



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 AM UTC

PDB ID : 3CL2 / pdb_00003cl2
Title : N1 Neuraminidase N294S + Oseltamivir
Authors : Collins, P.; Haire, L.F.; Lin, Y.P.; Liu, J.; Russell, R.J.; Walker, P.A.; Skehel, J.J.; Martin, S.R.; Hay, A.J.; Gamblin, S.J.
Deposited on : 2008-03-18
Resolution : 2.54 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

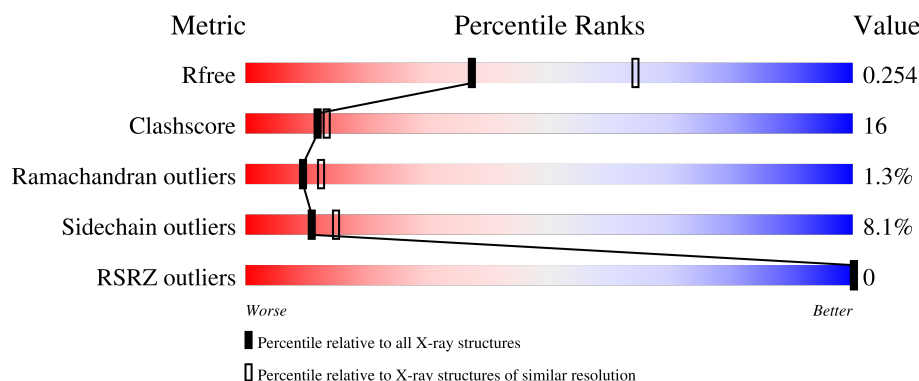
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	385	
1	B	385	
1	C	385	
1	D	385	
1	E	385	

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Mol	Chain	Length	Quality of chain
1	F	385	 72%22%5%
1	G	385	 71%22%6%
1	H	385	 72%21%6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23840 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
			2960	1857	509	573	21			
1	B	385	Total	C	N	O	S	0	0	0
			2960	1857	509	573	21			
1	C	385	Total	C	N	O	S	0	0	0
			2960	1857	509	573	21			
1	D	385	Total	C	N	O	S	0	0	0
			2960	1857	509	573	21			
1	E	385	Total	C	N	O	S	0	0	0
			2960	1857	509	573	21			
1	F	385	Total	C	N	O	S	0	0	0
			2960	1857	509	573	21			
1	G	385	Total	C	N	O	S	0	0	0
			2960	1857	509	573	21			
1	H	385	Total	C	N	O	S	0	0	0
			2960	1857	509	573	21			

There are 16 discrepancies between the modelled and reference sequences:

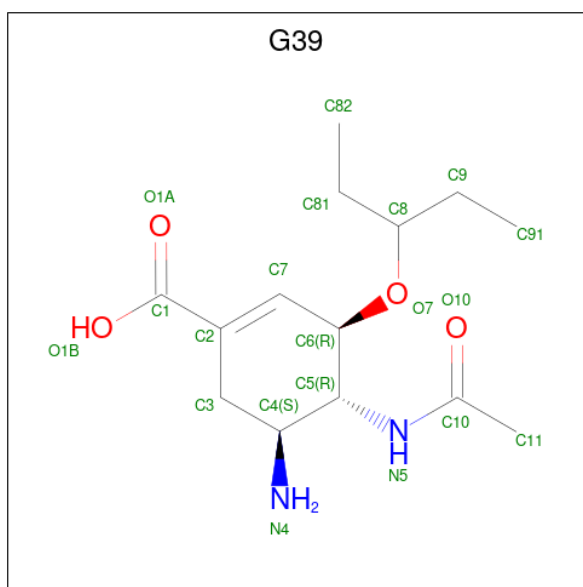
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	TYR	HIS	conflict	UNP Q6DPL2
A	294	SER	ASN	engineered mutation	UNP Q6DPL2
B	252	TYR	HIS	conflict	UNP Q6DPL2
B	294	SER	ASN	engineered mutation	UNP Q6DPL2
C	252	TYR	HIS	conflict	UNP Q6DPL2
C	294	SER	ASN	engineered mutation	UNP Q6DPL2
D	252	TYR	HIS	conflict	UNP Q6DPL2
D	294	SER	ASN	engineered mutation	UNP Q6DPL2
E	252	TYR	HIS	conflict	UNP Q6DPL2
E	294	SER	ASN	engineered mutation	UNP Q6DPL2
F	252	TYR	HIS	conflict	UNP Q6DPL2
F	294	SER	ASN	engineered mutation	UNP Q6DPL2
G	252	TYR	HIS	conflict	UNP Q6DPL2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	294	SER	ASN	engineered mutation	UNP Q6DPL2
H	252	TYR	HIS	conflict	UNP Q6DPL2
H	294	SER	ASN	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).

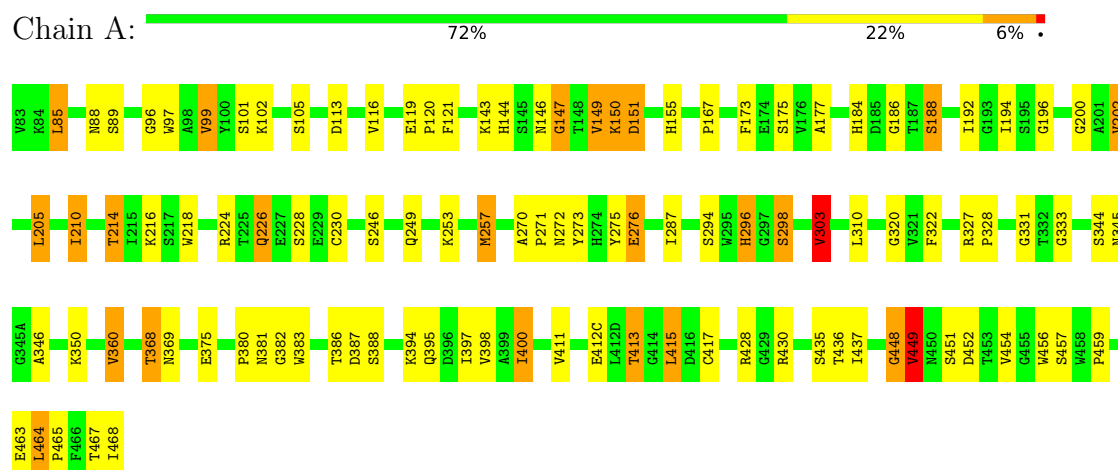


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	14	2	4		
2	B	1	Total	C	N	O	0	0
			20	14	2	4		
2	C	1	Total	C	N	O	0	0
			20	14	2	4		
2	D	1	Total	C	N	O	0	0
			20	14	2	4		
2	E	1	Total	C	N	O	0	0
			20	14	2	4		
2	F	1	Total	C	N	O	0	0
			20	14	2	4		
2	G	1	Total	C	N	O	0	0
			20	14	2	4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

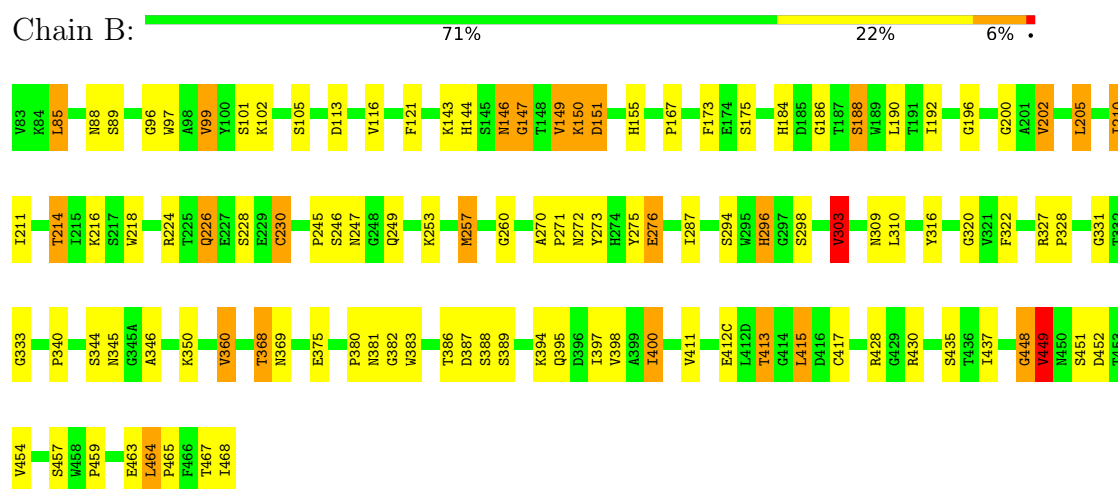
3 Residue-property plots

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.

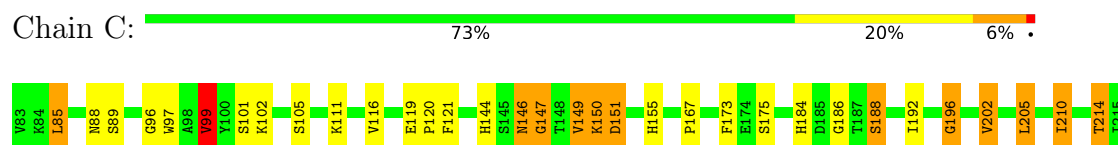
• Molecule 1: Neuraminidase

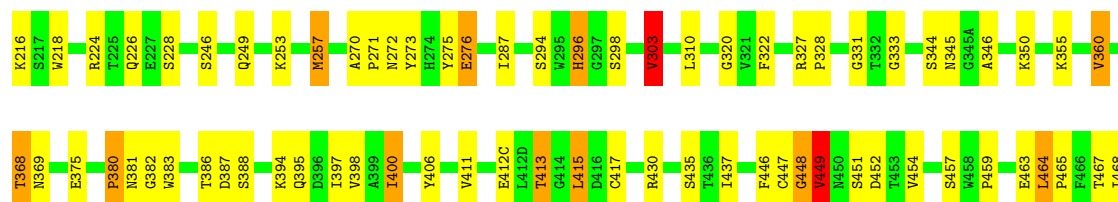


• Molecule 1: Neuraminidase



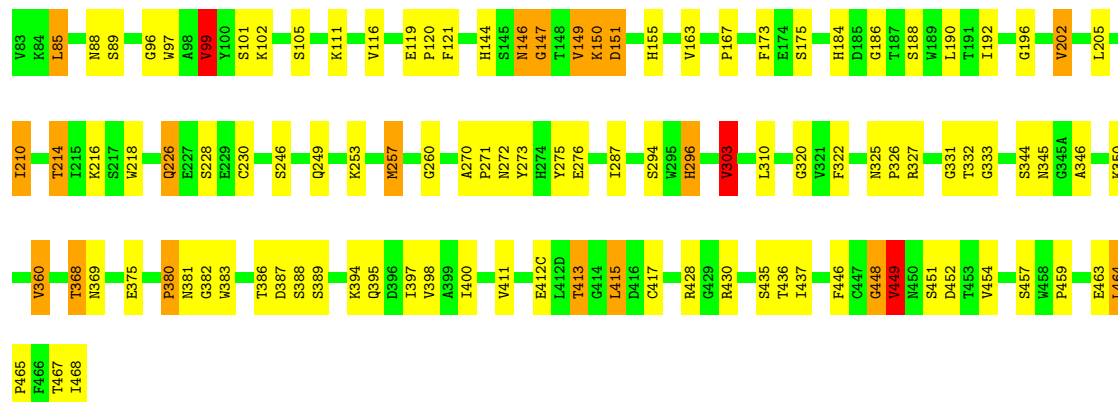
• Molecule 1: Neuraminidase





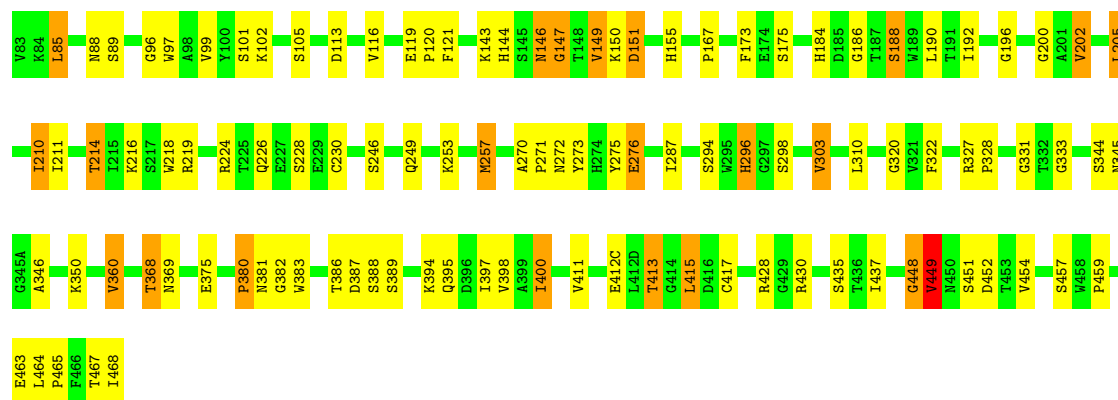
• Molecule 1: Neuraminidase

Chain D: 72% 22% 5% •



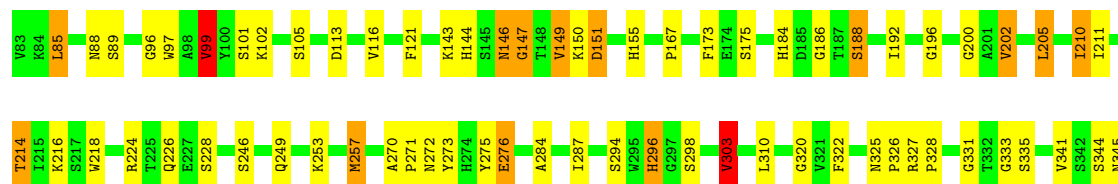
• Molecule 1: Neuraminidase

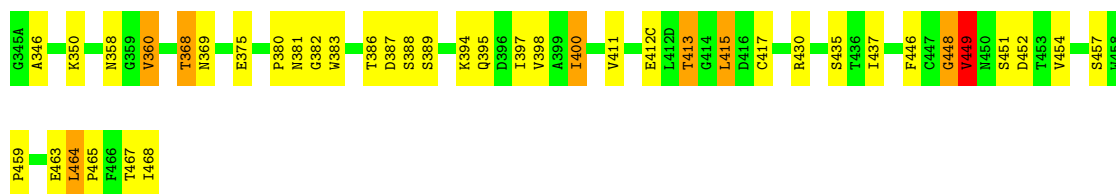
Chain E: 72% 22% 5% •



• Molecule 1: Neuraminidase

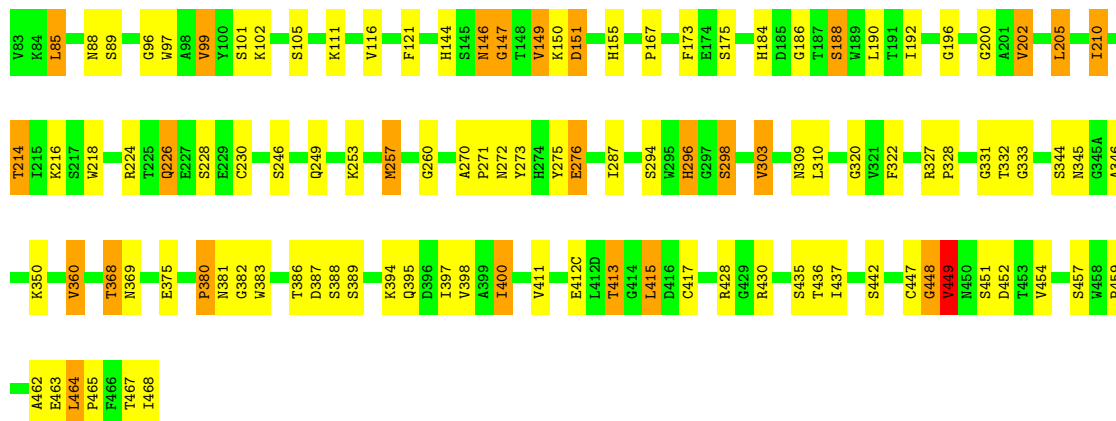
Chain F: 72% 22% 5% •





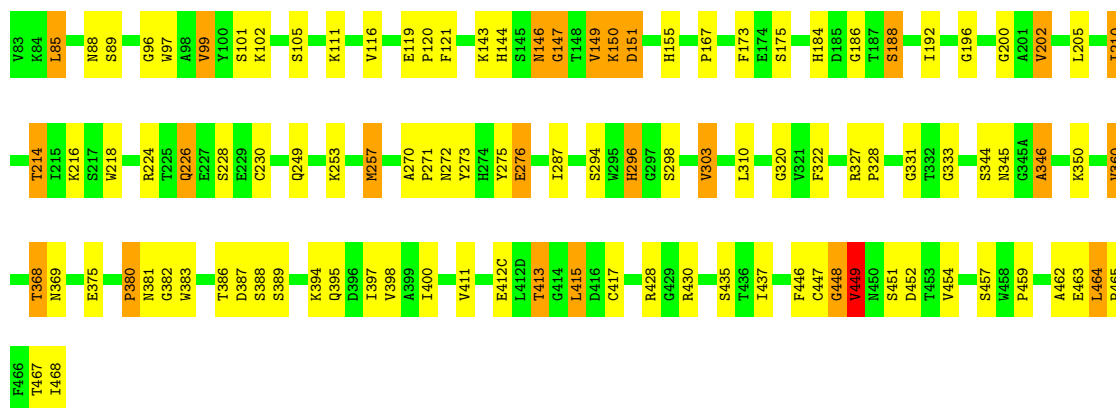
● Molecule 1: Neuraminidase

Chain G: 71% 22% 6%



● Molecule 1: Neuraminidase

Chain H: 72% 21% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	290.65Å 290.65Å 133.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 2.54 29.85 – 2.54	Depositor EDS
% Data completeness (in resolution range)	90.4 (29.85-2.54) 91.2 (29.85-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239 , 0.263 0.230 , 0.254	Depositor DCC
R_{free} test set	9674 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	23840	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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	0.55	0/3043	0.90	7/4138 (0.2%)
1	B	0.54	0/3043	0.91	7/4138 (0.2%)
1	C	0.55	0/3043	0.89	8/4138 (0.2%)
1	D	0.54	0/3043	0.89	8/4138 (0.2%)
1	E	0.54	0/3043	0.90	4/4138 (0.1%)
1	F	0.55	0/3043	0.89	6/4138 (0.1%)
1	G	0.54	0/3043	0.89	6/4138 (0.1%)
1	H	0.56	0/3043	0.90	6/4138 (0.1%)
All	All	0.55	0/24344	0.90	52/33104 (0.2%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	GLN	N-CA-C	6.94	118.85	111.28
1	D	246	SER	N-CA-C	-6.41	105.21	113.16
1	A	246	SER	N-CA-C	-6.37	105.47	113.18
1	B	246	SER	N-CA-C	-6.08	105.82	113.18
1	F	226	GLN	N-CA-C	6.06	117.97	111.36
1	F	196	GLY	CA-C-N	6.00	125.91	119.85
1	F	196	GLY	C-N-CA	6.00	125.91	119.85
1	A	226	GLN	N-CA-C	5.99	117.81	111.28
1	B	226	GLN	N-CA-C	5.86	117.75	111.36
1	D	380	PRO	N-CA-C	-5.83	102.66	111.41
1	A	196	GLY	CA-C-N	5.79	125.69	119.85
1	A	196	GLY	C-N-CA	5.79	125.69	119.85
1	H	196	GLY	CA-C-N	5.70	126.18	120.14
1	H	196	GLY	C-N-CA	5.70	126.18	120.14
1	D	226	GLN	N-CA-C	5.68	117.48	111.28
1	C	246	SER	N-CA-C	-5.65	106.34	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	226	GLN	N-CA-C	5.61	117.39	111.28
1	C	196	GLY	CA-C-N	5.61	125.51	119.85
1	C	196	GLY	C-N-CA	5.61	125.51	119.85
1	F	303	VAL	CB-CA-C	-5.54	101.53	110.28
1	G	226	GLN	N-CA-C	5.50	117.35	111.36
1	G	246	SER	N-CA-C	-5.49	106.53	113.18
1	C	150	LYS	N-CA-C	5.48	117.71	111.02
1	D	196	GLY	CA-C-N	5.47	125.38	119.85
1	D	196	GLY	C-N-CA	5.47	125.38	119.85
1	C	303	VAL	CB-CA-C	-5.46	101.65	110.28
1	A	303	VAL	CB-CA-C	-5.43	101.69	110.28
1	B	99	VAL	CB-CA-C	-5.43	102.74	111.59
1	E	196	GLY	CA-C-N	5.43	125.33	119.85
1	E	196	GLY	C-N-CA	5.43	125.33	119.85
1	G	380	PRO	N-CA-C	-5.37	103.36	111.41
1	B	196	GLY	CA-C-N	5.37	125.27	119.85
1	B	196	GLY	C-N-CA	5.37	125.27	119.85
1	F	99	VAL	CB-CA-C	-5.35	102.86	111.59
1	E	246	SER	N-CA-C	-5.33	106.73	113.18
1	F	246	SER	N-CA-C	-5.31	106.78	113.20
1	H	380	PRO	N-CA-C	-5.30	103.47	111.41
1	D	99	VAL	CB-CA-C	-5.29	102.69	111.32
1	E	380	PRO	N-CA-C	-5.28	103.49	111.41
1	C	380	PRO	N-CA-C	-5.26	103.52	111.41
1	H	150	LYS	N-CA-C	5.24	117.42	111.02
1	B	303	VAL	CB-CA-C	-5.24	102.01	110.28
1	C	99	VAL	CB-CA-C	-5.24	103.06	111.59
1	D	303	VAL	CB-CA-C	-5.21	102.04	110.28
1	B	150	LYS	N-CA-C	5.20	117.35	111.11
1	G	196	GLY	CA-C-N	5.17	125.62	120.14
1	G	196	GLY	C-N-CA	5.17	125.62	120.14
1	A	99	VAL	CB-CA-C	-5.15	102.92	111.32
1	D	150	LYS	N-CA-C	5.14	117.30	111.02
1	H	346	ALA	N-CA-C	5.12	116.55	111.07
1	G	99	VAL	CB-CA-C	-5.09	103.02	111.32
1	A	150	LYS	N-CA-C	5.04	117.17	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2960	0	2782	108	0
1	B	2960	0	2782	110	0
1	C	2960	0	2782	106	0
1	D	2960	0	2782	105	0
1	E	2960	0	2782	115	0
1	F	2960	0	2782	118	1
1	G	2960	0	2782	115	0
1	H	2960	0	2782	114	0
2	A	20	0	23	0	0
2	B	20	0	23	0	0
2	C	20	0	23	1	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	23840	0	22440	730	1

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 16.

All (730) 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:A:452:ASP:O	1:C:214:THR:HG21	1.39	1.19
1:F:216:LYS:NZ	1:G:452:ASP:HB2	1.60	1.14
1:E:216:LYS:NZ	1:H:452:ASP:HB2	1.63	1.13
1:F:452:ASP:O	1:H:214:THR:HG21	1.50	1.12
1:F:214:THR:HG21	1:G:452:ASP:O	1.48	1.11
1:B:216:LYS:NZ	1:C:452:ASP:HB2	1.66	1.10
1:B:452:ASP:O	1:D:214:THR:HG21	1.51	1.08
1:G:249:GLN:NE2	1:G:272:ASN:H	1.51	1.08
1:A:413:THR:HG22	1:A:415:LEU:H	1.18	1.08
1:B:214:THR:HG21	1:C:452:ASP:O	1.54	1.07
1:A:216:LYS:NZ	1:D:452:ASP:HB2	1.73	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:413:THR:HG22	1:G:415:LEU:H	1.20	1.04
1:H:249:GLN:NE2	1:H:272:ASN:H	1.54	1.03
1:C:413:THR:HG22	1:C:415:LEU:H	1.22	1.03
1:E:452:ASP:O	1:G:214:THR:HG21	1.56	1.02
1:B:413:THR:HG22	1:B:415:LEU:H	1.22	1.02
1:A:214:THR:HG21	1:D:452:ASP:O	1.61	1.00
1:D:249:GLN:NE2	1:D:272:ASN:H	1.60	0.99
1:B:216:LYS:HZ3	1:C:452:ASP:HB2	1.24	0.99
1:F:413:THR:HG22	1:F:415:LEU:H	1.25	0.99
1:H:413:THR:HG22	1:H:415:LEU:H	1.26	0.98
1:B:249:GLN:NE2	1:B:272:ASN:H	1.61	0.98
1:F:144:HIS:HE1	1:G:463:GLU:H	1.11	0.97
1:D:413:THR:HG22	1:D:415:LEU:H	1.29	0.97
1:A:249:GLN:NE2	1:A:272:ASN:H	1.63	0.96
1:E:216:LYS:HZ3	1:H:452:ASP:HB2	1.32	0.95
1:F:249:GLN:NE2	1:F:272:ASN:H	1.64	0.95
1:A:144:HIS:HE1	1:D:463:GLU:H	1.14	0.95
1:C:249:GLN:NE2	1:C:272:ASN:H	1.65	0.94
1:E:413:THR:HG22	1:E:415:LEU:H	1.30	0.94
1:G:150:LYS:O	1:G:151:ASP:HB2	1.68	0.93
1:B:150:LYS:O	1:B:151:ASP:HB2	1.65	0.93
1:E:214:THR:HB	1:H:451:SER:OG	1.69	0.92
1:D:150:LYS:O	1:D:151:ASP:HB2	1.67	0.92
1:E:214:THR:HG21	1:H:452:ASP:O	1.70	0.92
1:E:249:GLN:NE2	1:E:272:ASN:H	1.67	0.92
1:E:150:LYS:O	1:E:151:ASP:HB2	1.70	0.92
1:F:150:LYS:O	1:F:151:ASP:HB2	1.70	0.92
1:B:144:HIS:HE1	1:C:463:GLU:H	1.11	0.91
1:H:150:LYS:O	1:H:151:ASP:HB2	1.69	0.91
1:E:216:LYS:HZ2	1:H:452:ASP:HB2	1.36	0.91
1:E:144:HIS:HE1	1:H:463:GLU:H	1.14	0.91
1:C:150:LYS:O	1:C:151:ASP:HB2	1.72	0.90
1:A:249:GLN:HE21	1:A:272:ASN:H	1.18	0.89
1:F:216:LYS:HZ3	1:G:452:ASP:HB2	1.24	0.89
1:F:216:LYS:HZ2	1:G:452:ASP:HB2	1.38	0.89
1:F:413:THR:HG21	1:F:415:LEU:HD22	1.55	0.88
1:A:150:LYS:O	1:A:151:ASP:HB2	1.73	0.88
1:A:413:THR:HG21	1:A:415:LEU:HD22	1.56	0.88
1:B:249:GLN:HE21	1:B:272:ASN:H	1.18	0.87
1:F:85:LEU:HD12	1:F:412(C):GLU:HG3	1.56	0.87
1:G:249:GLN:HE21	1:G:272:ASN:H	1.17	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ASP:HB2	1:D:216:LYS:NZ	1.89	0.86
1:D:249:GLN:HE21	1:D:272:ASN:H	1.17	0.86
1:A:452:ASP:HB2	1:C:216:LYS:NZ	1.90	0.86
1:H:249:GLN:HE21	1:H:272:ASN:H	1.19	0.86
1:H:413:THR:HG21	1:H:415:LEU:HD22	1.57	0.86
1:B:413:THR:HG21	1:B:415:LEU:HD22	1.58	0.85
1:E:249:GLN:HE21	1:E:272:ASN:H	1.24	0.85
1:G:413:THR:HG21	1:G:415:LEU:HD22	1.56	0.85
1:D:413:THR:HG21	1:D:415:LEU:HD22	1.57	0.85
1:C:413:THR:HG21	1:C:415:LEU:HD22	1.59	0.85
1:F:249:GLN:HE21	1:F:272:ASN:H	1.24	0.85
1:A:85:LEU:HD12	1:A:412(C):GLU:HG3	1.58	0.84
1:E:413:THR:HG21	1:E:415:LEU:HD22	1.59	0.83
1:A:216:LYS:HZ2	1:D:452:ASP:HB2	1.40	0.83
1:E:85:LEU:HD12	1:E:412(C):GLU:HG3	1.60	0.83
1:F:144:HIS:CE1	1:G:463:GLU:H	1.96	0.83
1:D:85:LEU:HD12	1:D:412(C):GLU:HG3	1.59	0.83
1:B:144:HIS:CE1	1:C:463:GLU:H	1.97	0.83
1:C:249:GLN:HE21	1:C:272:ASN:H	1.24	0.82
1:H:85:LEU:HD12	1:H:412(C):GLU:HG3	1.60	0.82
1:F:214:THR:HB	1:G:451:SER:OG	1.79	0.82
1:D:89:SER:OG	1:D:417:CYS:HA	1.80	0.81
1:E:200:GLY:O	1:H:454:VAL:HG11	1.78	0.81
1:E:210:ILE:HD12	1:H:413:THR:HA	1.61	0.81
1:A:214:THR:HB	1:D:451:SER:OG	1.80	0.81
1:C:85:LEU:HD12	1:C:412(C):GLU:HG3	1.60	0.81
1:A:413:THR:HG22	1:A:415:LEU:N	1.96	0.80
1:B:85:LEU:HD12	1:B:412(C):GLU:HG3	1.64	0.80
1:G:413:THR:HG22	1:G:415:LEU:N	1.96	0.80
1:G:249:GLN:NE2	1:G:272:ASN:N	2.29	0.80
1:E:144:HIS:CE1	1:H:463:GLU:H	2.00	0.80
1:A:216:LYS:HZ3	1:D:452:ASP:HB2	1.43	0.80
1:E:452:ASP:HB2	1:G:216:LYS:NZ	1.96	0.80
1:F:452:ASP:HB2	1:H:216:LYS:NZ	1.97	0.80
1:B:89:SER:OG	1:B:417:CYS:HA	1.81	0.79
1:C:89:SER:OG	1:C:417:CYS:HA	1.82	0.79
1:G:89:SER:OG	1:G:417:CYS:HA	1.82	0.79
1:B:200:GLY:O	1:C:454:VAL:HG11	1.82	0.79
1:G:85:LEU:HD12	1:G:412(C):GLU:HG3	1.63	0.79
1:F:200:GLY:O	1:G:454:VAL:HG11	1.83	0.79
1:F:216:LYS:NZ	1:G:452:ASP:CB	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:SER:OG	1:E:417:CYS:HA	1.83	0.79
1:H:89:SER:OG	1:H:417:CYS:HA	1.82	0.78
1:F:463:GLU:H	1:H:144:HIS:HE1	1.30	0.78
1:H:249:GLN:NE2	1:H:272:ASN:N	2.31	0.77
1:B:214:THR:HB	1:C:451:SER:OG	1.83	0.77
1:B:413:THR:HG22	1:B:415:LEU:N	1.98	0.77
1:G:397:ILE:HG22	1:G:398:VAL:HG23	1.67	0.77
1:A:89:SER:OG	1:A:417:CYS:HA	1.85	0.77
1:H:413:THR:HG22	1:H:415:LEU:N	2.00	0.76
1:B:216:LYS:NZ	1:C:452:ASP:CB	2.47	0.76
1:F:89:SER:OG	1:F:417:CYS:HA	1.85	0.76
1:A:144:HIS:CE1	1:D:463:GLU:H	2.03	0.75
1:A:397:ILE:HG22	1:A:398:VAL:HG23	1.67	0.75
1:C:413:THR:HG22	1:C:415:LEU:N	1.99	0.75
1:B:216:LYS:HZ2	1:C:452:ASP:HB2	1.48	0.75
1:F:413:THR:HG22	1:F:415:LEU:N	2.01	0.74
1:H:413:THR:HG21	1:H:415:LEU:HB2	1.69	0.74
1:D:413:THR:HG22	1:D:415:LEU:N	2.03	0.74
1:E:184:HIS:HD2	1:E:186:GLY:H	1.36	0.74
1:F:184:HIS:HD2	1:F:186:GLY:H	1.37	0.73
1:B:249:GLN:NE2	1:B:272:ASN:N	2.36	0.73
1:C:97:TRP:H	1:C:395:GLN:HE22	1.35	0.72
1:C:413:THR:HG21	1:C:415:LEU:HB2	1.71	0.72
1:E:463:GLU:H	1:G:144:HIS:HE1	1.36	0.72
1:G:413:THR:HG21	1:G:415:LEU:HB2	1.71	0.72
1:E:413:THR:HG22	1:E:415:LEU:N	2.03	0.72
1:D:249:GLN:NE2	1:D:272:ASN:N	2.36	0.72
1:G:249:GLN:NE2	1:G:271:PRO:HA	2.05	0.72
1:B:397:ILE:HG22	1:B:398:VAL:HG23	1.71	0.71
1:F:102:LYS:HZ2	1:H:155:HIS:HD2	1.38	0.71
1:A:200:GLY:O	1:D:454:VAL:HG11	1.90	0.71
1:D:331:GLY:O	1:D:388:SER:HB3	1.90	0.71
1:F:143:LYS:HE3	1:G:463:GLU:HG3	1.73	0.71
1:B:97:TRP:H	1:B:395:GLN:HE22	1.36	0.71
1:B:463:GLU:H	1:D:144:HIS:HE1	1.35	0.70
1:G:249:GLN:HE22	1:G:271:PRO:HA	1.57	0.70
1:H:249:GLN:NE2	1:H:271:PRO:HA	2.07	0.70
1:E:397:ILE:HG22	1:E:398:VAL:HG23	1.72	0.70
1:H:397:ILE:HG22	1:H:398:VAL:HG23	1.74	0.70
1:G:184:HIS:HD2	1:G:186:GLY:H	1.38	0.70
1:E:143:LYS:HE3	1:H:463:GLU:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:VAL:HG13	1:G:383:TRP:HE3	1.57	0.70
1:F:184:HIS:CD2	1:F:186:GLY:H	2.10	0.70
1:F:144:HIS:HE1	1:G:463:GLU:N	1.89	0.69
1:F:413:THR:CG2	1:F:415:LEU:HD22	2.22	0.69
1:A:452:ASP:HB2	1:C:216:LYS:HZ3	1.57	0.69
1:B:143:LYS:HE3	1:C:463:GLU:HG3	1.75	0.69
1:A:454:VAL:HG22	1:C:202:VAL:CG1	2.22	0.69
1:F:464:LEU:HB3	1:F:465:PRO:HA	1.73	0.69
1:B:452:ASP:HB2	1:D:216:LYS:HZ2	1.57	0.69
1:E:331:GLY:O	1:E:388:SER:HB3	1.91	0.69
1:A:331:GLY:O	1:A:388:SER:HB3	1.92	0.69
1:G:413:THR:CG2	1:G:415:LEU:HD22	2.22	0.69
1:A:249:GLN:NE2	1:A:272:ASN:N	2.39	0.69
1:D:360:VAL:HG13	1:D:383:TRP:HE3	1.58	0.69
1:H:249:GLN:HE22	1:H:271:PRO:HA	1.58	0.69
1:D:397:ILE:HG22	1:D:398:VAL:HG23	1.75	0.69
1:G:97:TRP:H	1:G:395:GLN:HE22	1.40	0.69
1:B:413:THR:HG21	1:B:415:LEU:HB2	1.74	0.68
1:E:464:LEU:HB3	1:E:465:PRO:HA	1.74	0.68
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.76	0.68
1:F:413:THR:HG21	1:F:415:LEU:HB2	1.74	0.68
1:E:155:HIS:HD2	1:H:102:LYS:HZ2	1.41	0.68
1:H:413:THR:CG2	1:H:415:LEU:HB2	2.23	0.68
1:D:413:THR:CG2	1:D:415:LEU:HD22	2.24	0.68
1:A:210:ILE:HD12	1:D:413:THR:HA	1.76	0.68
1:A:452:ASP:CB	1:C:216:LYS:NZ	2.56	0.68
1:B:102:LYS:HZ2	1:D:155:HIS:HD2	1.42	0.68
1:C:228:SER:HB3	1:C:350:LYS:HE2	1.76	0.68
1:F:397:ILE:HG22	1:F:398:VAL:HG23	1.75	0.68
1:G:413:THR:CG2	1:G:415:LEU:HB2	2.24	0.68
1:A:413:THR:HG21	1:A:415:LEU:HB2	1.75	0.68
1:A:143:LYS:HE3	1:D:463:GLU:HG3	1.75	0.67
1:C:397:ILE:HG22	1:C:398:VAL:HG23	1.76	0.67
1:H:413:THR:CG2	1:H:415:LEU:HD22	2.25	0.67
1:B:331:GLY:O	1:B:388:SER:HB3	1.95	0.67
1:E:413:THR:HG21	1:E:415:LEU:HB2	1.75	0.67
1:E:184:HIS:CD2	1:E:186:GLY:H	2.12	0.67
1:G:331:GLY:O	1:G:388:SER:HB3	1.95	0.67
1:H:360:VAL:HG13	1:H:383:TRP:HE3	1.59	0.67
1:A:184:HIS:HD2	1:A:186:GLY:H	1.41	0.67
1:A:464:LEU:HB3	1:A:465:PRO:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:THR:CG2	1:B:415:LEU:HD22	2.24	0.67
1:D:464:LEU:HB3	1:D:465:PRO:HA	1.75	0.67
1:B:216:LYS:HZ3	1:C:452:ASP:CB	2.03	0.67
1:C:360:VAL:HG13	1:C:383:TRP:HE3	1.60	0.67
1:C:413:THR:CG2	1:C:415:LEU:HB2	2.25	0.67
1:C:464:LEU:HB3	1:C:465:PRO:HA	1.76	0.67
1:G:184:HIS:CD2	1:G:186:GLY:H	2.12	0.67
1:A:413:THR:CG2	1:A:415:LEU:HD22	2.24	0.67
1:H:464:LEU:HB3	1:H:465:PRO:HA	1.77	0.67
1:B:464:LEU:HB3	1:B:465:PRO:HA	1.78	0.66
1:F:97:TRP:H	1:F:395:GLN:HE22	1.42	0.66
1:F:216:LYS:HZ2	1:G:452:ASP:CB	2.07	0.66
1:G:464:LEU:HB3	1:G:465:PRO:HA	1.77	0.66
1:B:202:VAL:CG1	1:C:454:VAL:HG22	2.25	0.66
1:D:413:THR:HG21	1:D:415:LEU:HB2	1.77	0.66
1:H:97:TRP:H	1:H:395:GLN:HE22	1.42	0.66
1:C:249:GLN:HE22	1:C:271:PRO:HA	1.60	0.66
1:D:249:GLN:NE2	1:D:271:PRO:HA	2.10	0.66
1:E:144:HIS:HE1	1:H:463:GLU:N	1.91	0.66
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.76	0.66
1:B:452:ASP:CB	1:D:216:LYS:NZ	2.58	0.66
1:C:249:GLN:NE2	1:C:271:PRO:HA	2.11	0.66
1:F:360:VAL:HG13	1:F:383:TRP:HE3	1.61	0.66
1:H:184:HIS:HD2	1:H:186:GLY:H	1.42	0.65
1:B:454:VAL:HG22	1:D:202:VAL:CG1	2.26	0.65
1:D:184:HIS:CD2	1:D:186:GLY:H	2.15	0.65
1:E:102:LYS:HZ2	1:G:155:HIS:HD2	1.42	0.65
1:D:184:HIS:HD2	1:D:186:GLY:H	1.43	0.65
1:B:144:HIS:HE1	1:C:463:GLU:N	1.90	0.65
1:A:97:TRP:H	1:A:395:GLN:HE22	1.43	0.65
1:A:249:GLN:NE2	1:A:271:PRO:HA	2.11	0.65
1:A:463:GLU:H	1:C:144:HIS:HE1	1.44	0.65
1:E:360:VAL:HG13	1:E:383:TRP:HE3	1.60	0.65
1:F:249:GLN:NE2	1:F:272:ASN:N	2.40	0.65
1:F:331:GLY:O	1:F:388:SER:HB3	1.95	0.65
1:A:249:GLN:HE22	1:A:271:PRO:HA	1.62	0.65
1:C:184:HIS:HD2	1:C:186:GLY:H	1.44	0.65
1:E:249:GLN:NE2	1:E:272:ASN:N	2.42	0.65
1:E:228:SER:HB3	1:E:350:LYS:HE2	1.78	0.65
1:B:360:VAL:HG13	1:B:383:TRP:HE3	1.61	0.65
1:D:228:SER:HB3	1:D:350:LYS:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:THR:CG2	1:C:415:LEU:HD22	2.27	0.64
1:E:452:ASP:HB2	1:G:216:LYS:HZ2	1.62	0.64
1:B:184:HIS:HD2	1:B:186:GLY:H	1.45	0.64
1:B:452:ASP:HB2	1:D:216:LYS:HZ3	1.61	0.64
1:E:216:LYS:NZ	1:H:452:ASP:CB	2.53	0.64
1:A:228:SER:HB3	1:A:350:LYS:CE	2.28	0.64
1:E:413:THR:CG2	1:E:415:LEU:HD22	2.28	0.64
1:H:184:HIS:CD2	1:H:186:GLY:H	2.16	0.64
1:A:184:HIS:CD2	1:A:186:GLY:H	2.17	0.63
1:F:155:HIS:HD2	1:G:102:LYS:HZ2	1.47	0.63
1:G:228:SER:HB3	1:G:350:LYS:HE2	1.79	0.63
1:C:331:GLY:O	1:C:388:SER:HB3	1.98	0.63
1:D:249:GLN:HE22	1:D:271:PRO:HA	1.63	0.63
1:F:210:ILE:HD12	1:G:413:THR:HA	1.79	0.63
1:A:413:THR:CG2	1:A:415:LEU:HB2	2.29	0.63
1:E:211:ILE:HD12	1:H:447:CYS:HB2	1.80	0.63
1:F:228:SER:HB3	1:F:350:LYS:HE2	1.79	0.63
1:A:360:VAL:HG13	1:A:383:TRP:HE3	1.61	0.63
1:C:184:HIS:CD2	1:C:186:GLY:H	2.17	0.63
1:F:452:ASP:HB2	1:H:216:LYS:HZ3	1.62	0.63
1:B:184:HIS:CD2	1:B:186:GLY:H	2.16	0.62
1:B:413:THR:CG2	1:B:415:LEU:HB2	2.29	0.62
1:F:413:THR:CG2	1:F:415:LEU:HB2	2.28	0.62
1:H:228:SER:HB3	1:H:350:LYS:HE2	1.79	0.62
1:A:144:HIS:HE1	1:D:463:GLU:N	1.93	0.62
1:E:413:THR:CG2	1:E:415:LEU:HB2	2.28	0.62
1:B:249:GLN:NE2	1:B:271:PRO:HA	2.15	0.62
1:F:211:ILE:HD12	1:G:447:CYS:HB2	1.81	0.62
1:F:463:GLU:H	1:H:144:HIS:CE1	2.14	0.62
1:D:97:TRP:H	1:D:395:GLN:HE22	1.45	0.62
1:E:249:GLN:HE22	1:E:271:PRO:HA	1.64	0.62
1:A:452:ASP:HB2	1:C:216:LYS:HZ2	1.64	0.62
1:C:249:GLN:NE2	1:C:272:ASN:N	2.41	0.62
1:F:249:GLN:HE22	1:F:271:PRO:HA	1.64	0.62
1:F:454:VAL:HG22	1:H:202:VAL:CG1	2.31	0.61
1:B:228:SER:HB3	1:B:350:LYS:CE	2.31	0.61
1:E:97:TRP:H	1:E:395:GLN:HE22	1.48	0.61
1:E:249:GLN:NE2	1:E:271:PRO:HA	2.15	0.61
1:F:249:GLN:NE2	1:F:271:PRO:HA	2.15	0.61
1:E:452:ASP:HB2	1:G:216:LYS:HZ3	1.65	0.61
1:D:413:THR:CG2	1:D:415:LEU:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:GLY:O	1:D:448:GLY:O	2.19	0.60
1:F:202:VAL:CG1	1:G:454:VAL:HG22	2.30	0.60
1:A:155:HIS:HD2	1:D:102:LYS:HZ2	1.48	0.60
1:A:216:LYS:NZ	1:D:452:ASP:CB	2.58	0.60
1:D:333:GLY:H	1:D:386:THR:HG22	1.67	0.60
1:D:228:SER:HB3	1:D:350:LYS:CE	2.31	0.60
1:C:333:GLY:H	1:C:386:THR:HG22	1.66	0.60
1:A:454:VAL:HG22	1:C:202:VAL:HG11	1.83	0.60
1:F:102:LYS:NZ	1:H:155:HIS:HD2	2.00	0.60
1:F:454:VAL:HG11	1:H:200:GLY:O	2.02	0.60
1:A:216:LYS:HZ2	1:D:452:ASP:CB	2.13	0.59
1:F:451:SER:OG	1:H:214:THR:HB	2.02	0.59
1:E:454:VAL:HG22	1:G:202:VAL:CG1	2.32	0.59
1:C:228:SER:HB3	1:C:350:LYS:CE	2.32	0.59
1:B:97:TRP:N	1:B:395:GLN:HE22	2.01	0.59
1:B:249:GLN:HE22	1:B:271:PRO:HA	1.67	0.59
1:G:105:SER:HB3	1:G:167:PRO:HD2	1.85	0.59
1:G:368:THR:HG22	1:G:369:ASN:OD1	2.03	0.59
1:F:452:ASP:HB2	1:H:216:LYS:HZ2	1.69	0.58
1:E:451:SER:OG	1:G:214:THR:HB	2.02	0.58
1:G:360:VAL:CG1	1:G:383:TRP:HE3	2.16	0.58
1:D:146:ASN:ND2	1:D:437:ILE:HB	2.18	0.58
1:B:155:HIS:HD2	1:C:102:LYS:HZ2	1.49	0.58
1:E:463:GLU:H	1:G:144:HIS:CE1	2.20	0.58
1:F:228:SER:HB3	1:F:350:LYS:CE	2.34	0.58
1:G:413:THR:HG21	1:G:415:LEU:CD2	2.32	0.58
1:H:368:THR:HG22	1:H:369:ASN:OD1	2.04	0.58
1:C:368:THR:HG22	1:C:369:ASN:OD1	2.03	0.58
1:D:105:SER:HB3	1:D:167:PRO:HD2	1.86	0.58
1:C:448:GLY:O	1:C:449:VAL:HB	2.04	0.58
1:H:331:GLY:O	1:H:388:SER:HB3	2.04	0.58
1:F:275:TYR:CE2	1:F:303:VAL:HG22	2.38	0.57
1:B:294:SER:O	1:B:346:ALA:O	2.22	0.57
1:E:448:GLY:O	1:E:449:VAL:HB	2.04	0.57
1:G:322:PHE:HB2	1:G:327:ARG:HD2	1.85	0.57
1:H:228:SER:HB3	1:H:350:LYS:CE	2.34	0.57
1:G:146:ASN:ND2	1:G:437:ILE:HB	2.20	0.57
1:H:105:SER:HB3	1:H:167:PRO:HD2	1.86	0.57
1:D:368:THR:HG22	1:D:369:ASN:OD1	2.05	0.57
1:A:333:GLY:H	1:A:386:THR:HG22	1.69	0.57
1:A:105:SER:HB3	1:A:167:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:SER:HB3	1:E:350:LYS:CE	2.35	0.57
1:F:368:THR:HG22	1:F:369:ASN:OD1	2.05	0.57
1:G:228:SER:HB3	1:G:350:LYS:CE	2.35	0.57
1:A:218:TRP:CE2	1:A:253:LYS:HE3	2.40	0.56
1:A:96:GLY:O	1:A:448:GLY:O	2.23	0.56
1:A:452:ASP:CB	1:C:216:LYS:HZ3	2.15	0.56
1:B:105:SER:HB3	1:B:167:PRO:HD2	1.87	0.56
1:C:218:TRP:CE2	1:C:253:LYS:HE3	2.40	0.56
1:F:333:GLY:H	1:F:386:THR:HG22	1.70	0.56
1:C:146:ASN:ND2	1:C:437:ILE:HB	2.21	0.56
1:A:294:SER:O	1:A:346:ALA:O	2.23	0.56
1:E:457:SER:O	1:E:459:PRO:HD3	2.05	0.56
1:E:192:ILE:HD11	1:E:257:MET:HE1	1.88	0.56
1:E:368:THR:HG22	1:E:369:ASN:OD1	2.06	0.56
1:G:344:SER:O	1:G:345:ASN:HB2	2.05	0.56
1:B:368:THR:HG22	1:B:369:ASN:OD1	2.06	0.56
1:B:381:ASN:O	1:B:387:ASP:OD1	2.24	0.56
1:B:454:VAL:HG22	1:D:202:VAL:HG11	1.87	0.56
1:F:150:LYS:O	1:F:151:ASP:CB	2.51	0.56
1:H:360:VAL:CG1	1:H:383:TRP:HE3	2.18	0.56
1:E:452:ASP:CB	1:G:216:LYS:NZ	2.68	0.56
1:F:105:SER:HB3	1:F:167:PRO:HD2	1.87	0.56
1:G:448:GLY:O	1:G:449:VAL:HB	2.06	0.56
1:F:413:THR:HA	1:H:210:ILE:HD12	1.87	0.55
1:H:275:TYR:CE2	1:H:303:VAL:HG22	2.41	0.55
1:B:210:ILE:HD12	1:C:413:THR:HA	1.88	0.55
1:B:275:TYR:CE2	1:B:303:VAL:HG22	2.40	0.55
1:D:457:SER:O	1:D:459:PRO:HD3	2.07	0.55
1:F:413:THR:HG21	1:F:415:LEU:CD2	2.32	0.55
1:B:360:VAL:CG1	1:B:383:TRP:HE3	2.19	0.55
1:E:294:SER:O	1:E:346:ALA:O	2.24	0.55
1:F:173:PHE:CZ	1:G:101:SER:HA	2.41	0.55
1:H:146:ASN:HD22	1:H:147:GLY:H	1.55	0.55
1:A:448:GLY:O	1:A:449:VAL:HB	2.06	0.55
1:A:333:GLY:H	1:A:386:THR:CG2	2.20	0.55
1:C:105:SER:HB3	1:C:167:PRO:HD2	1.89	0.55
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.89	0.55
1:E:380:PRO:O	1:E:381:ASN:C	2.49	0.55
1:A:146:ASN:HD22	1:A:147:GLY:H	1.54	0.55
1:H:150:LYS:O	1:H:151:ASP:CB	2.51	0.55
1:A:368:THR:HG22	1:A:369:ASN:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.88	0.55
1:E:322:PHE:HB2	1:E:327:ARG:HD2	1.89	0.55
1:F:452:ASP:CB	1:H:216:LYS:NZ	2.68	0.55
1:C:360:VAL:CG1	1:C:383:TRP:HE3	2.19	0.54
1:D:360:VAL:CG1	1:D:383:TRP:HE3	2.19	0.54
1:E:467:THR:O	1:E:468:ILE:HB	2.07	0.54
1:E:216:LYS:HZ2	1:H:452:ASP:CB	2.14	0.54
1:E:360:VAL:CG1	1:E:383:TRP:HE3	2.19	0.54
1:E:381:ASN:O	1:E:387:ASP:OD1	2.25	0.54
1:F:216:LYS:HZ3	1:G:452:ASP:CB	2.09	0.54
1:A:381:ASN:O	1:A:387:ASP:OD1	2.25	0.54
1:A:452:ASP:CB	1:C:216:LYS:HZ2	2.18	0.54
1:B:202:VAL:HG12	1:C:454:VAL:HG22	1.89	0.54
1:D:413:THR:HG21	1:D:415:LEU:CD2	2.35	0.54
1:E:105:SER:HB3	1:E:167:PRO:HD2	1.88	0.54
1:F:202:VAL:HG12	1:G:454:VAL:HG22	1.88	0.54
1:G:97:TRP:N	1:G:395:GLN:HE22	2.04	0.54
1:G:467:THR:O	1:G:468:ILE:HB	2.06	0.54
1:D:380:PRO:O	1:D:381:ASN:C	2.51	0.54
1:H:322:PHE:HB2	1:H:327:ARG:HD2	1.89	0.54
1:B:463:GLU:H	1:D:144:HIS:CE1	2.22	0.54
1:B:467:THR:O	1:B:468:ILE:HB	2.08	0.54
1:A:202:VAL:CG1	1:D:454:VAL:HG22	2.37	0.54
1:E:146:ASN:ND2	1:E:437:ILE:HB	2.23	0.54
1:A:360:VAL:CG1	1:A:383:TRP:HE3	2.21	0.53
1:C:322:PHE:HB2	1:C:327:ARG:HD2	1.90	0.53
1:D:150:LYS:O	1:D:151:ASP:CB	2.49	0.53
1:H:467:THR:O	1:H:468:ILE:HB	2.08	0.53
1:A:413:THR:HG21	1:A:415:LEU:CD2	2.34	0.53
1:C:97:TRP:N	1:C:395:GLN:HE22	2.05	0.53
1:F:360:VAL:CG1	1:F:383:TRP:HE3	2.21	0.53
1:G:333:GLY:H	1:G:386:THR:HG22	1.74	0.53
1:H:96:GLY:O	1:H:448:GLY:O	2.27	0.53
1:H:457:SER:O	1:H:459:PRO:HD3	2.09	0.53
1:D:218:TRP:CE2	1:D:253:LYS:HE3	2.43	0.53
1:H:146:ASN:ND2	1:H:437:ILE:HB	2.24	0.53
1:A:102:LYS:HZ2	1:C:155:HIS:HD2	1.55	0.53
1:A:333:GLY:N	1:A:386:THR:CG2	2.71	0.53
1:C:96:GLY:O	1:C:448:GLY:O	2.27	0.53
1:E:155:HIS:CD2	1:H:102:LYS:HZ2	2.26	0.53
1:G:381:ASN:O	1:G:387:ASP:OD1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ASN:O	1:C:387:ASP:OD1	2.27	0.53
1:A:322:PHE:HB2	1:A:327:ARG:HD2	1.89	0.53
1:A:380:PRO:O	1:A:381:ASN:C	2.52	0.53
1:B:96:GLY:O	1:B:448:GLY:O	2.26	0.53
1:F:214:THR:CG2	1:G:452:ASP:O	2.39	0.53
1:F:322:PHE:HB2	1:F:327:ARG:HD2	1.91	0.53
1:D:192:ILE:HD11	1:D:257:MET:HE1	1.91	0.52
1:F:467:THR:O	1:F:468:ILE:HB	2.08	0.52
1:G:192:ILE:HD11	1:G:257:MET:HE1	1.91	0.52
1:G:249:GLN:HE22	1:G:272:ASN:N	2.06	0.52
1:A:452:ASP:CG	1:C:216:LYS:HZ2	2.17	0.52
1:C:294:SER:O	1:C:346:ALA:O	2.27	0.52
1:F:294:SER:O	1:F:346:ALA:O	2.27	0.52
1:G:375:GLU:OE1	1:G:394:LYS:HE3	2.08	0.52
1:D:448:GLY:O	1:D:449:VAL:HB	2.09	0.52
1:A:97:TRP:N	1:A:395:GLN:HE22	2.07	0.52
1:A:275:TYR:CE2	1:A:303:VAL:HG22	2.44	0.52
1:C:380:PRO:O	1:C:381:ASN:C	2.52	0.52
1:F:333:GLY:H	1:F:386:THR:CG2	2.23	0.52
1:F:381:ASN:O	1:F:387:ASP:OD1	2.26	0.52
1:D:467:THR:O	1:D:468:ILE:HB	2.08	0.52
1:F:113:ASP:OD1	1:G:111:LYS:HE2	2.10	0.52
1:H:287:ILE:N	1:H:287:ILE:HD12	2.25	0.52
1:H:381:ASN:O	1:H:387:ASP:OD1	2.27	0.52
1:H:413:THR:HG21	1:H:415:LEU:CD2	2.34	0.52
1:A:192:ILE:HD11	1:A:257:MET:HE1	1.92	0.52
1:D:226:GLN:HE22	1:D:230:CYS:HA	1.74	0.52
1:C:270:ALA:HB1	1:C:273:TYR:HB2	1.91	0.52
1:G:275:TYR:CE2	1:G:303:VAL:HG22	2.44	0.52
1:H:294:SER:O	1:H:346:ALA:O	2.27	0.52
1:A:467:THR:O	1:A:468:ILE:HB	2.10	0.52
1:B:448:GLY:O	1:B:449:VAL:HB	2.07	0.52
1:B:452:ASP:CB	1:D:216:LYS:HZ3	2.18	0.52
1:B:452:ASP:CB	1:D:216:LYS:HZ2	2.19	0.52
1:E:173:PHE:CZ	1:H:101:SER:HA	2.45	0.52
1:E:333:GLY:H	1:E:386:THR:HG22	1.75	0.52
1:B:333:GLY:H	1:B:386:THR:HG22	1.75	0.52
1:A:413:THR:HA	1:C:210:ILE:HD12	1.91	0.51
1:B:216:LYS:HZ2	1:C:452:ASP:CB	2.16	0.51
1:A:451:SER:OG	1:C:214:THR:HB	2.10	0.51
1:C:413:THR:HG21	1:C:415:LEU:CD2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ILE:HD11	1:C:257:MET:HE1	1.91	0.51
1:D:294:SER:O	1:D:346:ALA:O	2.28	0.51
1:F:146:ASN:ND2	1:F:437:ILE:HB	2.24	0.51
1:E:454:VAL:HG11	1:G:200:GLY:O	2.10	0.51
1:G:96:GLY:O	1:G:448:GLY:O	2.28	0.51
1:G:192:ILE:HG12	1:G:205:LEU:HD22	1.92	0.51
1:C:333:GLY:N	1:C:386:THR:CG2	2.74	0.51
1:E:275:TYR:CE2	1:E:303:VAL:HG22	2.44	0.51
1:H:375:GLU:OE1	1:H:394:LYS:HE3	2.11	0.51
1:B:146:ASN:ND2	1:B:437:ILE:HB	2.26	0.51
1:F:344:SER:O	1:F:345:ASN:HB2	2.10	0.51
1:E:96:GLY:O	1:E:448:GLY:O	2.28	0.51
1:B:270:ALA:HB1	1:B:273:TYR:HB2	1.93	0.51
1:B:451:SER:OG	1:D:214:THR:HB	2.11	0.50
1:C:457:SER:O	1:C:459:PRO:HD3	2.10	0.50
1:H:97:TRP:N	1:H:395:GLN:HE22	2.08	0.50
1:D:333:GLY:N	1:D:386:THR:CG2	2.74	0.50
1:E:375:GLU:OE1	1:E:394:LYS:HE3	2.12	0.50
1:A:113:ASP:OD1	1:D:111:LYS:HE2	2.12	0.50
1:F:380:PRO:O	1:F:381:ASN:C	2.52	0.50
1:H:146:ASN:ND2	1:H:147:GLY:H	2.09	0.50
1:F:96:GLY:O	1:F:448:GLY:O	2.28	0.50
1:F:101:SER:HA	1:H:173:PHE:CZ	2.46	0.50
1:C:320:GLY:HA3	1:C:331:GLY:O	2.12	0.50
1:A:226:GLN:HE22	1:A:230:CYS:HA	1.77	0.50
1:D:344:SER:O	1:D:345:ASN:HB2	2.10	0.50
1:E:97:TRP:N	1:E:395:GLN:HE22	2.10	0.50
1:E:413:THR:HG21	1:E:415:LEU:CD2	2.37	0.50
1:F:270:ALA:HB1	1:F:273:TYR:HB2	1.93	0.50
1:G:298:SER:OG	1:G:328:PRO:HD3	2.11	0.50
1:G:380:PRO:O	1:G:381:ASN:C	2.54	0.50
1:B:413:THR:HG21	1:B:415:LEU:CD2	2.34	0.50
1:D:270:ALA:HB1	1:D:273:TYR:HB2	1.94	0.50
1:F:375:GLU:OE1	1:F:394:LYS:HE3	2.12	0.50
1:G:294:SER:O	1:G:346:ALA:O	2.29	0.50
1:H:387:ASP:OD2	1:H:389:SER:O	2.29	0.50
1:E:413:THR:HA	1:G:210:ILE:HD12	1.93	0.50
1:H:270:ALA:HB1	1:H:273:TYR:HB2	1.94	0.50
1:D:333:GLY:C	1:D:386:THR:HG23	2.37	0.49
1:E:320:GLY:HA3	1:E:331:GLY:O	2.13	0.49
1:E:452:ASP:CB	1:G:216:LYS:HZ2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:GLY:N	1:F:386:THR:CG2	2.75	0.49
1:G:332:THR:HG22	1:G:386:THR:HG21	1.93	0.49
1:H:448:GLY:O	1:H:449:VAL:HB	2.11	0.49
1:A:146:ASN:ND2	1:A:147:GLY:H	2.10	0.49
1:D:381:ASN:O	1:D:387:ASP:OD1	2.31	0.49
1:A:320:GLY:HA3	1:A:331:GLY:O	2.13	0.49
1:B:320:GLY:HA3	1:B:331:GLY:O	2.13	0.49
1:F:448:GLY:O	1:F:449:VAL:HB	2.12	0.49
1:F:457:SER:O	1:F:459:PRO:HD3	2.12	0.49
1:H:298:SER:OG	1:H:328:PRO:HD3	2.13	0.49
1:A:101:SER:HA	1:C:173:PHE:CZ	2.47	0.49
1:A:155:HIS:HD2	1:D:102:LYS:NZ	2.10	0.49
1:B:428:ARG:NH1	1:B:464:LEU:HG	2.28	0.49
1:D:333:GLY:H	1:D:386:THR:CG2	2.24	0.49
1:F:146:ASN:HD22	1:F:147:GLY:H	1.59	0.49
1:B:192:ILE:HD11	1:B:257:MET:HE1	1.95	0.49
1:B:457:SER:O	1:B:459:PRO:HD3	2.11	0.49
1:E:216:LYS:HD3	1:H:452:ASP:OD2	2.12	0.49
1:E:144:HIS:CE1	1:H:462:ALA:HA	2.48	0.49
1:E:146:ASN:HD22	1:E:147:GLY:H	1.60	0.49
1:E:270:ALA:HB1	1:E:273:TYR:HB2	1.93	0.49
1:D:146:ASN:HD22	1:D:147:GLY:H	1.61	0.49
1:F:102:LYS:HZ2	1:H:155:HIS:CD2	2.24	0.49
1:F:320:GLY:HA3	1:F:331:GLY:O	2.13	0.48
1:G:360:VAL:HG13	1:G:383:TRP:CE3	2.44	0.48
1:A:375:GLU:OE1	1:A:394:LYS:HE3	2.14	0.48
1:G:146:ASN:HD22	1:G:147:GLY:H	1.62	0.48
1:C:150:LYS:O	1:C:151:ASP:CB	2.53	0.48
1:C:467:THR:O	1:C:468:ILE:HB	2.13	0.48
1:D:320:GLY:HA3	1:D:331:GLY:O	2.13	0.48
1:G:149:VAL:HG21	1:G:430:ARG:CZ	2.44	0.48
1:G:270:ALA:HB1	1:G:273:TYR:HB2	1.95	0.48
1:H:386:THR:HG22	1:H:386:THR:O	2.12	0.48
1:B:218:TRP:CE2	1:B:253:LYS:HE3	2.48	0.48
1:B:375:GLU:OE1	1:B:394:LYS:HE3	2.13	0.48
1:E:224:ARG:NE	1:E:276:GLU:OE1	2.43	0.48
1:G:457:SER:O	1:G:459:PRO:HD3	2.14	0.48
1:H:344:SER:O	1:H:345:ASN:HB2	2.12	0.48
1:A:457:SER:O	1:A:459:PRO:HD3	2.12	0.48
1:D:272:ASN:O	1:D:296:HIS:HE1	1.97	0.48
1:F:97:TRP:N	1:F:395:GLN:HE22	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:LYS:O	1:G:151:ASP:CB	2.49	0.48
1:B:146:ASN:HD22	1:B:147:GLY:H	1.60	0.48
1:B:380:PRO:O	1:B:381:ASN:C	2.57	0.48
1:E:101:SER:HA	1:G:173:PHE:CZ	2.49	0.48
1:G:400:ILE:H	1:G:400:ILE:HG13	1.48	0.48
1:A:149:VAL:HG21	1:A:430:ARG:CZ	2.43	0.47
1:A:452:ASP:OD2	1:C:216:LYS:NZ	2.43	0.47
1:B:89:SER:HG	1:B:417:CYS:HA	1.78	0.47
1:B:387:ASP:OD2	1:B:389:SER:O	2.32	0.47
1:E:272:ASN:O	1:E:296:HIS:HE1	1.97	0.47
1:H:192:ILE:HD11	1:H:257:MET:HE1	1.95	0.47
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.95	0.47
1:B:272:ASN:O	1:B:296:HIS:HE1	1.96	0.47
1:C:275:TYR:CE2	1:C:303:VAL:HG22	2.49	0.47
1:E:155:HIS:HD2	1:H:102:LYS:NZ	2.08	0.47
1:A:173:PHE:CZ	1:D:101:SER:HA	2.49	0.47
1:D:386:THR:HG22	1:D:386:THR:O	2.14	0.47
1:E:210:ILE:CD1	1:H:413:THR:HA	2.39	0.47
1:A:386:THR:HG22	1:A:386:THR:O	2.15	0.47
1:B:413:THR:HA	1:D:210:ILE:HD12	1.95	0.47
1:C:146:ASN:HD22	1:C:147:GLY:H	1.61	0.47
1:F:146:ASN:ND2	1:F:147:GLY:H	2.13	0.47
1:H:249:GLN:HE22	1:H:272:ASN:N	2.08	0.47
1:B:173:PHE:CZ	1:C:101:SER:HA	2.50	0.47
1:D:275:TYR:CE2	1:D:303:VAL:HG22	2.49	0.47
1:B:333:GLY:N	1:B:386:THR:CG2	2.78	0.47
1:C:333:GLY:N	1:C:386:THR:HG22	2.30	0.47
1:G:333:GLY:H	1:G:386:THR:CG2	2.28	0.47
1:A:224:ARG:NE	1:A:276:GLU:OE1	2.45	0.47
1:D:375:GLU:OE1	1:D:394:LYS:HE3	2.15	0.47
1:F:218:TRP:CE2	1:F:253:LYS:HE3	2.50	0.47
1:A:146:ASN:ND2	1:A:437:ILE:HB	2.30	0.46
1:A:192:ILE:HG12	1:A:205:LEU:HD22	1.97	0.46
1:H:320:GLY:HA3	1:H:331:GLY:O	2.14	0.46
1:A:150:LYS:O	1:A:151:ASP:CB	2.52	0.46
1:B:113:ASP:OD1	1:C:111:LYS:HE2	2.15	0.46
1:C:333:GLY:H	1:C:386:THR:CG2	2.26	0.46
1:F:400:ILE:H	1:F:400:ILE:HG13	1.49	0.46
1:B:333:GLY:H	1:B:386:THR:CG2	2.28	0.46
1:B:146:ASN:ND2	1:B:147:GLY:H	2.14	0.46
1:B:298:SER:OG	1:B:328:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:TYR:OH	2:C:802:G39:C2	2.64	0.46
1:D:287:ILE:N	1:D:287:ILE:HD12	2.30	0.46
1:H:149:VAL:HG21	1:H:430:ARG:CZ	2.45	0.46
1:B:149:VAL:HG21	1:B:430:ARG:CZ	2.45	0.46
1:E:214:THR:HB	1:H:451:SER:HG	1.77	0.46
1:E:298:SER:OG	1:E:328:PRO:HD3	2.16	0.46
1:G:218:TRP:CE2	1:G:253:LYS:HE3	2.51	0.46
1:H:218:TRP:CE2	1:H:253:LYS:HE3	2.51	0.46
1:A:344:SER:O	1:A:345:ASN:HB2	2.14	0.46
1:D:146:ASN:ND2	1:D:147:GLY:H	2.14	0.46
1:E:85:LEU:HD13	1:E:186:GLY:CA	2.46	0.46
1:B:344:SER:O	1:B:345:ASN:HB2	2.15	0.46
1:E:113:ASP:OD1	1:H:111:LYS:HE2	2.16	0.46
1:A:287:ILE:N	1:A:287:ILE:HD12	2.31	0.46
1:F:386:THR:HG22	1:F:386:THR:O	2.16	0.46
1:A:428:ARG:NH1	1:A:464:LEU:HG	2.31	0.46
1:B:184:HIS:CE1	1:B:188:SER:HA	2.51	0.46
1:B:192:ILE:HG12	1:B:205:LEU:HD22	1.98	0.46
1:C:119:GLU:N	1:C:120:PRO:HD3	2.30	0.46
1:E:400:ILE:H	1:E:400:ILE:HG13	1.49	0.46
1:C:272:ASN:O	1:C:296:HIS:HE1	1.99	0.45
1:E:333:GLY:N	1:E:386:THR:CG2	2.79	0.45
1:F:287:ILE:N	1:F:287:ILE:HD12	2.31	0.45
1:F:452:ASP:CB	1:H:216:LYS:HZ3	2.28	0.45
1:H:380:PRO:O	1:H:381:ASN:C	2.56	0.45
1:E:344:SER:O	1:E:345:ASN:HB2	2.16	0.45
1:F:105:SER:CB	1:F:167:PRO:HD2	2.47	0.45
1:C:149:VAL:HG21	1:C:430:ARG:CZ	2.46	0.45
1:C:386:THR:HG22	1:C:386:THR:O	2.16	0.45
1:D:97:TRP:N	1:D:395:GLN:HE22	2.13	0.45
1:G:184:HIS:CE1	1:G:188:SER:HA	2.52	0.45
1:C:333:GLY:C	1:C:386:THR:HG23	2.41	0.45
1:E:121:PHE:CG	1:E:228:SER:HA	2.51	0.45
1:G:272:ASN:O	1:G:296:HIS:HE1	1.98	0.45
1:G:333:GLY:N	1:G:386:THR:CG2	2.80	0.45
1:E:216:LYS:HD3	1:H:452:ASP:CG	2.41	0.45
1:H:333:GLY:H	1:H:386:THR:HG22	1.81	0.45
1:G:224:ARG:NE	1:G:276:GLU:OE1	2.43	0.45
1:C:344:SER:O	1:C:345:ASN:HB2	2.16	0.45
1:F:387:ASP:OD2	1:F:389:SER:O	2.35	0.45
1:A:184:HIS:CE1	1:A:188:SER:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:VAL:HG13	1:D:383:TRP:CE3	2.46	0.45
1:E:428:ARG:NH1	1:E:464:LEU:HG	2.32	0.45
1:B:150:LYS:O	1:B:151:ASP:CB	2.47	0.44
1:B:463:GLU:O	1:B:463:GLU:HG3	2.17	0.44
1:E:218:TRP:CE2	1:E:253:LYS:HE3	2.53	0.44
1:F:275:TYR:CE2	1:F:303:VAL:CG2	3.00	0.44
1:A:272:ASN:O	1:A:296:HIS:HE1	2.00	0.44
1:E:146:ASN:ND2	1:E:147:GLY:H	2.15	0.44
1:F:216:LYS:HZ2	1:G:452:ASP:CG	2.25	0.44
1:G:320:GLY:HA3	1:G:331:GLY:O	2.17	0.44
1:B:85:LEU:HD13	1:B:186:GLY:CA	2.48	0.44
1:B:224:ARG:NE	1:B:276:GLU:OE1	2.48	0.44
1:C:99:VAL:HA	1:C:446:PHE:CD2	2.53	0.44
1:C:121:PHE:CG	1:C:228:SER:HA	2.53	0.44
1:C:287:ILE:HD12	1:C:287:ILE:N	2.32	0.44
1:C:375:GLU:OE1	1:C:394:LYS:HE3	2.17	0.44
1:F:298:SER:OG	1:F:328:PRO:HD3	2.18	0.44
1:F:463:GLU:HG3	1:H:143:LYS:HE3	1.99	0.44
1:D:333:GLY:N	1:D:386:THR:HG22	2.32	0.44
1:E:149:VAL:HG21	1:E:430:ARG:CZ	2.48	0.44
1:E:454:VAL:HG22	1:G:202:VAL:HG11	1.98	0.44
1:B:121:PHE:CG	1:B:228:SER:HA	2.53	0.44
1:F:192:ILE:HG12	1:F:205:LEU:HD22	1.99	0.44
1:A:105:SER:CB	1:A:167:PRO:HD2	2.48	0.44
1:B:211:ILE:HD12	1:C:447:CYS:HB2	2.00	0.44
1:B:275:TYR:CE2	1:B:303:VAL:CG2	3.01	0.44
1:F:149:VAL:HG21	1:F:430:ARG:CZ	2.48	0.44
1:E:333:GLY:H	1:E:386:THR:CG2	2.31	0.44
1:F:272:ASN:O	1:F:296:HIS:HE1	2.01	0.44
1:F:454:VAL:HG22	1:H:202:VAL:HG11	1.99	0.44
1:G:387:ASP:OD2	1:G:389:SER:O	2.36	0.44
1:H:333:GLY:H	1:H:386:THR:CG2	2.31	0.44
1:B:249:GLN:HE22	1:B:272:ASN:N	2.16	0.43
1:C:85:LEU:HD13	1:C:186:GLY:CA	2.48	0.43
1:F:144:HIS:CE1	1:G:462:ALA:HA	2.53	0.43
1:F:192:ILE:HD11	1:F:257:MET:HE1	2.00	0.43
1:G:85:LEU:HD13	1:G:186:GLY:CA	2.48	0.43
1:G:121:PHE:CG	1:G:228:SER:HA	2.53	0.43
1:H:184:HIS:CE1	1:H:188:SER:HA	2.53	0.43
1:E:202:VAL:CG1	1:H:454:VAL:HG22	2.47	0.43
1:C:298:SER:OG	1:C:328:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLU:N	1:E:120:PRO:HD3	2.33	0.43
1:E:287:ILE:HD12	1:E:287:ILE:N	2.33	0.43
1:B:287:ILE:N	1:B:287:ILE:HD12	2.33	0.43
1:E:463:GLU:O	1:E:463:GLU:HG3	2.17	0.43
1:B:105:SER:CB	1:B:167:PRO:HD2	2.48	0.43
1:D:387:ASP:OD2	1:D:389:SER:O	2.37	0.43
1:E:190:LEU:HD21	1:E:257:MET:HE3	2.00	0.43
1:G:105:SER:CB	1:G:167:PRO:HD2	2.49	0.43
1:A:400:ILE:H	1:A:400:ILE:HG13	1.48	0.43
1:C:224:ARG:NE	1:C:276:GLU:OE1	2.45	0.43
1:E:184:HIS:CE1	1:E:188:SER:HA	2.53	0.43
1:H:226:GLN:HE22	1:H:230:CYS:HA	1.83	0.43
1:B:155:HIS:HD2	1:C:102:LYS:NZ	2.16	0.43
1:E:192:ILE:HG12	1:E:205:LEU:HD22	2.00	0.43
1:F:452:ASP:CB	1:H:216:LYS:HZ2	2.28	0.43
1:F:224:ARG:NE	1:F:276:GLU:OE1	2.47	0.43
1:G:226:GLN:HE22	1:G:230:CYS:HA	1.83	0.43
1:H:121:PHE:CG	1:H:228:SER:HA	2.54	0.43
1:A:224:ARG:NH1	1:A:276:GLU:OE1	2.51	0.42
1:H:272:ASN:O	1:H:296:HIS:HE1	2.02	0.42
1:F:99:VAL:HA	1:F:446:PHE:CD2	2.55	0.42
1:D:149:VAL:HG21	1:D:430:ARG:CZ	2.49	0.42
1:E:387:ASP:OD2	1:E:389:SER:O	2.37	0.42
1:F:205:LEU:HD23	1:F:205:LEU:N	2.34	0.42
1:H:99:VAL:HA	1:H:446:PHE:CD2	2.55	0.42
1:A:85:LEU:HD13	1:A:186:GLY:CA	2.49	0.42
1:E:386:THR:HG22	1:E:386:THR:O	2.19	0.42
1:F:85:LEU:HD13	1:F:186:GLY:CA	2.50	0.42
1:F:325:ASN:HA	1:F:326:PRO:C	2.44	0.42
1:F:452:ASP:OD2	1:H:216:LYS:NZ	2.49	0.42
1:A:119:GLU:N	1:A:120:PRO:HD3	2.35	0.42
1:E:192:ILE:HD11	1:E:257:MET:CE	2.49	0.42
1:E:218:TRP:CD1	1:E:219:ARG:HG2	2.55	0.42
1:A:463:GLU:HG3	1:A:463:GLU:O	2.19	0.42
1:D:121:PHE:CG	1:D:228:SER:HA	2.55	0.42
1:D:463:GLU:HG3	1:D:463:GLU:O	2.18	0.42
1:G:386:THR:HG22	1:G:386:THR:O	2.18	0.42
1:A:298:SER:OG	1:A:328:PRO:HD3	2.20	0.42
1:D:428:ARG:NH1	1:D:464:LEU:HG	2.33	0.42
1:F:121:PHE:CG	1:F:228:SER:HA	2.54	0.42
1:H:463:GLU:HG3	1:H:463:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:GLU:N	1:H:144:HIS:HE1	2.07	0.42
1:A:436:THR:HG21	1:A:464:LEU:HD13	2.02	0.42
1:G:146:ASN:ND2	1:G:147:GLY:H	2.16	0.42
1:A:121:PHE:CG	1:A:228:SER:HA	2.54	0.42
1:D:85:LEU:HD13	1:D:186:GLY:HA2	2.02	0.42
1:A:333:GLY:C	1:A:386:THR:HG23	2.45	0.41
1:B:386:THR:HG22	1:B:386:THR:O	2.20	0.41
1:B:400:ILE:H	1:B:400:ILE:HG13	1.48	0.41
1:H:119:GLU:N	1:H:120:PRO:HD3	2.35	0.41
1:B:226:GLN:HE22	1:B:230:CYS:HA	1.85	0.41
1:D:85:LEU:HD13	1:D:186:GLY:CA	2.50	0.41
1:D:190:LEU:HD13	1:D:260:GLY:HA2	2.02	0.41
1:D:332:THR:HG22	1:D:386:THR:HG21	2.03	0.41
1:E:457:SER:C	1:E:459:PRO:HD3	2.45	0.41
1:H:333:GLY:N	1:H:386:THR:CG2	2.83	0.41
1:E:184:HIS:HD2	1:E:186:GLY:N	2.12	0.41
1:C:184:HIS:CE1	1:C:188:SER:HA	2.55	0.41
1:D:457:SER:C	1:D:459:PRO:HD3	2.45	0.41
1:E:150:LYS:O	1:E:151:ASP:CB	2.51	0.41
1:A:205:LEU:HD23	1:A:205:LEU:N	2.35	0.41
1:D:436:THR:HG21	1:D:464:LEU:HD13	2.02	0.41
1:E:105:SER:CB	1:E:167:PRO:HD2	2.50	0.41
1:F:216:LYS:CE	1:G:452:ASP:OD2	2.69	0.41
1:F:216:LYS:HD3	1:G:452:ASP:OD2	2.20	0.41
1:G:428:ARG:NH1	1:G:464:LEU:HG	2.35	0.41
1:A:85:LEU:HD13	1:A:186:GLY:HA2	2.01	0.41
1:B:101:SER:HA	1:D:173:PHE:CZ	2.56	0.41
1:B:245:PRO:C	1:B:247:ASN:H	2.28	0.41
1:E:224:ARG:NH1	1:E:276:GLU:OE1	2.53	0.41
1:H:428:ARG:NH1	1:H:464:LEU:HG	2.35	0.41
1:B:190:LEU:HD13	1:B:260:GLY:HA2	2.01	0.41
1:C:205:LEU:N	1:C:205:LEU:HD23	2.35	0.41
1:C:355:LYS:HD2	1:C:383:TRP:CD2	2.55	0.41
1:D:249:GLN:HE22	1:D:272:ASN:N	2.17	0.41
1:D:325:ASN:HA	1:D:326:PRO:C	2.46	0.41
1:H:224:ARG:NE	1:H:276:GLU:OE1	2.46	0.41
1:B:85:LEU:HD13	1:B:186:GLY:HA2	2.01	0.41
1:B:216:LYS:HZ2	1:C:452:ASP:CG	2.29	0.41
1:E:226:GLN:HE22	1:E:230:CYS:HA	1.86	0.41
1:E:452:ASP:CB	1:G:216:LYS:HZ3	2.33	0.41
1:F:155:HIS:HD2	1:G:102:LYS:NZ	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:HIS:HD2	1:F:186:GLY:N	2.12	0.41
1:F:335:SER:HB3	1:F:341:VAL:CG2	2.51	0.41
1:G:190:LEU:HD13	1:G:260:GLY:HA2	2.02	0.41
1:G:287:ILE:HD12	1:G:287:ILE:N	2.35	0.41
1:G:436:THR:HG21	1:G:464:LEU:HD13	2.02	0.41
1:H:413:THR:HG22	1:H:415:LEU:HB2	2.02	0.41
1:F:184:HIS:CE1	1:F:188:SER:HA	2.56	0.41
1:A:456:TRP:CE3	1:C:196:GLY:HA2	2.56	0.40
1:C:275:TYR:CE2	1:C:303:VAL:CG2	3.03	0.40
1:F:360:VAL:HG13	1:F:383:TRP:CE3	2.49	0.40
1:A:149:VAL:H	1:A:149:VAL:HG23	1.58	0.40
1:B:316:TYR:CZ	1:B:340:PRO:HG3	2.57	0.40
1:C:400:ILE:H	1:C:400:ILE:HG13	1.46	0.40
1:D:119:GLU:N	1:D:120:PRO:HD3	2.36	0.40
1:F:386:THR:O	1:F:387:ASP:C	2.64	0.40
1:G:85:LEU:HD13	1:G:186:GLY:HA2	2.02	0.40
1:G:332:THR:CG2	1:G:386:THR:HG21	2.51	0.40
1:H:457:SER:C	1:H:459:PRO:HD3	2.46	0.40
1:A:177:ALA:HA	1:A:194:ILE:O	2.22	0.40
1:D:99:VAL:HA	1:D:446:PHE:CD2	2.57	0.40
1:E:102:LYS:NZ	1:G:155:HIS:HD2	2.14	0.40
1:H:105:SER:CB	1:H:167:PRO:HD2	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:ALA:O	1:F:358:ASN:ND2[4_455]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/385 (100%)	357 (93%)	21 (6%)	5 (1%)	9	12
1	B	383/385 (100%)	359 (94%)	19 (5%)	5 (1%)	9	12
1	C	383/385 (100%)	356 (93%)	22 (6%)	5 (1%)	9	12
1	D	383/385 (100%)	357 (93%)	21 (6%)	5 (1%)	9	12
1	E	383/385 (100%)	357 (93%)	21 (6%)	5 (1%)	9	12
1	F	383/385 (100%)	354 (92%)	24 (6%)	5 (1%)	9	12
1	G	383/385 (100%)	359 (94%)	19 (5%)	5 (1%)	9	12
1	H	383/385 (100%)	358 (94%)	20 (5%)	5 (1%)	9	12
All	All	3064/3080 (100%)	2857 (93%)	167 (6%)	40 (1%)	9	12

All (40) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	D	449	VAL
1	E	449	VAL
1	F	449	VAL
1	G	449	VAL
1	H	449	VAL
1	B	382	GLY
1	A	382	GLY
1	D	382	GLY
1	G	382	GLY
1	C	382	GLY
1	E	382	GLY
1	F	382	GLY
1	H	382	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/329 (100%)	303 (92%)	26 (8%)	11	16
1	B	329/329 (100%)	301 (92%)	28 (8%)	10	13
1	C	329/329 (100%)	303 (92%)	26 (8%)	11	16
1	D	329/329 (100%)	302 (92%)	27 (8%)	10	14
1	E	329/329 (100%)	304 (92%)	25 (8%)	12	17
1	F	329/329 (100%)	303 (92%)	26 (8%)	11	16
1	G	329/329 (100%)	300 (91%)	29 (9%)	9	12
1	H	329/329 (100%)	303 (92%)	26 (8%)	11	16
All	All	2632/2632 (100%)	2419 (92%)	213 (8%)	11	15

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	88	ASN

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Mol	Chain	Res	Type
1	A	99	VAL
1	A	116	VAL
1	A	149	VAL
1	A	175	SER
1	A	188	SER
1	A	202	VAL
1	A	205	LEU
1	A	210	ILE
1	A	214	THR
1	A	257	MET
1	A	276	GLU
1	A	296	HIS
1	A	298	SER
1	A	303	VAL
1	A	310	LEU
1	A	360	VAL
1	A	368	THR
1	A	400	ILE
1	A	411	VAL
1	A	413	THR
1	A	415	LEU
1	A	435	SER
1	A	449	VAL
1	A	464	LEU
1	B	85	LEU
1	B	88	ASN
1	B	99	VAL
1	B	116	VAL
1	B	146	ASN
1	B	149	VAL
1	B	175	SER
1	B	188	SER
1	B	202	VAL
1	B	205	LEU
1	B	210	ILE
1	B	214	THR
1	B	230	CYS
1	B	257	MET
1	B	276	GLU
1	B	296	HIS
1	B	303	VAL
1	B	309	ASN

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Mol	Chain	Res	Type
1	B	310	LEU
1	B	360	VAL
1	B	368	THR
1	B	400	ILE
1	B	411	VAL
1	B	413	THR
1	B	415	LEU
1	B	435	SER
1	B	449	VAL
1	B	464	LEU
1	C	85	LEU
1	C	88	ASN
1	C	99	VAL
1	C	116	VAL
1	C	146	ASN
1	C	149	VAL
1	C	175	SER
1	C	188	SER
1	C	202	VAL
1	C	205	LEU
1	C	210	ILE
1	C	214	THR
1	C	257	MET
1	C	276	GLU
1	C	296	HIS
1	C	303	VAL
1	C	310	LEU
1	C	360	VAL
1	C	368	THR
1	C	400	ILE
1	C	411	VAL
1	C	413	THR
1	C	415	LEU
1	C	435	SER
1	C	449	VAL
1	C	464	LEU
1	D	85	LEU
1	D	88	ASN
1	D	99	VAL
1	D	116	VAL
1	D	146	ASN
1	D	149	VAL

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Mol	Chain	Res	Type
1	D	163	VAL
1	D	175	SER
1	D	188	SER
1	D	202	VAL
1	D	205	LEU
1	D	210	ILE
1	D	214	THR
1	D	257	MET
1	D	276	GLU
1	D	296	HIS
1	D	303	VAL
1	D	310	LEU
1	D	360	VAL
1	D	368	THR
1	D	400	ILE
1	D	411	VAL
1	D	413	THR
1	D	415	LEU
1	D	435	SER
1	D	449	VAL
1	D	464	LEU
1	E	85	LEU
1	E	88	ASN
1	E	99	VAL
1	E	116	VAL
1	E	146	ASN
1	E	149	VAL
1	E	175	SER
1	E	188	SER
1	E	202	VAL
1	E	205	LEU
1	E	210	ILE
1	E	214	THR
1	E	257	MET
1	E	276	GLU
1	E	296	HIS
1	E	303	VAL
1	E	310	LEU
1	E	360	VAL
1	E	368	THR
1	E	400	ILE
1	E	411	VAL

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Mol	Chain	Res	Type
1	E	413	THR
1	E	415	LEU
1	E	435	SER
1	E	449	VAL
1	F	85	LEU
1	F	88	ASN
1	F	99	VAL
1	F	116	VAL
1	F	146	ASN
1	F	149	VAL
1	F	175	SER
1	F	188	SER
1	F	202	VAL
1	F	205	LEU
1	F	210	ILE
1	F	214	THR
1	F	257	MET
1	F	276	GLU
1	F	296	HIS
1	F	303	VAL
1	F	310	LEU
1	F	360	VAL
1	F	368	THR
1	F	400	ILE
1	F	411	VAL
1	F	413	THR
1	F	415	LEU
1	F	435	SER
1	F	449	VAL
1	F	464	LEU
1	G	85	LEU
1	G	88	ASN
1	G	99	VAL
1	G	116	VAL
1	G	146	ASN
1	G	149	VAL
1	G	175	SER
1	G	188	SER
1	G	202	VAL
1	G	205	LEU
1	G	210	ILE
1	G	214	THR

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Mol	Chain	Res	Type
1	G	257	MET
1	G	276	GLU
1	G	296	HIS
1	G	298	SER
1	G	303	VAL
1	G	309	ASN
1	G	310	LEU
1	G	360	VAL
1	G	368	THR
1	G	400	ILE
1	G	411	VAL
1	G	413	THR
1	G	415	LEU
1	G	435	SER
1	G	442	SER
1	G	449	VAL
1	G	464	LEU
1	H	85	LEU
1	H	88	ASN
1	H	99	VAL
1	H	116	VAL
1	H	146	ASN
1	H	149	VAL
1	H	175	SER
1	H	188	SER
1	H	202	VAL
1	H	205	LEU
1	H	210	ILE
1	H	214	THR
1	H	257	MET
1	H	276	GLU
1	H	296	HIS
1	H	303	VAL
1	H	310	LEU
1	H	360	VAL
1	H	368	THR
1	H	400	ILE
1	H	411	VAL
1	H	413	THR
1	H	415	LEU
1	H	435	SER
1	H	449	VAL

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Mol	Chain	Res	Type
1	H	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) 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	155	HIS
1	A	184	HIS
1	A	226	GLN
1	A	249	GLN
1	A	296	HIS
1	A	313	GLN
1	A	395	GLN
1	B	88	ASN
1	B	104	ASN
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	296	HIS
1	B	313	GLN
1	B	395	GLN
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	249	GLN
1	C	296	HIS
1	C	313	GLN
1	C	395	GLN
1	D	88	ASN
1	D	104	ASN
1	D	144	HIS
1	D	146	ASN

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Mol	Chain	Res	Type
1	D	155	HIS
1	D	184	HIS
1	D	226	GLN
1	D	249	GLN
1	D	296	HIS
1	D	313	GLN
1	D	395	GLN
1	E	88	ASN
1	E	104	ASN
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	296	HIS
1	E	313	GLN
1	E	325	ASN
1	E	395	GLN
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	296	HIS
1	F	313	GLN
1	F	395	GLN
1	G	88	ASN
1	G	104	ASN
1	G	144	HIS
1	G	146	ASN
1	G	155	HIS
1	G	184	HIS
1	G	226	GLN
1	G	249	GLN
1	G	296	HIS
1	G	313	GLN
1	G	395	GLN
1	H	88	ASN

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Mol	Chain	Res	Type
1	H	104	ASN
1	H	144	HIS
1	H	146	ASN
1	H	155	HIS
1	H	184	HIS
1	H	226	GLN
1	H	249	GLN
1	H	296	HIS
1	H	313	GLN
1	H	395	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	G	807	-	19,20,20	1.97	5 (26%)	20,27,27	1.68	6 (30%)
2	G39	A	800	-	19,20,20	1.99	6 (31%)	20,27,27	1.47	5 (25%)
2	G39	D	803	-	19,20,20	1.99	5 (26%)	20,27,27	1.32	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G39	F	806	-	19,20,20	2.09	6 (31%)	20,27,27	1.61	5 (25%)
2	G39	H	808	-	19,20,20	2.04	6 (31%)	20,27,27	1.51	6 (30%)
2	G39	E	805	-	19,20,20	2.14	6 (31%)	20,27,27	1.34	3 (15%)
2	G39	C	802	-	19,20,20	1.95	6 (31%)	20,27,27	1.38	4 (20%)
2	G39	B	801	-	19,20,20	1.98	7 (36%)	20,27,27	1.53	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	G	807	-	-	1/16/32/32	0/1/1/1
2	G39	A	800	-	-	1/16/32/32	0/1/1/1
2	G39	D	803	-	-	1/16/32/32	0/1/1/1
2	G39	F	806	-	-	1/16/32/32	0/1/1/1
2	G39	H	808	-	-	1/16/32/32	0/1/1/1
2	G39	E	805	-	-	1/16/32/32	0/1/1/1
2	G39	C	802	-	-	1/16/32/32	0/1/1/1
2	G39	B	801	-	-	1/16/32/32	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	805	G39	O1B-C1	-4.50	1.18	1.30
2	D	803	G39	O1B-C1	-4.27	1.18	1.30
2	C	802	G39	O1B-C1	-4.27	1.18	1.30
2	E	805	G39	C6-C7	4.26	1.56	1.50
2	B	801	G39	O1B-C1	-4.23	1.19	1.30
2	G	807	G39	O1B-C1	-4.18	1.19	1.30
2	F	806	G39	C6-C7	4.17	1.56	1.50
2	H	808	G39	C6-C7	4.13	1.56	1.50
2	H	808	G39	O1B-C1	-4.11	1.19	1.30
2	F	806	G39	O1B-C1	-4.09	1.19	1.30
2	A	800	G39	O1B-C1	-3.95	1.19	1.30
2	D	803	G39	C10-N5	3.87	1.46	1.34
2	A	800	G39	C10-N5	3.85	1.46	1.34
2	G	807	G39	C6-C7	3.84	1.55	1.50
2	C	802	G39	C10-N5	3.80	1.46	1.34
2	E	805	G39	C10-N5	3.76	1.46	1.34
2	F	806	G39	C10-N5	3.60	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	G39	C10-N5	3.57	1.45	1.34
2	A	800	G39	C6-C7	3.54	1.55	1.50
2	D	803	G39	C6-C7	3.45	1.55	1.50
2	C	802	G39	C6-C7	3.45	1.55	1.50
2	H	808	G39	C10-N5	3.44	1.45	1.34
2	B	801	G39	C6-C7	3.42	1.55	1.50
2	G	807	G39	C10-N5	3.23	1.44	1.34
2	H	808	G39	O7-C8	-3.15	1.40	1.44
2	F	806	G39	C3-C2	3.03	1.56	1.51
2	E	805	G39	C3-C2	2.96	1.56	1.51
2	A	800	G39	O7-C8	-2.88	1.40	1.44
2	D	803	G39	O7-C8	-2.87	1.40	1.44
2	E	805	G39	O7-C8	-2.86	1.41	1.44
2	G	807	G39	C3-C2	2.86	1.56	1.51
2	D	803	G39	C3-C2	2.82	1.56	1.51
2	B	801	G39	O7-C8	-2.81	1.41	1.44
2	F	806	G39	O7-C8	-2.75	1.41	1.44
2	C	802	G39	C3-C2	2.73	1.55	1.51
2	B	801	G39	C3-C2	2.66	1.55	1.51
2	A	800	G39	C3-C2	2.65	1.55	1.51
2	H	808	G39	C3-C2	2.55	1.55	1.51
2	F	806	G39	O10-C10	-2.52	1.17	1.23
2	C	802	G39	O7-C8	-2.51	1.41	1.44
2	G	807	G39	O7-C8	-2.49	1.41	1.44
2	A	800	G39	C1-C2	2.21	1.54	1.49
2	B	801	G39	O10-C10	-2.11	1.18	1.23
2	B	801	G39	C1-C2	2.06	1.53	1.49
2	E	805	G39	C1-C2	2.03	1.53	1.49
2	C	802	G39	C1-C2	2.01	1.53	1.49
2	H	808	G39	O10-C10	-2.00	1.18	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	807	G39	C5-N5-C10	-3.14	115.76	123.11
2	B	801	G39	C6-C5-N5	-2.98	107.79	111.13
2	F	806	G39	O1B-C1-C2	2.95	121.66	115.43
2	H	808	G39	C6-C5-N5	-2.89	107.90	111.13
2	G	807	G39	C6-C5-N5	-2.88	107.90	111.13
2	A	800	G39	O1B-C1-C2	2.84	121.43	115.43
2	G	807	G39	O1B-C1-C2	2.81	121.37	115.43
2	F	806	G39	C6-C5-N5	-2.79	108.00	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	808	G39	O1B-C1-C2	2.60	120.92	115.43
2	C	802	G39	C5-N5-C10	-2.56	117.11	123.11
2	A	800	G39	C6-C5-N5	-2.54	108.28	111.13
2	F	806	G39	C11-C10-N5	2.54	120.33	116.12
2	B	801	G39	O1B-C1-C2	2.52	120.76	115.43
2	E	805	G39	C5-N5-C10	-2.51	117.22	123.11
2	G	807	G39	O10-C10-N5	-2.47	117.62	121.98
2	D	803	G39	C6-C5-N5	-2.45	108.38	111.13
2	G	807	G39	C3-C2-C1	2.39	121.36	116.99
2	C	802	G39	O1B-C1-C2	2.38	120.46	115.43
2	A	800	G39	C3-C2-C1	2.38	121.35	116.99
2	D	803	G39	C5-N5-C10	-2.38	117.55	123.11
2	E	805	G39	O1B-C1-C2	2.35	120.39	115.43
2	E	805	G39	C3-C2-C1	2.33	121.26	116.99
2	B	801	G39	C5-N5-C10	-2.32	117.69	123.11
2	F	806	G39	C3-C2-C1	2.31	121.23	116.99
2	H	808	G39	C5-N5-C10	-2.31	117.70	123.11
2	C	802	G39	C6-C5-N5	-2.26	108.60	111.13
2	F	806	G39	O1A-C1-C2	-2.22	117.75	121.64
2	H	808	G39	C3-C2-C1	2.19	121.00	116.99
2	G	807	G39	O1A-C1-C2	-2.16	117.85	121.64
2	C	802	G39	C3-C2-C1	2.15	120.93	116.99
2	A	800	G39	O1A-C1-C2	-2.14	117.88	121.64
2	H	808	G39	C11-C10-N5	2.14	119.67	116.12
2	B	801	G39	C3-C2-C1	2.13	120.89	116.99
2	A	800	G39	C5-N5-C10	-2.11	118.16	123.11
2	D	803	G39	C3-C2-C1	2.11	120.85	116.99
2	B	801	G39	C11-C10-N5	2.10	119.60	116.12
2	H	808	G39	O1A-C1-C2	-2.07	118.01	121.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	E	805	G39	C9-C8-O7-C6
2	G	807	G39	C9-C8-O7-C6
2	D	803	G39	C9-C8-O7-C6
2	F	806	G39	C9-C8-O7-C6
2	H	808	G39	C9-C8-O7-C6

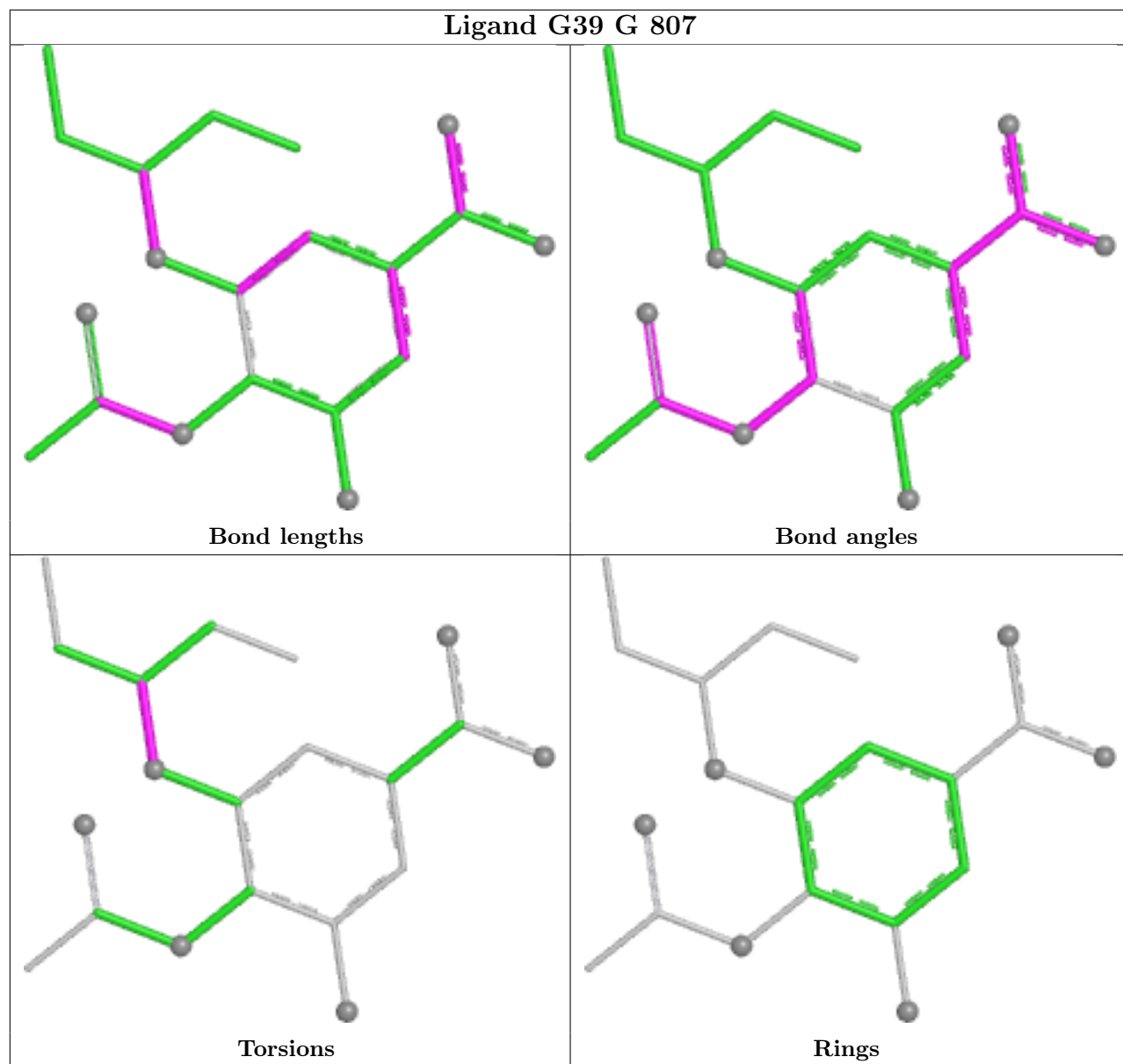
There are no ring outliers.

1 monomer is involved in 1 short contact:

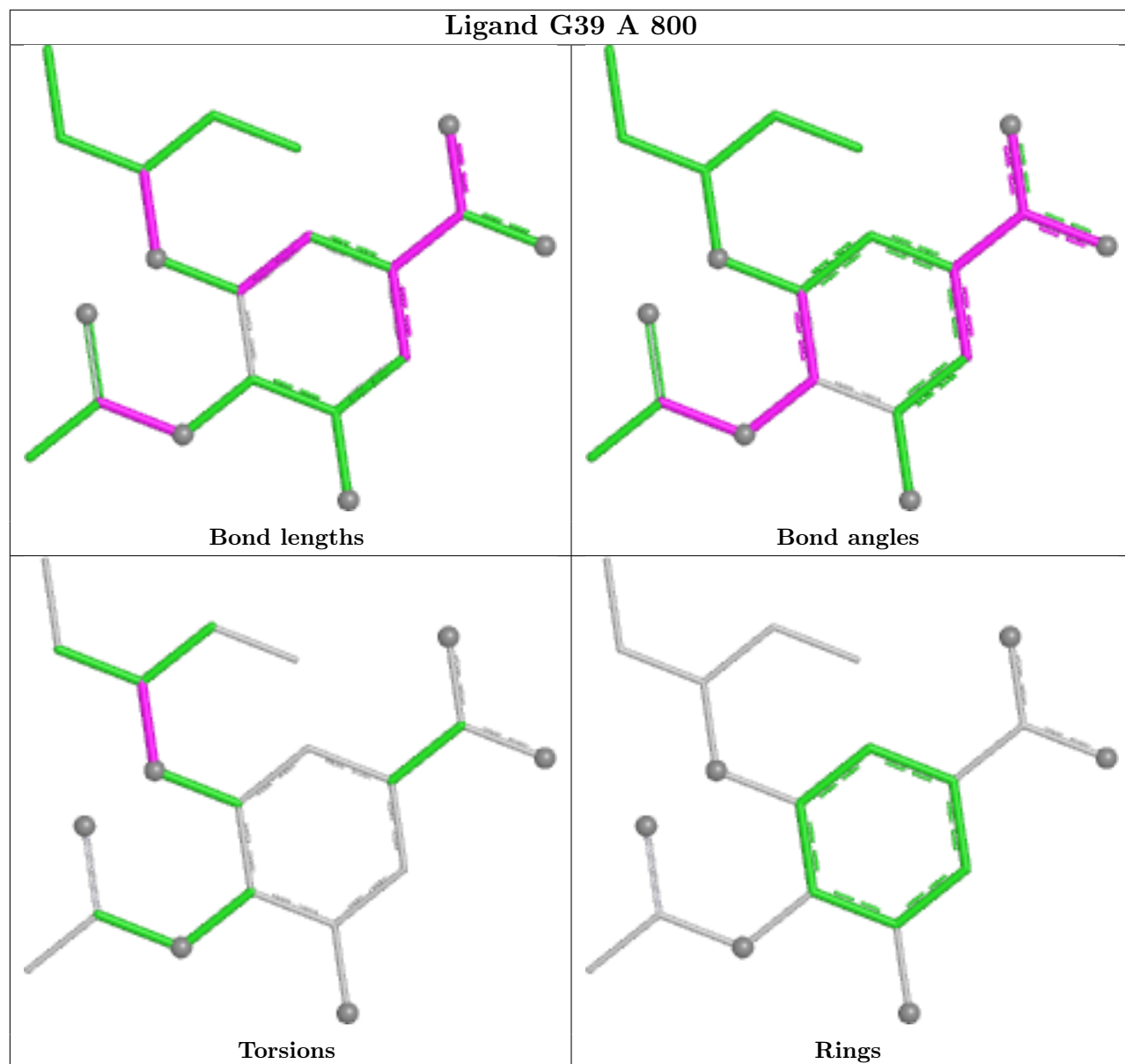
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	G39	1	0

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.

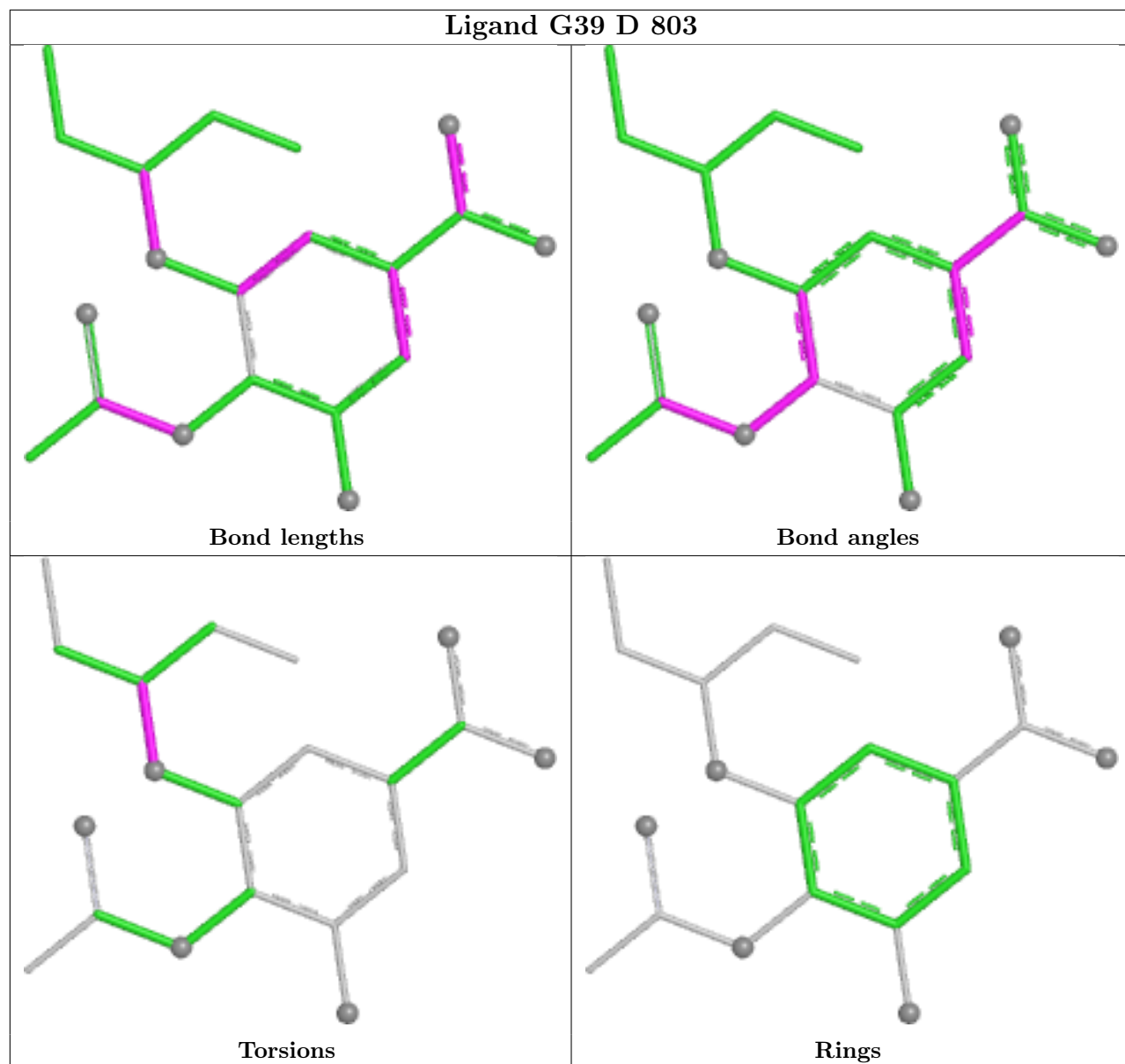
Ligand G39 G 807



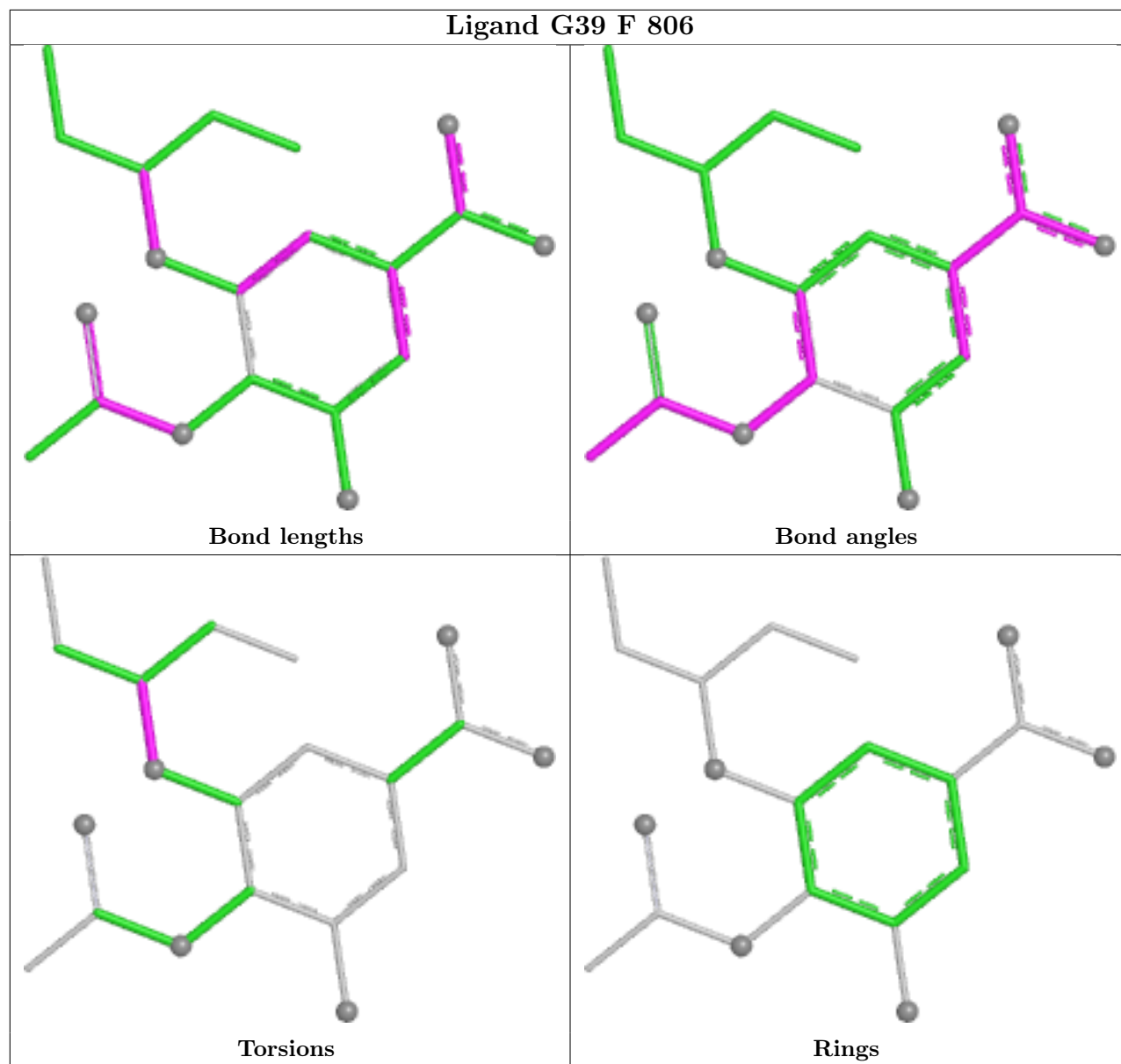
Ligand G39 A 800



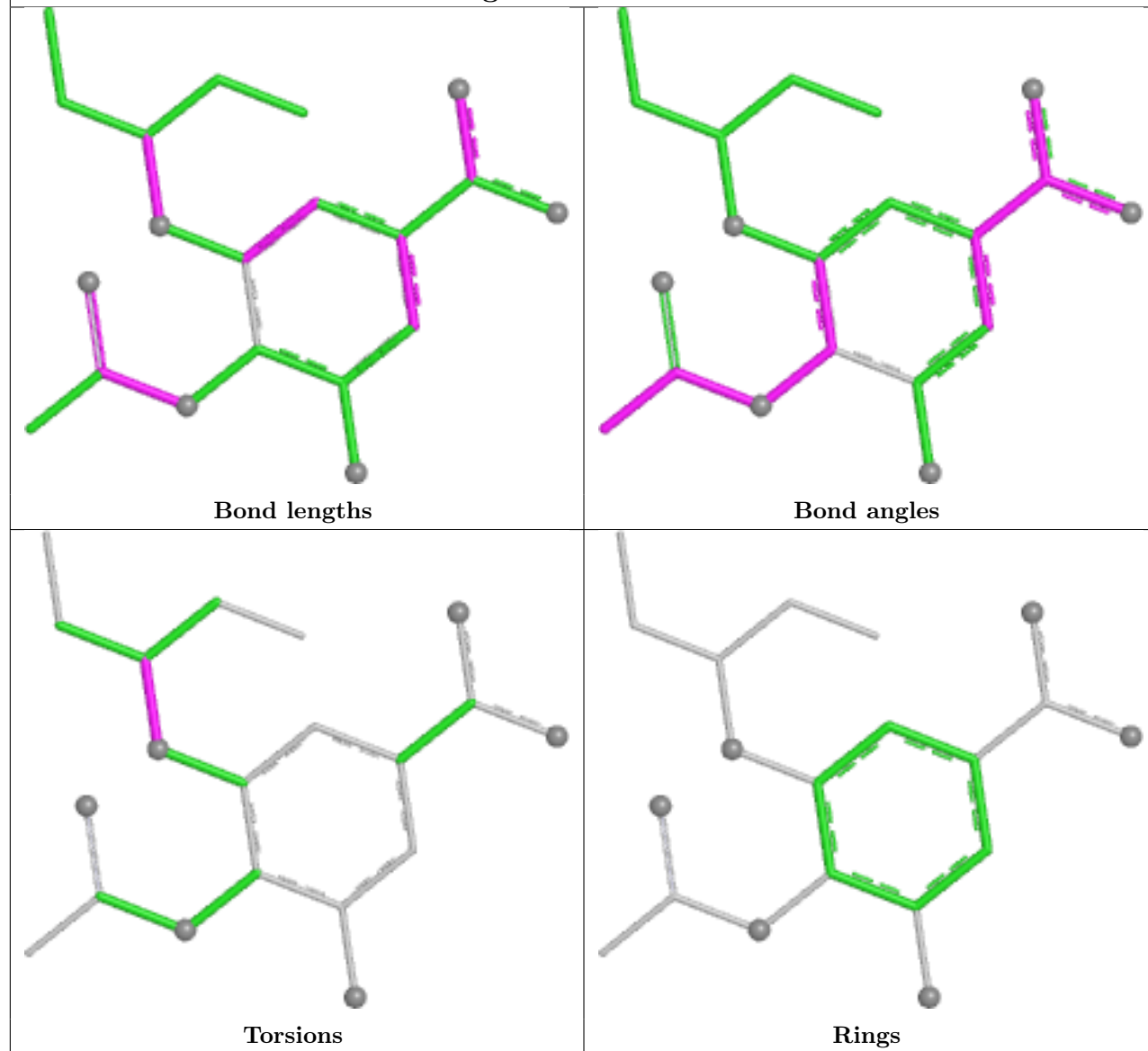
Ligand G39 D 803



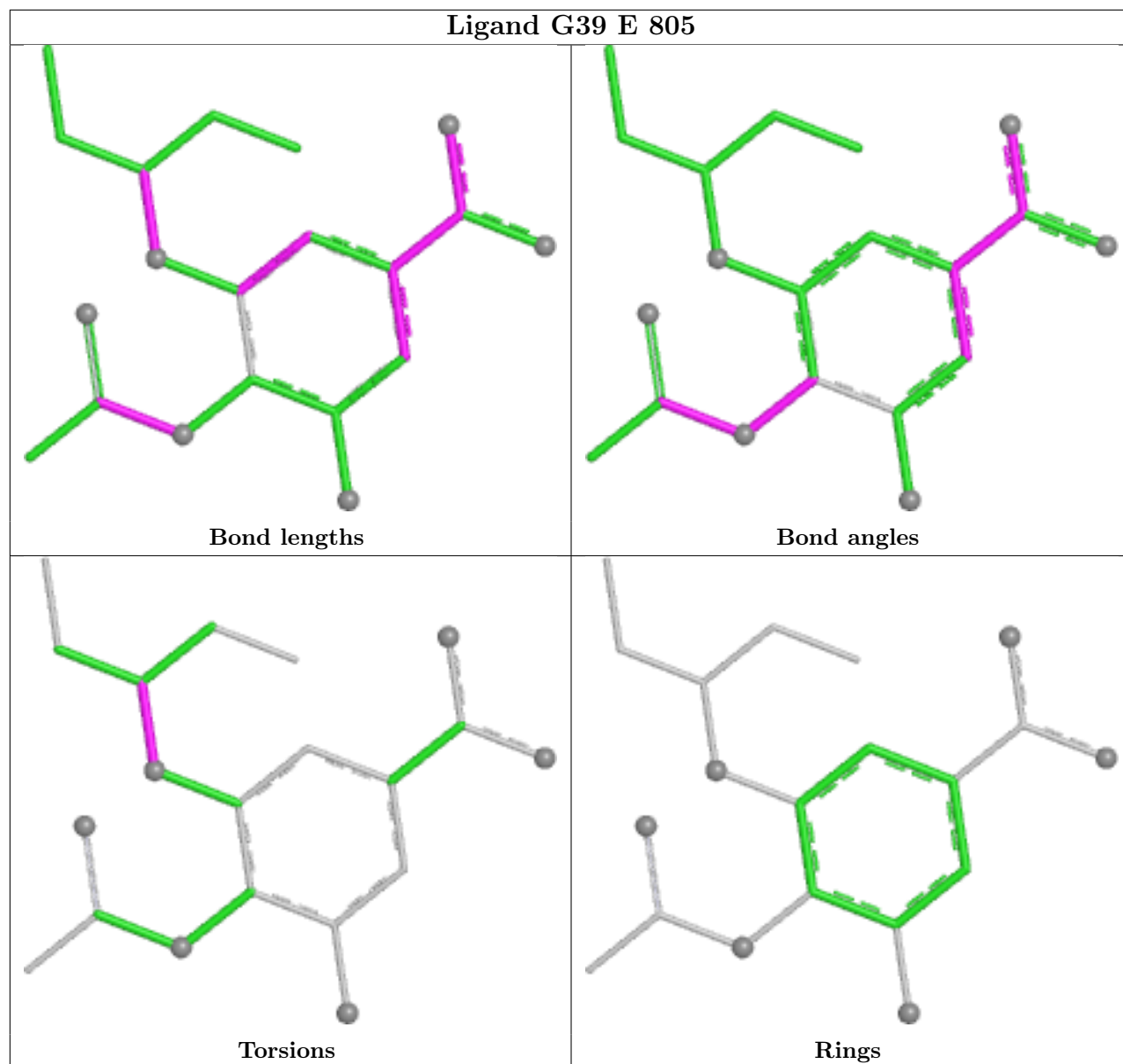
Ligand G39 F 806



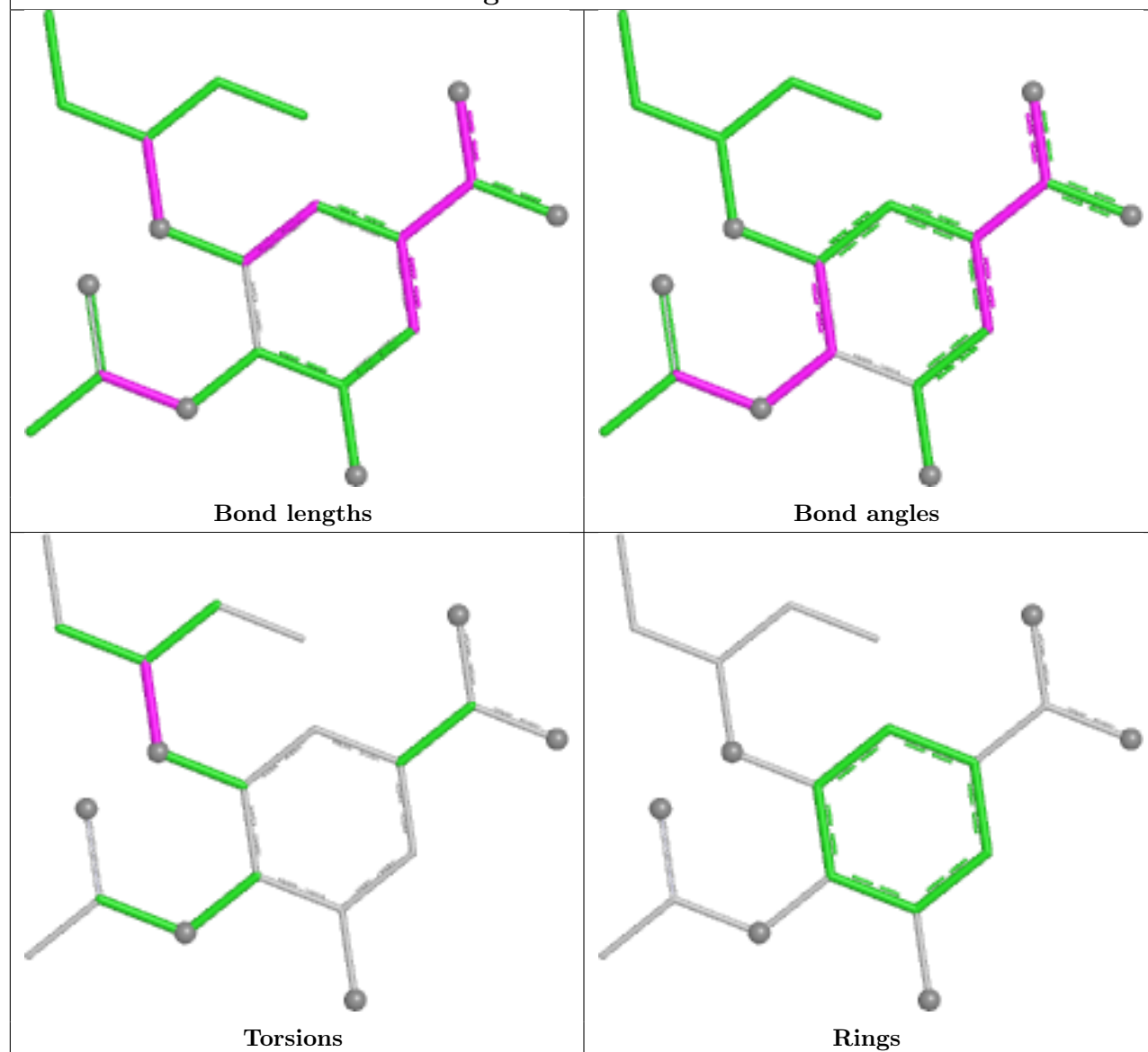
Ligand G39 H 808

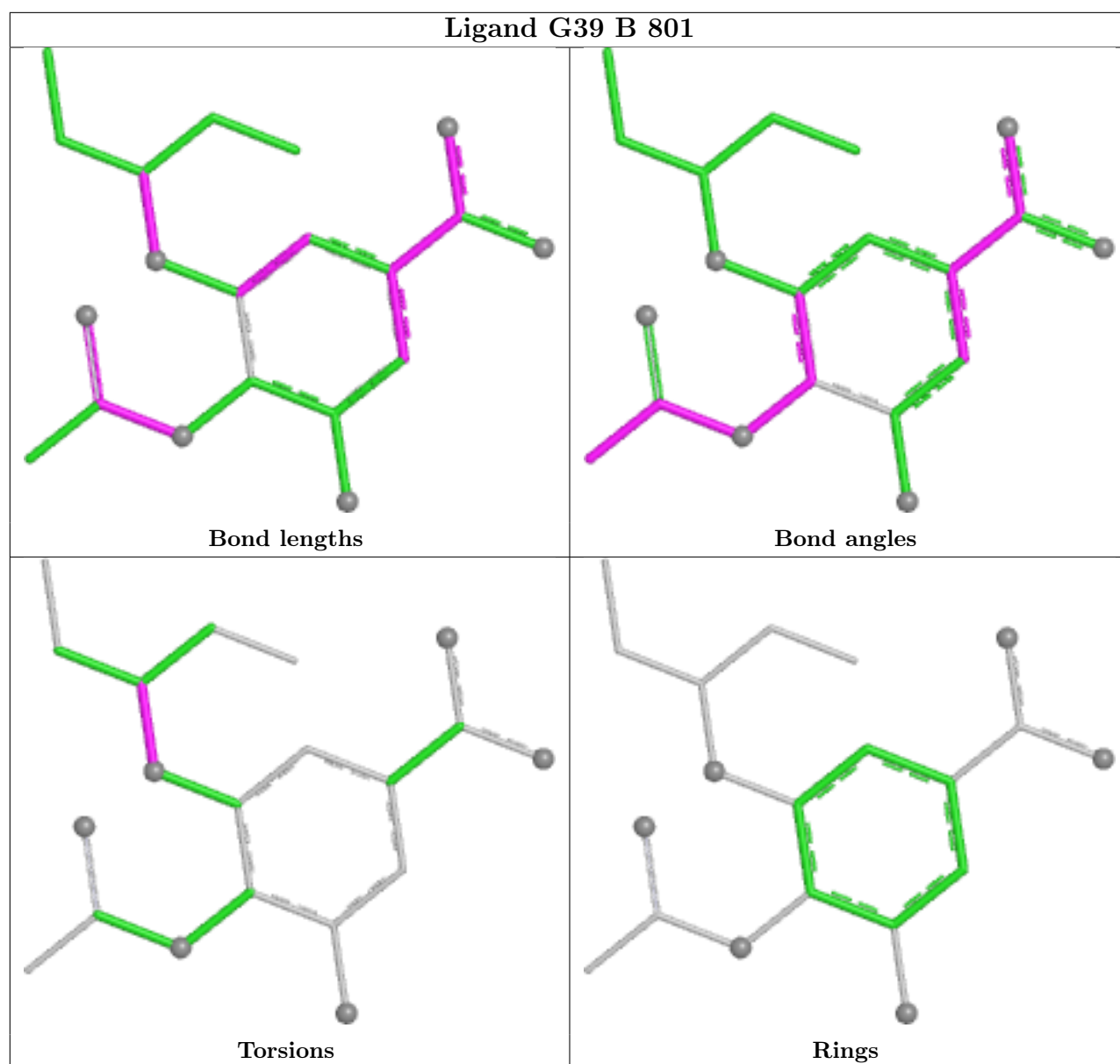


Ligand G39 E 805



Ligand G39 C 802





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	385/385 (100%)	-1.60	0 100 100	6, 16, 31, 57	0
1	B	385/385 (100%)	-1.59	0 100 100	6, 16, 32, 56	0
1	C	385/385 (100%)	-1.59	0 100 100	6, 15, 31, 62	0
1	D	385/385 (100%)	-1.57	0 100 100	7, 16, 31, 63	0
1	E	385/385 (100%)	-1.61	0 100 100	6, 15, 31, 64	0
1	F	385/385 (100%)	-1.62	0 100 100	6, 15, 30, 59	0
1	G	385/385 (100%)	-1.59	0 100 100	7, 15, 31, 63	0
1	H	385/385 (100%)	-1.60	0 100 100	4, 14, 29, 64	0
All	All	3080/3080 (100%)	-1.60	0 100 100	4, 15, 31, 64	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](#)

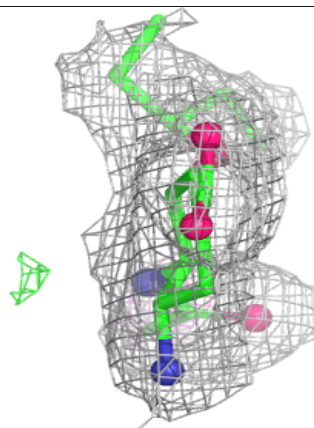
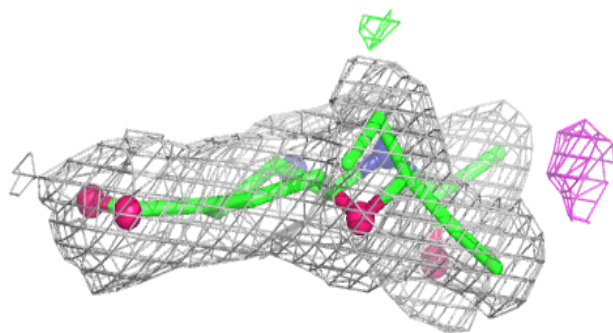
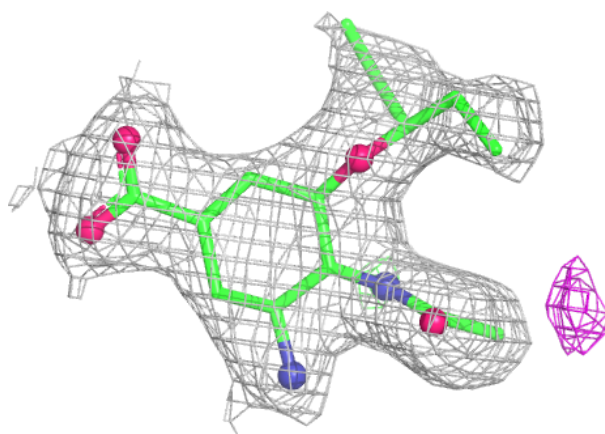
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	A	800	20/20	0.99	0.03	6,18,27,29	0
2	G39	B	801	20/20	0.99	0.03	6,16,24,25	0
2	G39	C	802	20/20	0.99	0.03	2,15,25,25	0
2	G39	D	803	20/20	0.99	0.03	4,18,26,28	0
2	G39	E	805	20/20	0.99	0.03	6,21,25,26	0
2	G39	G	807	20/20	0.99	0.03	7,19,23,24	0
2	G39	H	808	20/20	0.99	0.03	5,16,19,21	0
2	G39	F	806	20/20	1.00	0.03	6,15,23,25	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.

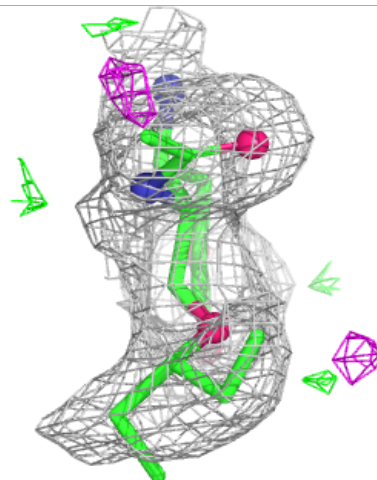
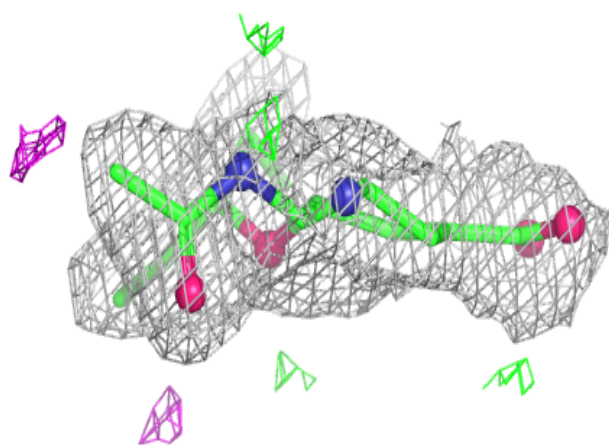
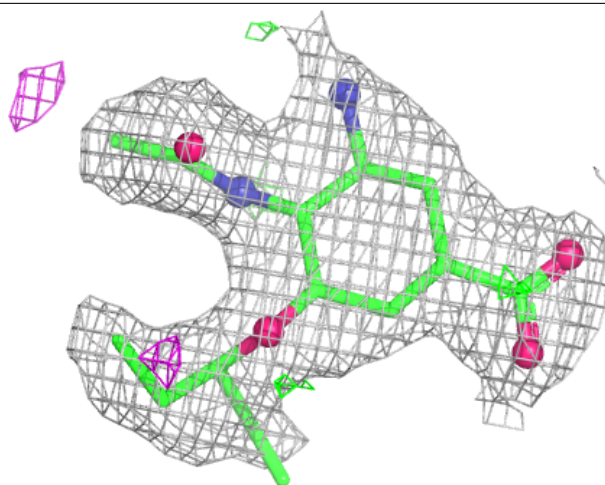
Electron density around G39 A 800:

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



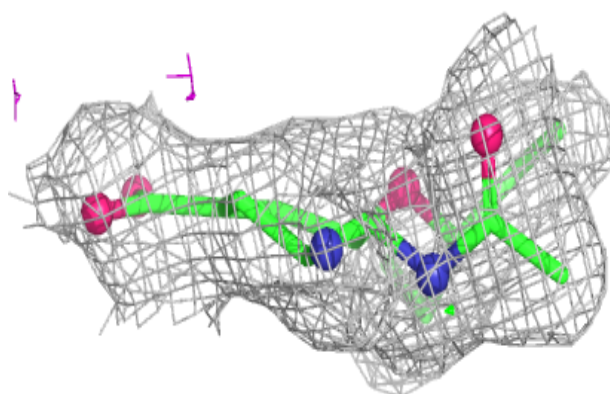
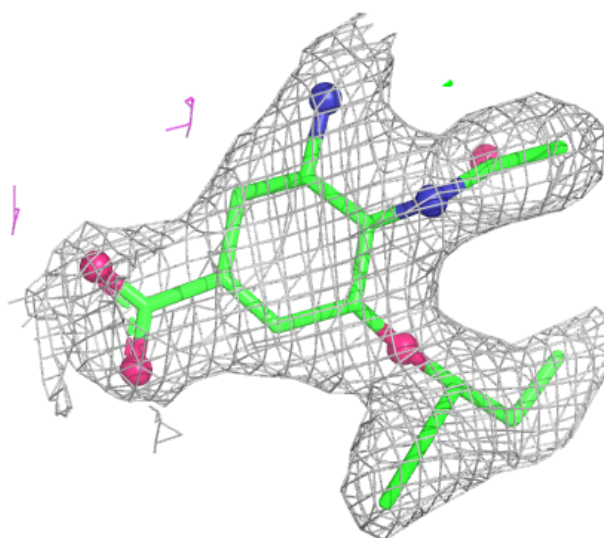
Electron density around G39 B 801:

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



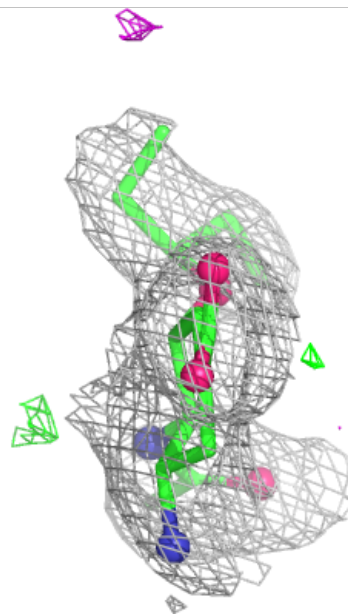
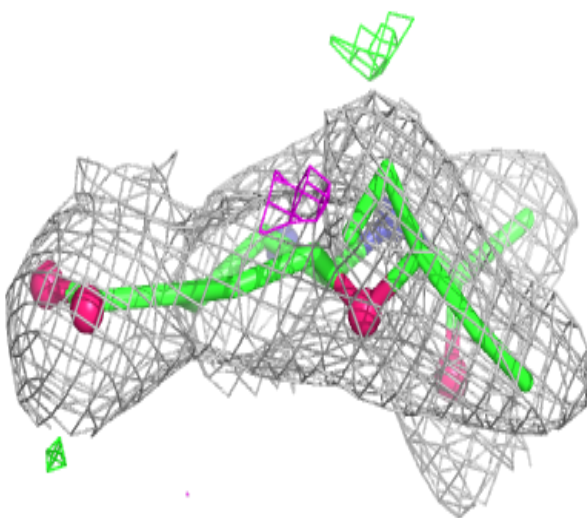
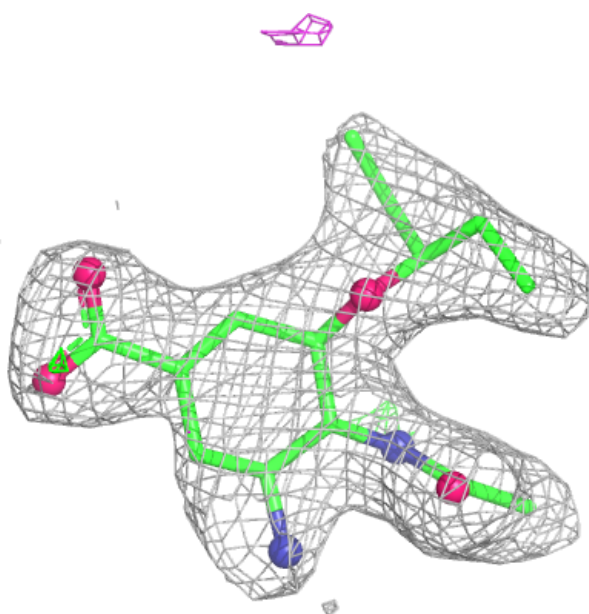
Electron density around G39 C 802:

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



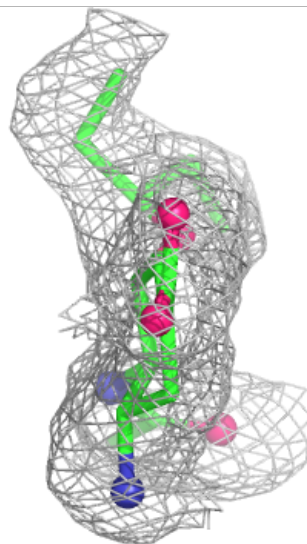
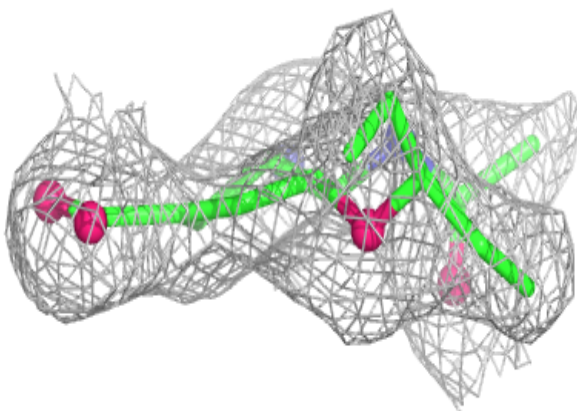
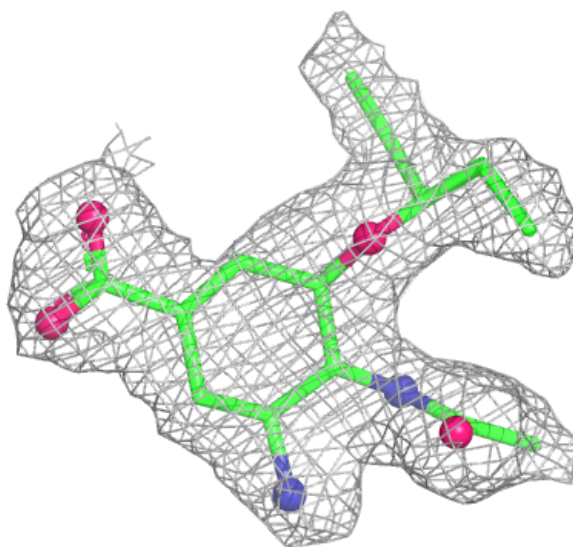
Electron density around G39 D 803:

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



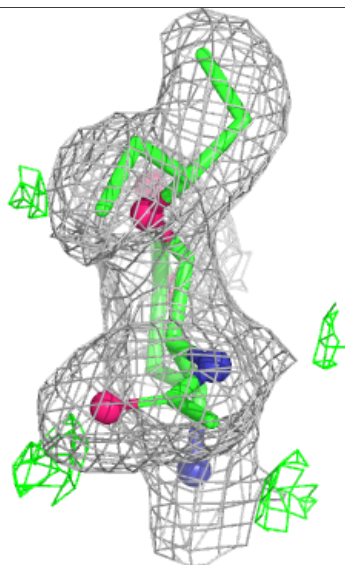
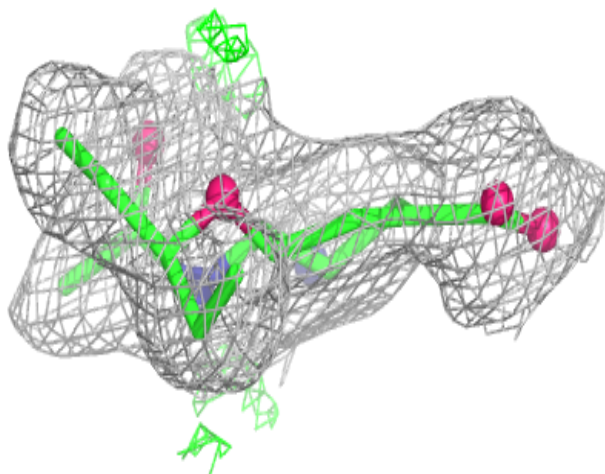
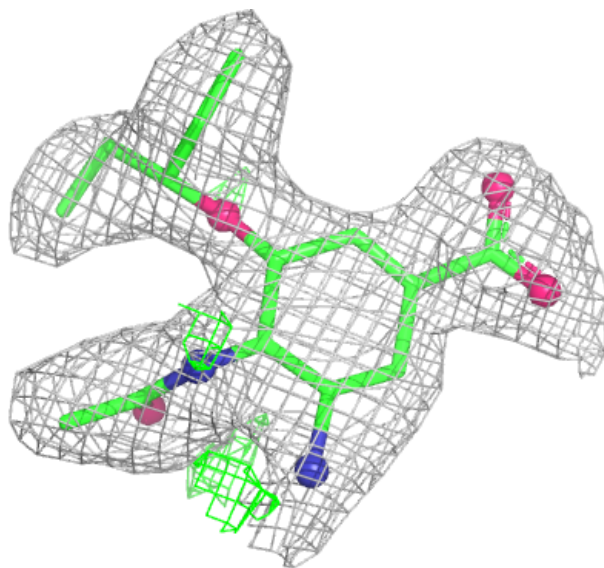
Electron density around G39 E 805:

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



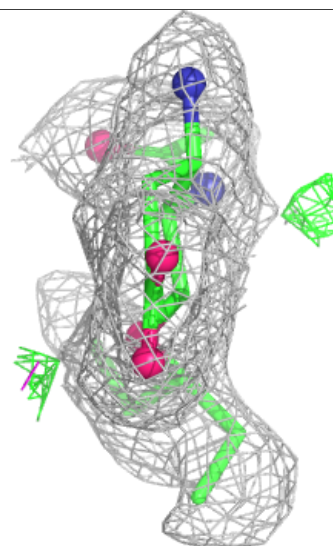
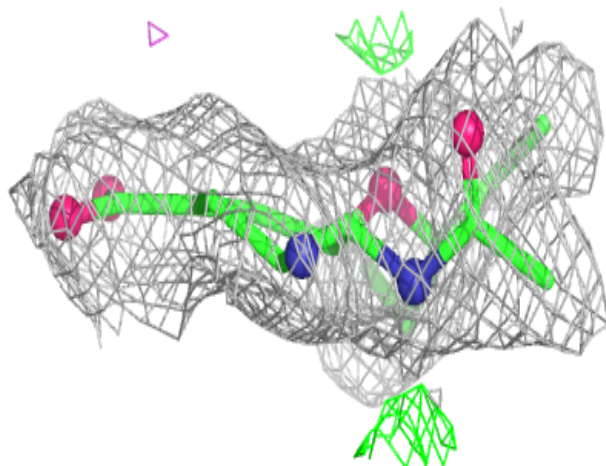
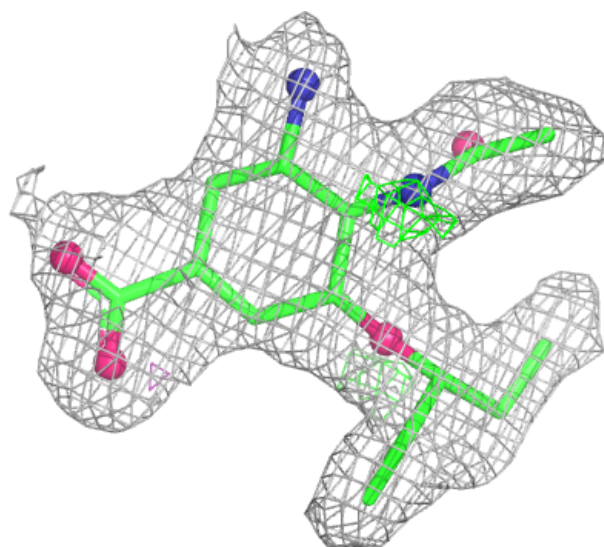
Electron density around G39 G 807:

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



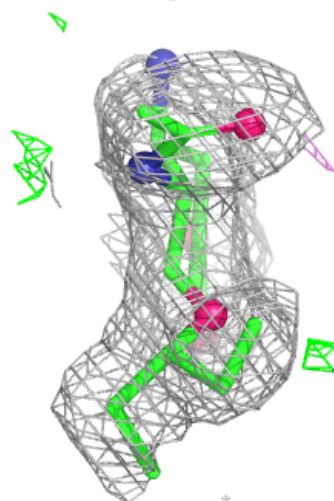
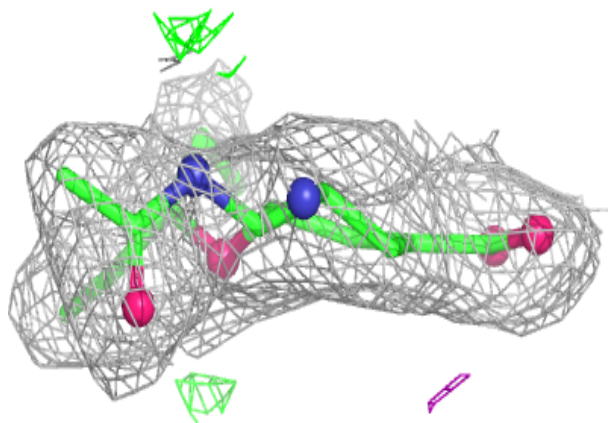
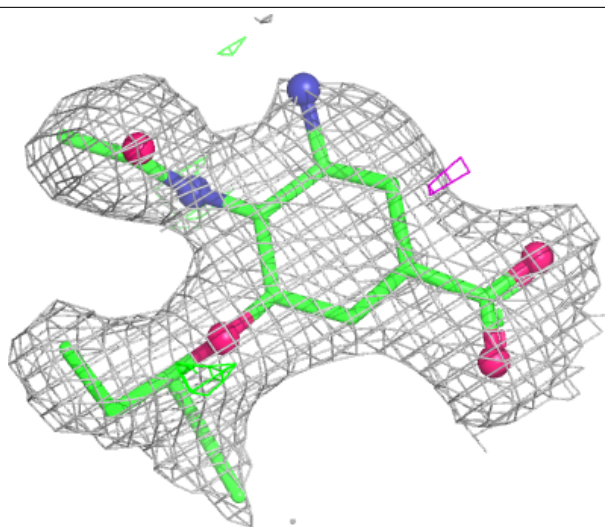
Electron density around G39 H 808:

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



Electron density around G39 F 806:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.