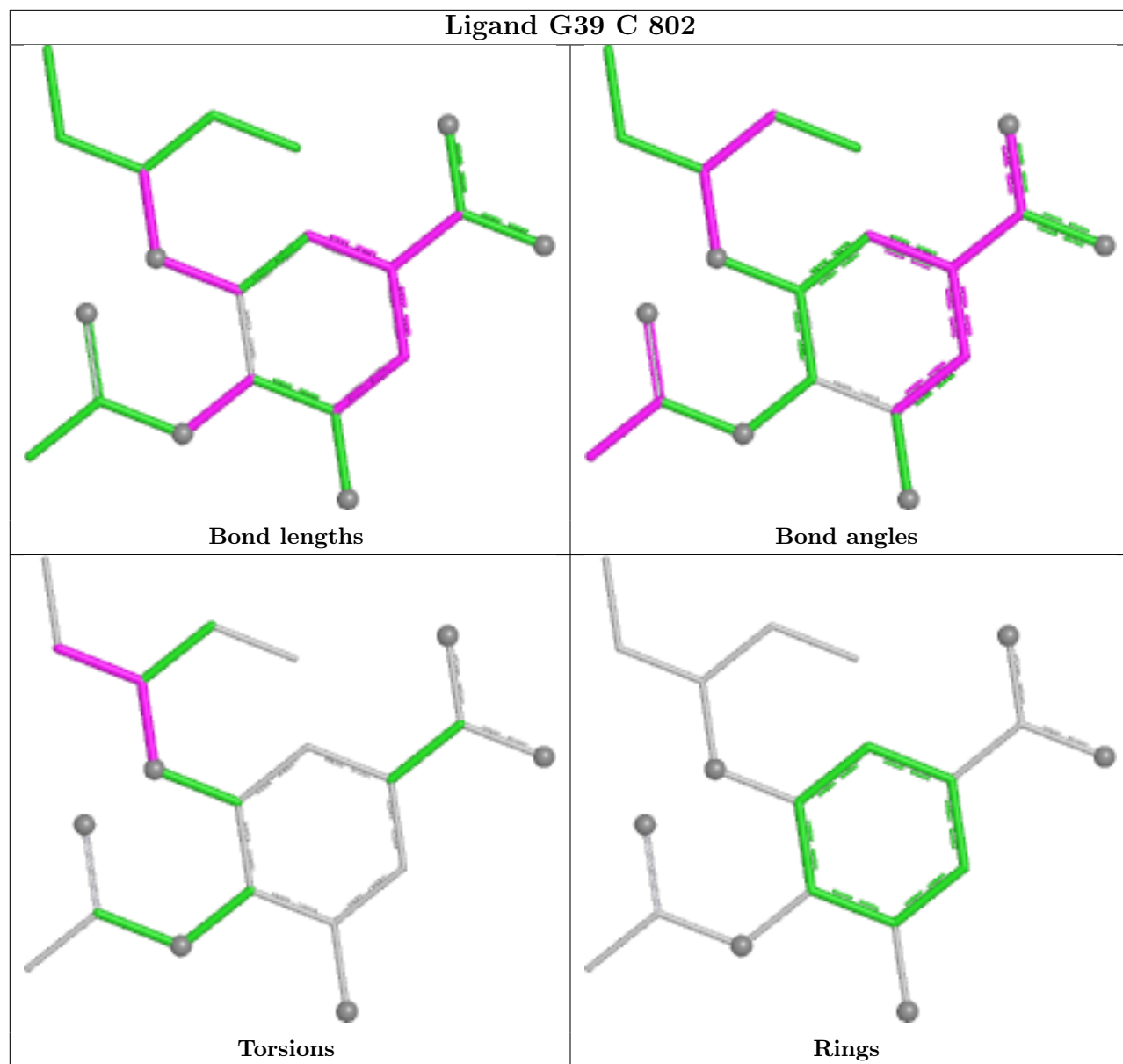
Ligand G39 D 803



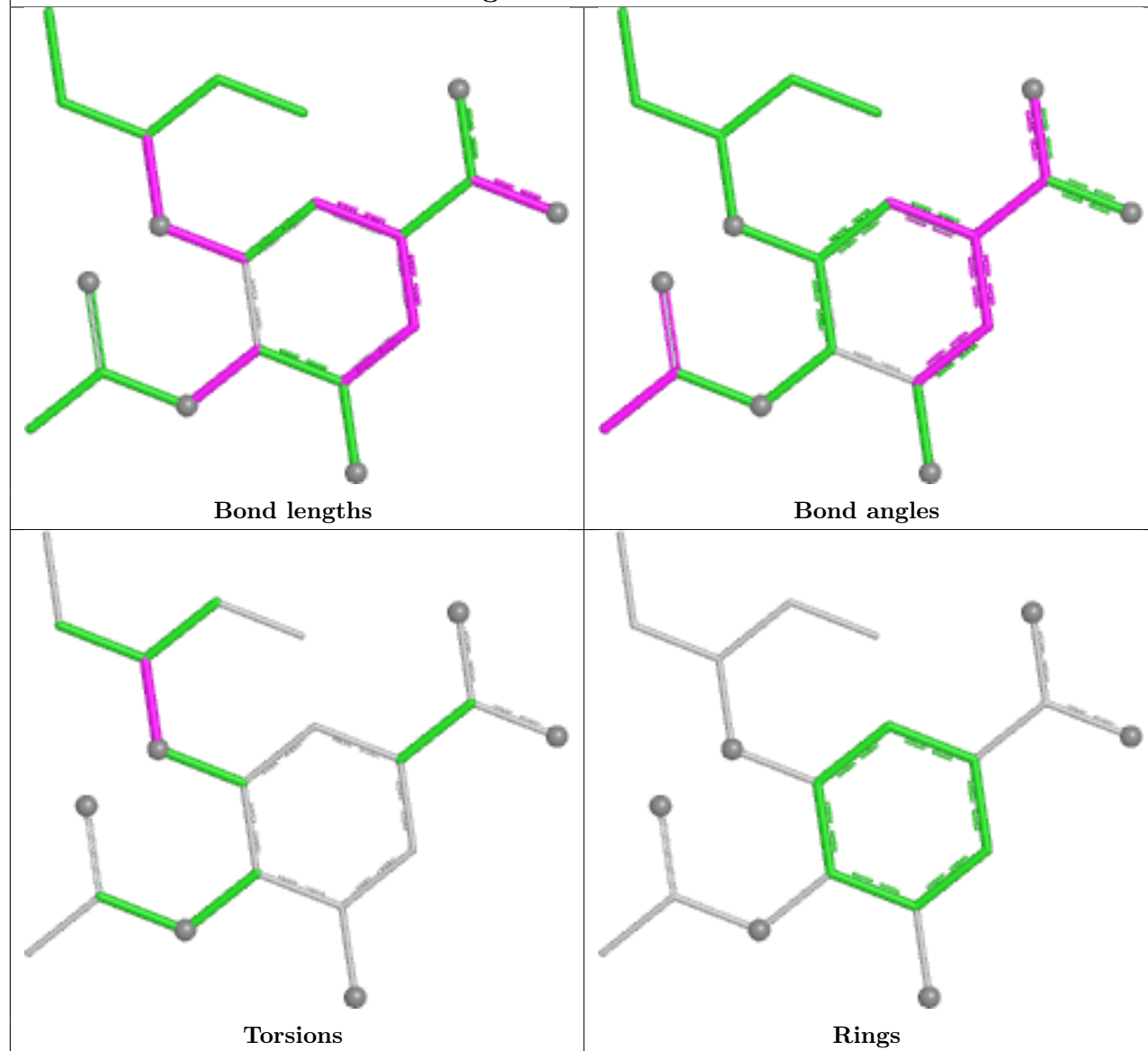
Ligand G39 B 801

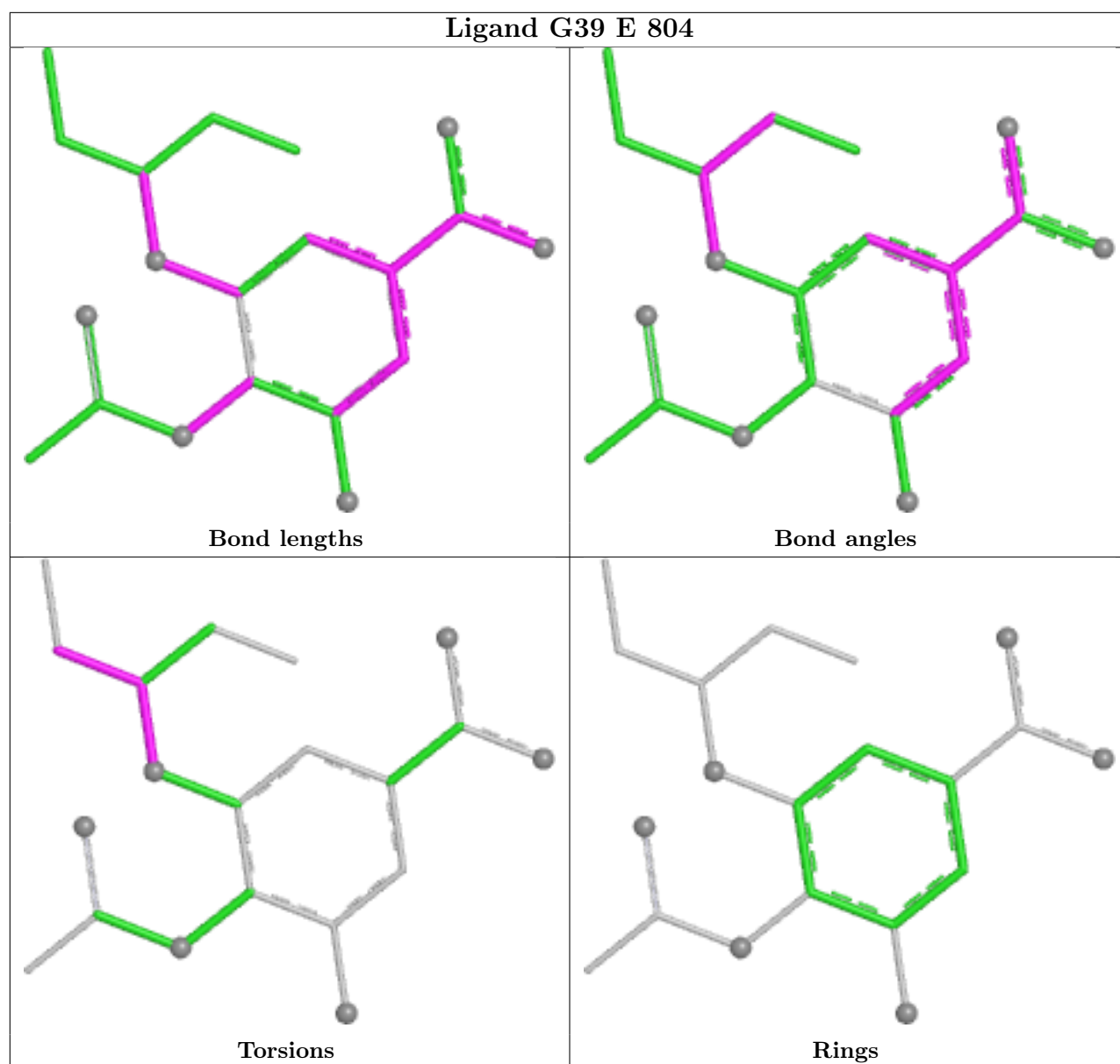


Ligand G39 C 802



Ligand G39 H 807





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	B	1
1	E	1
1	D	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	412:GLN	C	412(A):HIS	N	1.12
1	E	412:GLN	C	412(A):HIS	N	1.11
1	D	412:GLN	C	412(A):HIS	N	1.10
1	F	412:GLN	C	412(A):HIS	N	1.06

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%)	-1.65	0 100 100	9, 18, 28, 40	0
1	B	385/387 (99%)	-1.66	0 100 100	8, 18, 28, 40	0
1	C	385/387 (99%)	-1.64	0 100 100	10, 18, 28, 41	0
1	D	385/387 (99%)	-1.65	0 100 100	10, 18, 29, 43	0
1	E	385/387 (99%)	-1.60	0 100 100	15, 24, 33, 43	0
1	F	385/387 (99%)	-1.60	0 100 100	12, 25, 35, 44	0
1	G	385/387 (99%)	-1.63	0 100 100	9, 21, 32, 43	0
1	H	385/387 (99%)	-1.61	0 100 100	14, 23, 34, 44	0
All	All	3080/3096 (99%)	-1.63	0 100 100	8, 21, 32, 44	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](#)

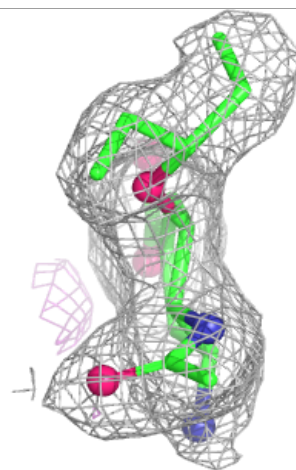
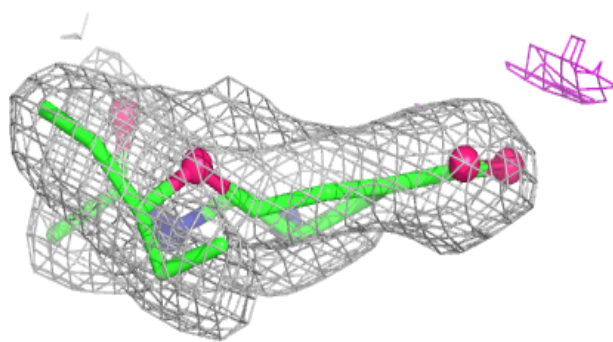
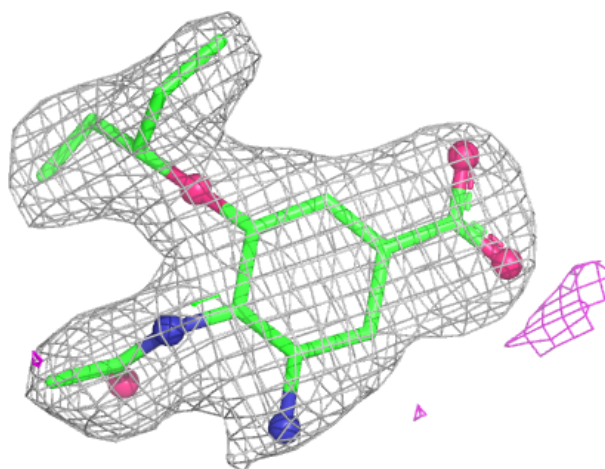
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	C	802	20/20	0.99	0.03	24,26,28,31	0
2	G39	D	803	20/20	0.99	0.03	17,22,23,24	0
2	G39	E	804	20/20	0.99	0.03	21,24,26,26	0
2	G39	F	805	20/20	0.99	0.03	25,29,32,33	0
2	G39	G	806	20/20	0.99	0.02	18,21,23,23	0
2	G39	H	807	20/20	0.99	0.03	20,27,29,29	0
2	G39	A	800	20/20	1.00	0.02	20,24,26,26	0
2	G39	B	801	20/20	1.00	0.02	17,25,29,30	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.

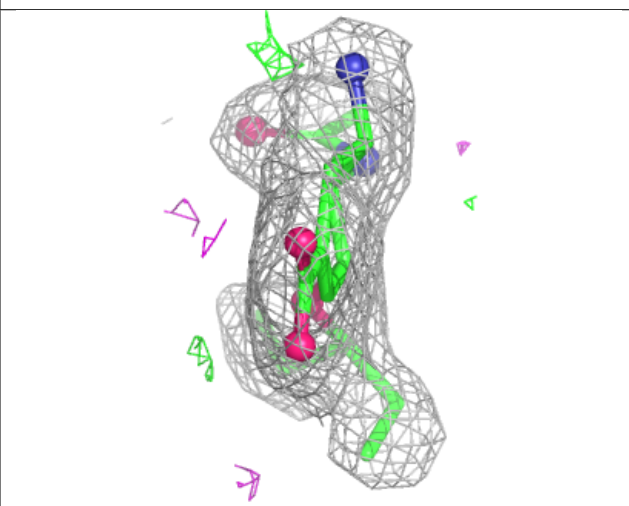
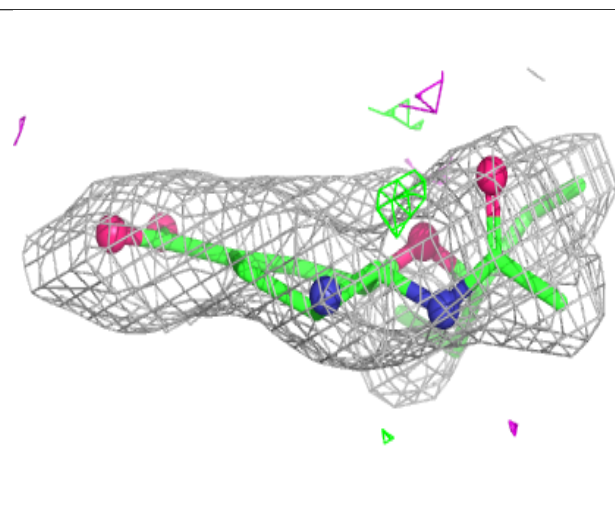
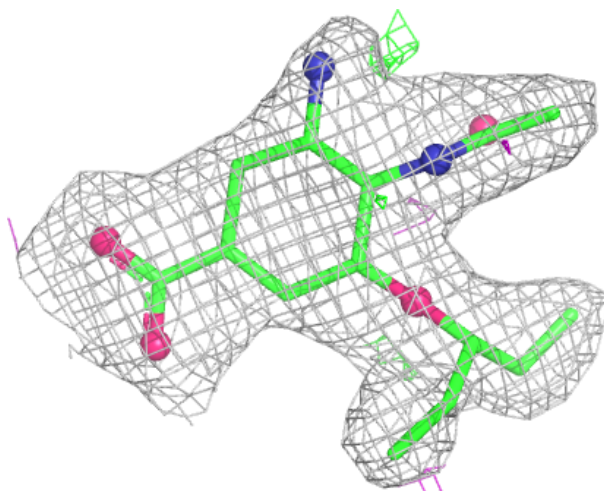
Electron density around G39 C 802:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



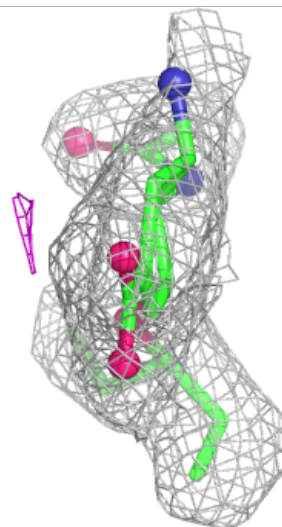
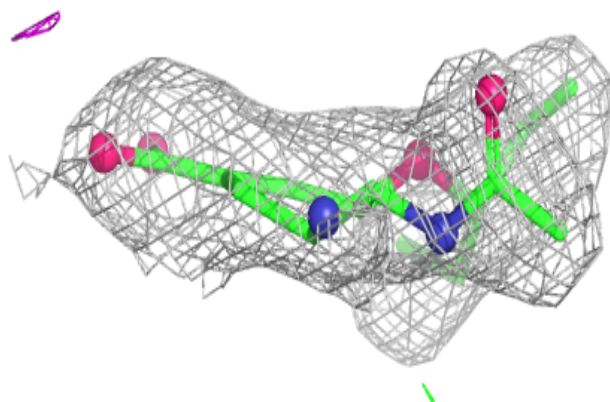
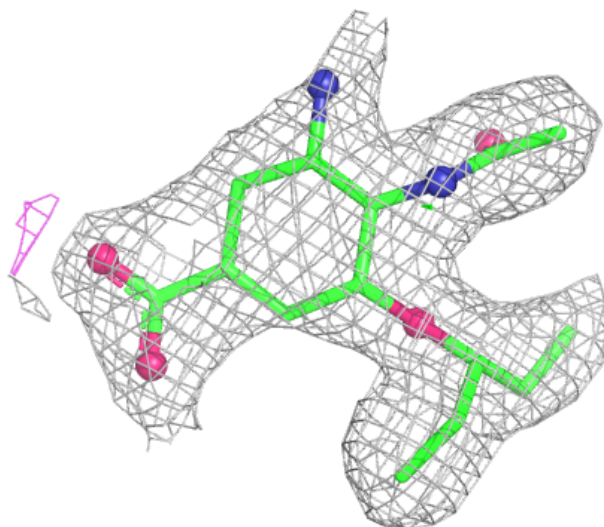
Electron density around G39 D 803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



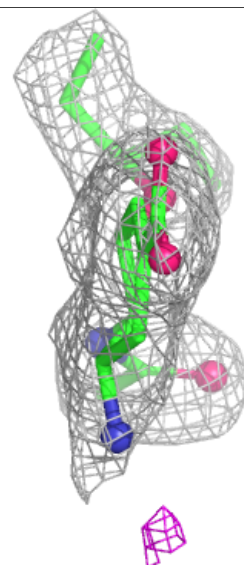
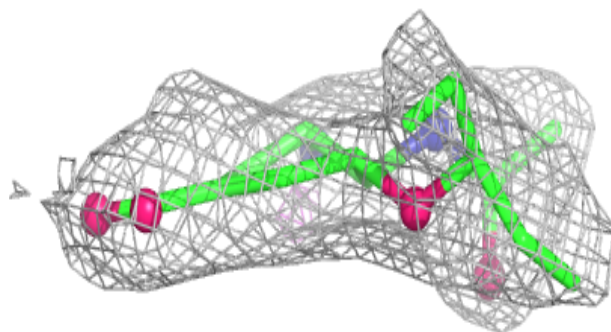
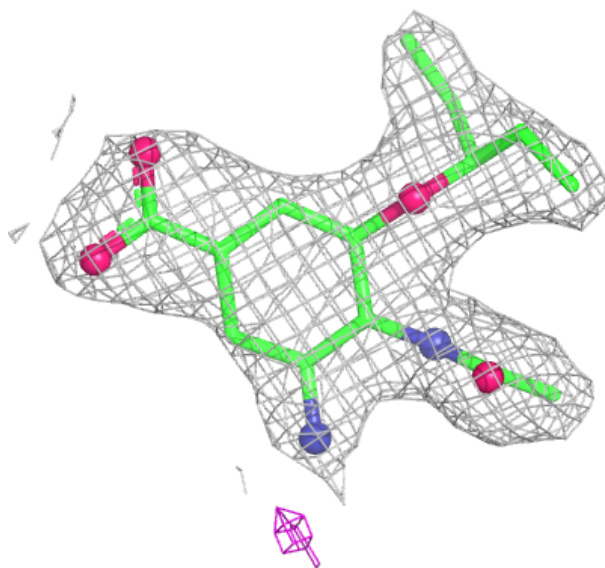
Electron density around G39 E 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



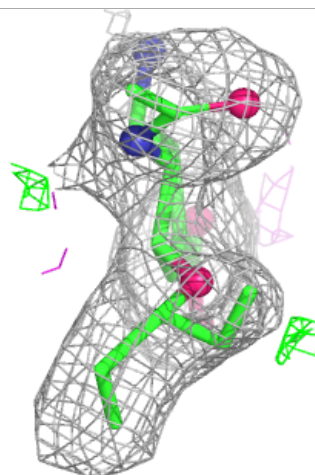
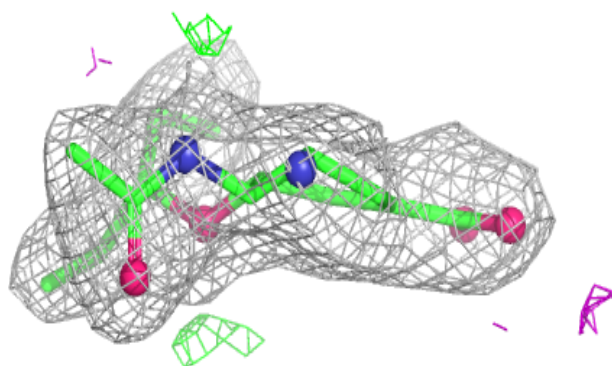
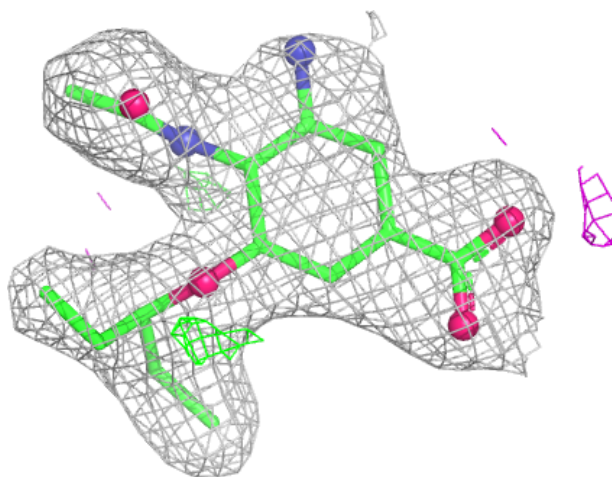
Electron density around G39 F 805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



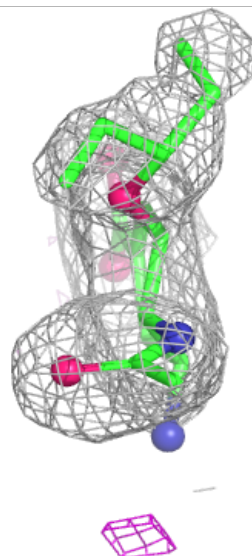
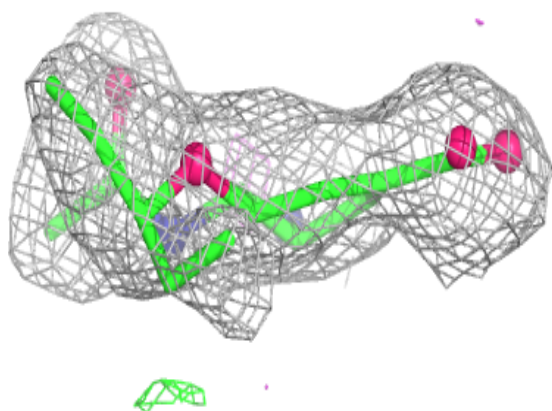
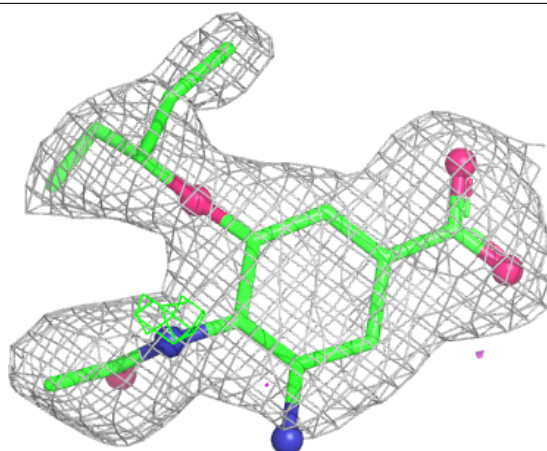
Electron density around G39 G 806:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



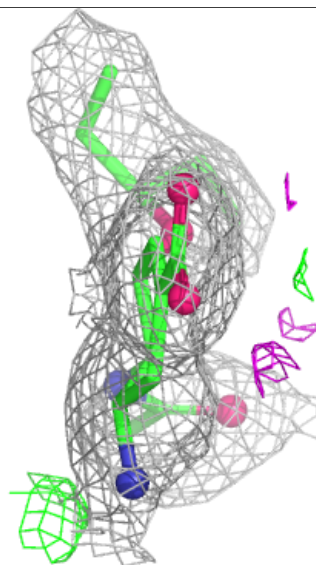
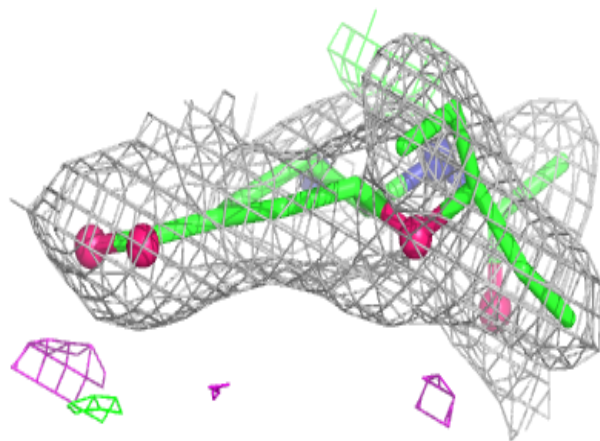
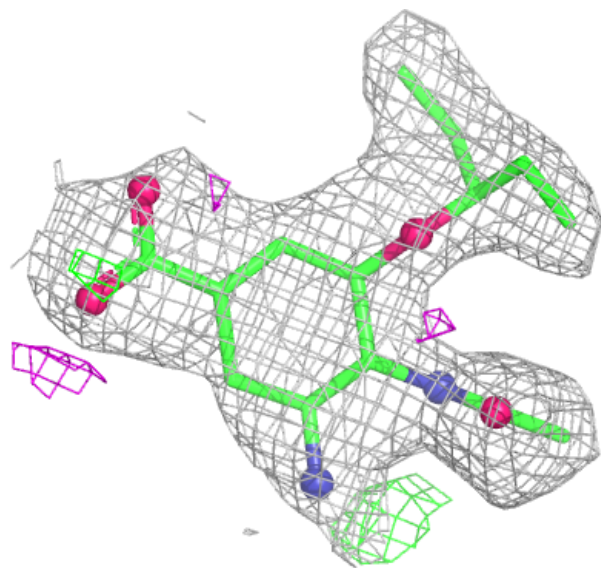
Electron density around G39 H 807:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



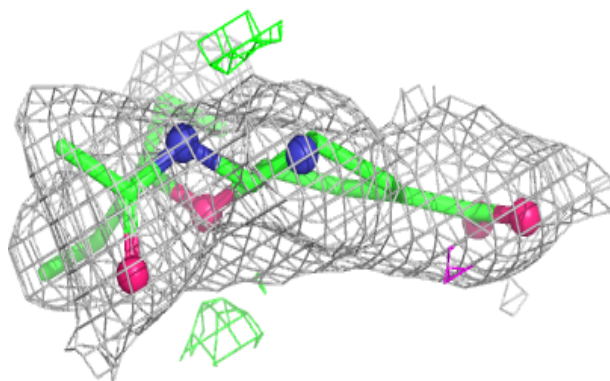
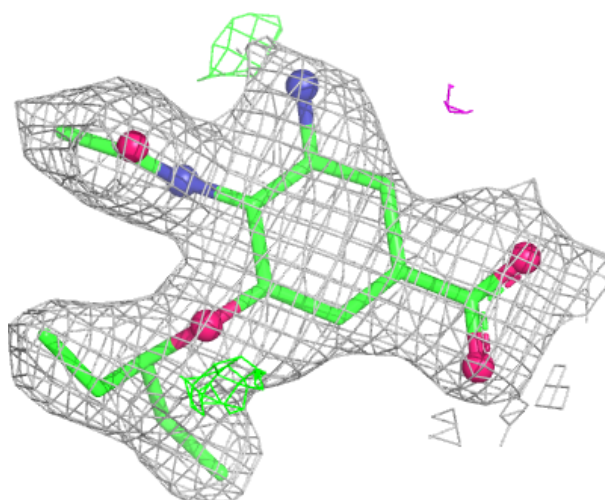
Electron density around G39 A 800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G39 B 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.