



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:44 PM UTC

PDB ID : 1GUL / pdb_00001gul
Title : HUMAN GLUTATHIONE TRANSFERASE A4-4 COMPLEX WITH
IODOBENZYL GLUTATHIONE
Authors : Bruns, C.M.; Hubatsch, I.; Ridderstrom, M.; Mannervik, B.; Tainer, J.A.
Deposited on : 1998-06-10
Resolution : 2.70 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

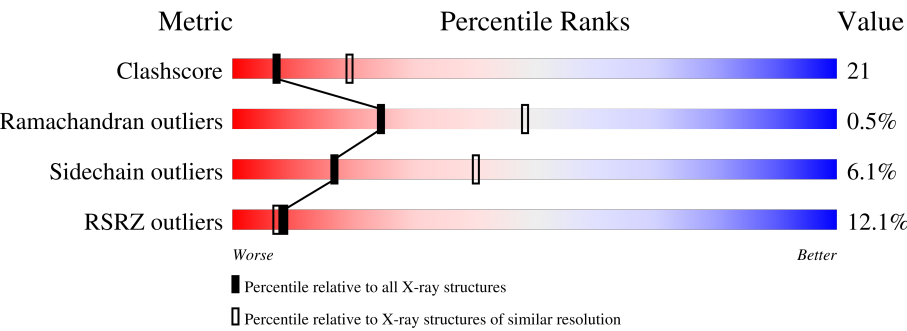
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	222	11% 57% 32% 7% ..
1	B	222	13% 58% 31% 7% ..
1	C	222	12% 55% 33% 8% ..
1	D	222	12% 56% 32% 8% ..
1	E	222	12% 57% 32% 7% ..
1	F	222	10% 56% 33% 7% ..
1	G	222	14% 55% 34% 8% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	222	11% 55% 33% 8% • •

2 Entry composition

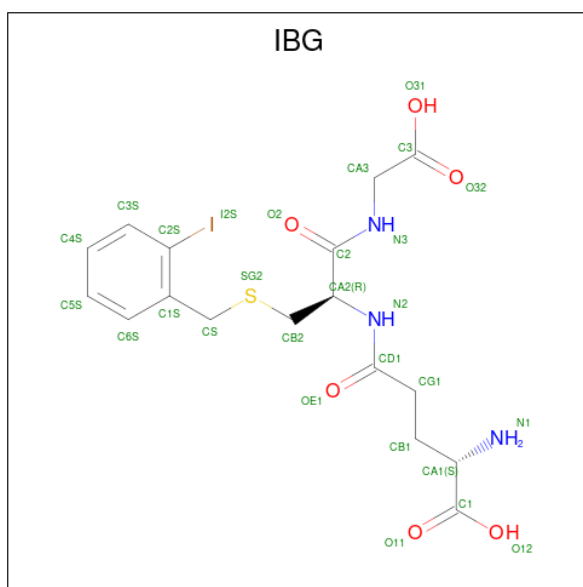
There are 3 unique types of molecules in this entry. The entry contains 14656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutathione S-transferase A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	B	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	C	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	D	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	E	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	F	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	G	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			
1	H	217	Total	C	N	O	S	0	0	0
			1777	1158	298	315	6			

- Molecule 2 is GAMMA-GLUTAMYL[S-(2-IODOBENZYL)CYSTEINYL]GLYCINE (CCD ID: IBG) (formula: C₁₇H₂₂IN₃O₆S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		
2	B	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		
2	C	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		
2	D	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		
2	E	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		
2	F	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		
2	G	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		
2	H	1	Total	C	I	N	O	S	0	0
			28	17	1	3	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	27	Total	O	0	0
			27	27		
3	C	27	Total	O	0	0
			27	27		
3	D	27	Total	O	0	0
			27	27		

Continued on next page...

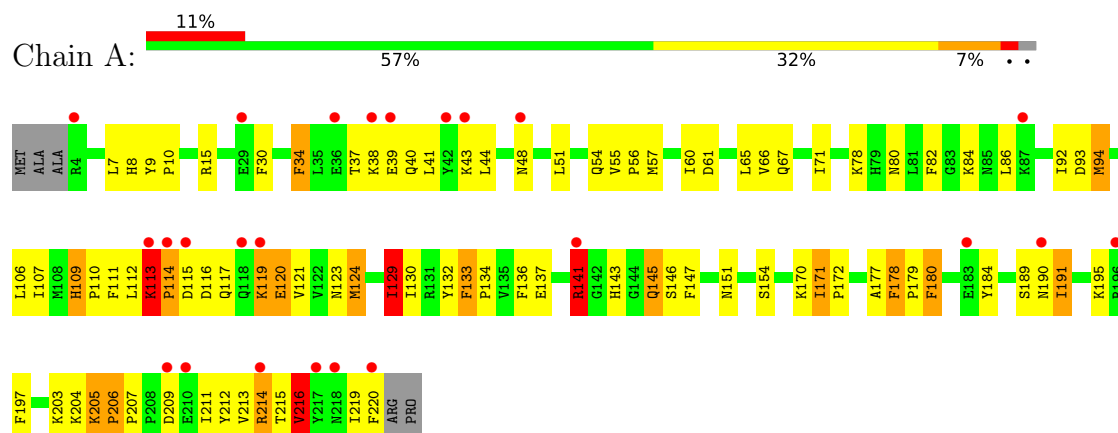
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	27	Total 27	O 27	0	0
3	F	27	Total 27	O 27	0	0
3	G	27	Total 27	O 27	0	0
3	H	27	Total 27	O 27	0	0

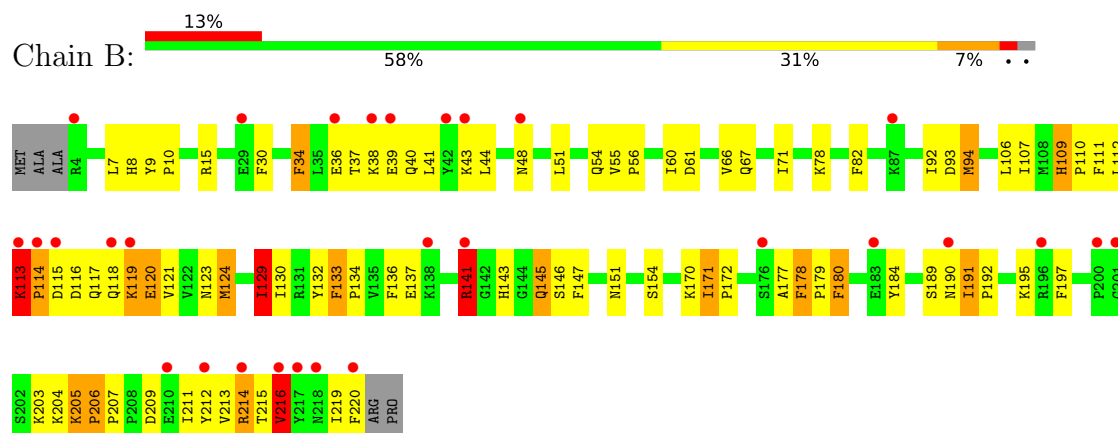
3 Residue-property plots [i](#)

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.

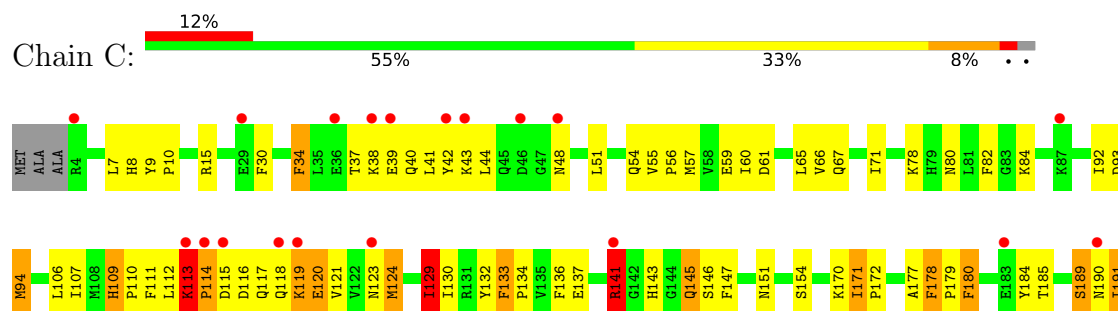
• Molecule 1: Glutathione S-transferase A4

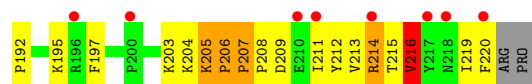


• Molecule 1: Glutathione S-transferase A4

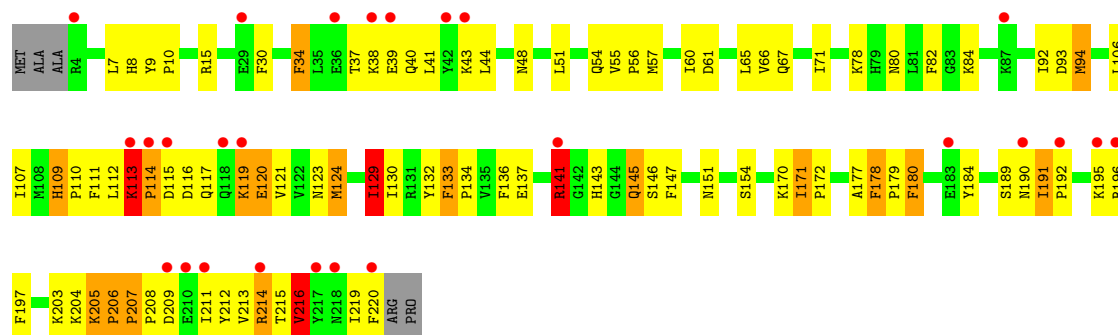


• Molecule 1: Glutathione S-transferase A4

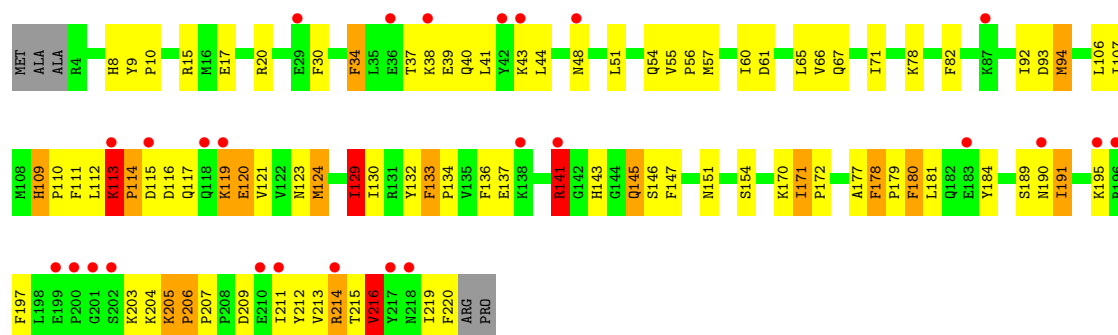




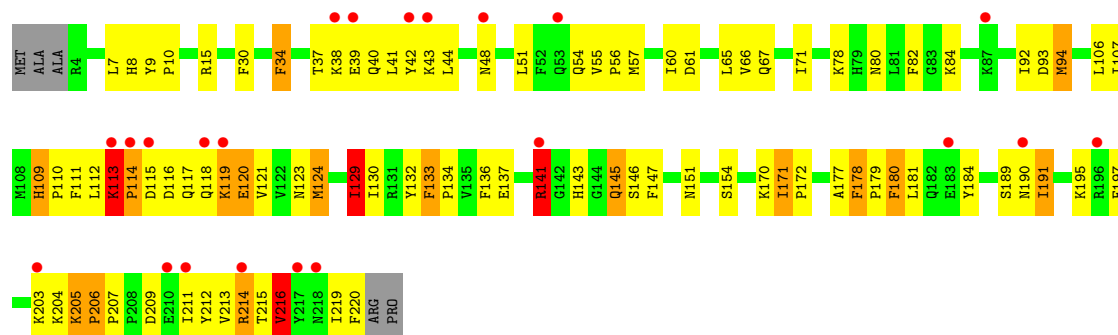
• Molecule 1: Glutathione S-transferase A4



• Molecule 1: Glutathione S-transferase A4

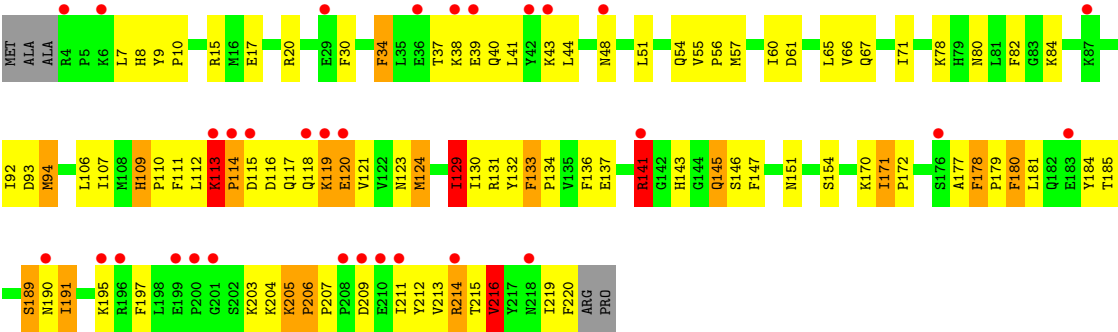


• Molecule 1: Glutathione S-transferase A4

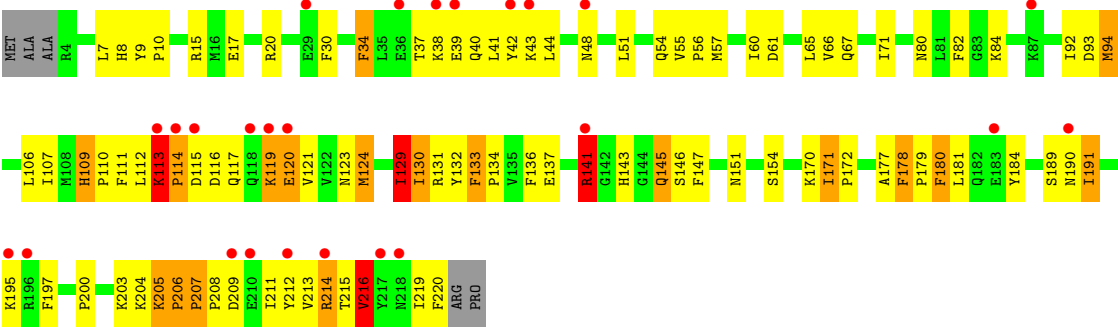


• Molecule 1: Glutathione S-transferase A4





● Molecule 1: Glutathione S-transferase A4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.30Å 156.10Å 101.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	160.00 – 2.70 110.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.0 (160.00-2.70) 86.1 (110.09-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.61Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.248 , 0.260 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14656	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: IBG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.63	4/1817 (0.2%)	1.94	43/2456 (1.8%)
1	B	1.63	4/1817 (0.2%)	1.94	43/2456 (1.8%)
1	C	1.63	4/1817 (0.2%)	1.94	43/2456 (1.8%)
1	D	1.63	4/1817 (0.2%)	1.94	43/2456 (1.8%)
1	E	1.63	4/1817 (0.2%)	1.94	43/2456 (1.8%)
1	F	1.63	4/1817 (0.2%)	1.94	43/2456 (1.8%)
1	G	1.63	4/1817 (0.2%)	1.94	44/2456 (1.8%)
1	H	1.63	4/1817 (0.2%)	1.94	43/2456 (1.8%)
All	All	1.63	32/14536 (0.2%)	1.94	345/19648 (1.8%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	207	PRO	CA-C	-5.77	1.46	1.52
1	B	207	PRO	CA-C	-5.75	1.46	1.52
1	D	207	PRO	CA-C	-5.72	1.46	1.52
1	G	207	PRO	CA-C	-5.71	1.46	1.52
1	C	207	PRO	CA-C	-5.70	1.46	1.52
1	A	207	PRO	CA-C	-5.70	1.46	1.52
1	H	207	PRO	CA-C	-5.68	1.46	1.52
1	E	207	PRO	CA-C	-5.65	1.47	1.52
1	C	191	ILE	C-N	-5.37	1.26	1.33
1	D	191	ILE	C-N	-5.36	1.26	1.33
1	G	121	VAL	CA-CB	-5.34	1.47	1.54
1	F	191	ILE	C-N	-5.34	1.26	1.33
1	B	191	ILE	C-N	-5.33	1.26	1.33
1	C	121	VAL	CA-CB	-5.31	1.47	1.54
1	E	191	ILE	C-N	-5.31	1.26	1.33
1	A	191	ILE	C-N	-5.30	1.26	1.33
1	G	191	ILE	C-N	-5.30	1.26	1.33
1	B	121	VAL	CA-CB	-5.29	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	121	VAL	CA-CB	-5.28	1.47	1.54
1	B	213	VAL	CA-CB	-5.27	1.48	1.54
1	A	121	VAL	CA-CB	-5.27	1.47	1.54
1	C	213	VAL	CA-CB	-5.26	1.48	1.54
1	E	121	VAL	CA-CB	-5.25	1.48	1.54
1	H	191	ILE	C-N	-5.25	1.26	1.33
1	D	121	VAL	CA-CB	-5.25	1.48	1.54
1	F	213	VAL	CA-CB	-5.24	1.48	1.54
1	F	121	VAL	CA-CB	-5.22	1.48	1.54
1	E	213	VAL	CA-CB	-5.21	1.48	1.54
1	A	213	VAL	CA-CB	-5.21	1.48	1.54
1	D	213	VAL	CA-CB	-5.20	1.48	1.54
1	H	213	VAL	CA-CB	-5.18	1.48	1.54
1	G	213	VAL	CA-CB	-5.17	1.48	1.54

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	133	PHE	CA-C-O	8.88	126.50	118.33
1	H	133	PHE	CA-C-O	8.85	126.47	118.33
1	B	133	PHE	CA-C-O	8.84	126.46	118.33
1	A	133	PHE	CA-C-O	8.82	126.44	118.33
1	C	133	PHE	CA-C-O	8.81	126.44	118.33
1	G	133	PHE	CA-C-O	8.81	126.43	118.33
1	E	133	PHE	CA-C-O	8.79	126.41	118.33
1	D	133	PHE	CA-C-O	8.78	126.41	118.33
1	G	147	PHE	CA-CB-CG	-8.49	105.31	113.80
1	E	147	PHE	CA-CB-CG	-8.48	105.31	113.80
1	F	147	PHE	CA-CB-CG	-8.48	105.32	113.80
1	C	147	PHE	CA-CB-CG	-8.47	105.33	113.80
1	D	147	PHE	CA-CB-CG	-8.47	105.33	113.80
1	A	147	PHE	CA-CB-CG	-8.46	105.33	113.80
1	B	147	PHE	CA-CB-CG	-8.45	105.35	113.80
1	D	220	PHE	CA-CB-CG	8.45	122.25	113.80
1	A	220	PHE	CA-CB-CG	8.41	122.22	113.80
1	F	220	PHE	CA-CB-CG	8.40	122.20	113.80
1	G	220	PHE	CA-CB-CG	8.40	122.20	113.80
1	B	220	PHE	CA-CB-CG	8.39	122.19	113.80
1	C	220	PHE	CA-CB-CG	8.39	122.19	113.80
1	H	147	PHE	CA-CB-CG	-8.39	105.41	113.80
1	E	220	PHE	CA-CB-CG	8.38	122.18	113.80
1	H	220	PHE	CA-CB-CG	8.37	122.17	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	PHE	N-CA-C	8.20	122.41	110.28
1	F	34	PHE	N-CA-C	8.20	122.41	110.28
1	E	34	PHE	N-CA-C	8.19	122.40	110.28
1	A	34	PHE	N-CA-C	8.19	122.39	110.28
1	C	34	PHE	N-CA-C	8.18	122.38	110.28
1	G	34	PHE	N-CA-C	8.18	122.38	110.28
1	H	34	PHE	N-CA-C	8.17	122.38	110.28
1	D	34	PHE	N-CA-C	8.16	122.36	110.28
1	G	120	GLU	CA-CB-CG	-8.14	97.82	114.10
1	B	120	GLU	CA-CB-CG	-8.13	97.83	114.10
1	D	120	GLU	CA-CB-CG	-8.13	97.84	114.10
1	F	120	GLU	CA-CB-CG	-8.13	97.84	114.10
1	A	120	GLU	CA-CB-CG	-8.12	97.85	114.10
1	E	120	GLU	CA-CB-CG	-8.13	97.85	114.10
1	C	120	GLU	CA-CB-CG	-8.12	97.85	114.10
1	H	120	GLU	CA-CB-CG	-8.10	97.91	114.10
1	C	129	ILE	CB-CA-C	-8.07	101.24	112.14
1	E	129	ILE	CB-CA-C	-8.07	101.24	112.14
1	A	129	ILE	CB-CA-C	-8.06	101.25	112.14
1	D	129	ILE	CB-CA-C	-8.06	101.25	112.14
1	B	129	ILE	CB-CA-C	-8.06	101.26	112.14
1	F	129	ILE	CB-CA-C	-8.06	101.26	112.14
1	H	129	ILE	CB-CA-C	-8.06	101.26	112.14
1	G	129	ILE	CB-CA-C	-8.04	101.28	112.14
1	E	207	PRO	N-CA-C	-7.51	101.54	110.70
1	C	207	PRO	N-CA-C	-7.48	101.58	110.70
1	A	207	PRO	N-CA-C	-7.48	101.58	110.70
1	G	207	PRO	N-CA-C	-7.47	101.58	110.70
1	F	207	PRO	N-CA-C	-7.47	101.59	110.70
1	B	207	PRO	N-CA-C	-7.46	101.60	110.70
1	D	207	PRO	N-CA-C	-7.46	101.60	110.70
1	H	207	PRO	N-CA-C	-7.45	101.61	110.70
1	H	171	ILE	CA-C-N	7.34	127.98	119.47
1	H	171	ILE	C-N-CA	7.34	127.98	119.47
1	B	171	ILE	CA-C-N	7.32	127.97	119.47
1	B	171	ILE	C-N-CA	7.32	127.97	119.47
1	C	171	ILE	CA-C-N	7.31	127.95	119.47
1	C	171	ILE	C-N-CA	7.31	127.95	119.47
1	F	171	ILE	CA-C-N	7.30	127.94	119.47
1	F	171	ILE	C-N-CA	7.30	127.94	119.47
1	A	171	ILE	CA-C-N	7.29	127.92	119.47
1	A	171	ILE	C-N-CA	7.29	127.92	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	ILE	CA-C-N	7.29	127.92	119.47
1	D	171	ILE	C-N-CA	7.29	127.92	119.47
1	E	171	ILE	CA-C-N	7.26	127.89	119.47
1	E	171	ILE	C-N-CA	7.26	127.89	119.47
1	G	171	ILE	CA-C-N	7.25	127.88	119.47
1	G	171	ILE	C-N-CA	7.25	127.88	119.47
1	H	191	ILE	CA-C-O	7.25	126.78	119.82
1	A	191	ILE	CA-C-O	7.22	126.76	119.82
1	D	191	ILE	CA-C-O	7.22	126.75	119.82
1	E	191	ILE	CA-C-O	7.22	126.75	119.82
1	C	191	ILE	CA-C-O	7.21	126.74	119.82
1	B	191	ILE	CA-C-O	7.21	126.74	119.82
1	G	191	ILE	CA-C-O	7.20	126.73	119.82
1	D	178	PHE	CA-C-N	7.19	127.03	119.05
1	D	178	PHE	C-N-CA	7.19	127.03	119.05
1	F	191	ILE	CA-C-O	7.19	126.72	119.82
1	H	178	PHE	CA-C-N	7.18	127.02	119.05
1	H	178	PHE	C-N-CA	7.18	127.02	119.05
1	G	178	PHE	CA-C-N	7.17	127.00	119.05
1	G	178	PHE	C-N-CA	7.17	127.00	119.05
1	E	190	ASN	N-CA-CB	7.16	121.69	110.46
1	G	190	ASN	N-CA-CB	7.15	121.69	110.46
1	E	178	PHE	CA-C-N	7.15	126.98	119.05
1	E	178	PHE	C-N-CA	7.15	126.98	119.05
1	B	178	PHE	CA-C-N	7.14	126.98	119.05
1	B	178	PHE	C-N-CA	7.14	126.98	119.05
1	A	178	PHE	CA-C-N	7.14	126.97	119.05
1	A	178	PHE	C-N-CA	7.14	126.97	119.05
1	F	190	ASN	N-CA-CB	7.14	121.66	110.46
1	H	190	ASN	N-CA-CB	7.13	121.66	110.46
1	A	190	ASN	N-CA-CB	7.13	121.65	110.46
1	C	178	PHE	CA-C-N	7.13	126.96	119.05
1	C	178	PHE	C-N-CA	7.13	126.96	119.05
1	D	190	ASN	N-CA-CB	7.13	121.65	110.46
1	D	180	PHE	CA-CB-CG	-7.12	106.68	113.80
1	B	190	ASN	N-CA-CB	7.12	121.64	110.46
1	F	178	PHE	CA-C-N	7.12	126.95	119.05
1	F	178	PHE	C-N-CA	7.12	126.95	119.05
1	C	190	ASN	N-CA-CB	7.11	121.63	110.46
1	C	180	PHE	CA-CB-CG	-7.10	106.70	113.80
1	B	180	PHE	CA-CB-CG	-7.09	106.70	113.80
1	E	180	PHE	CA-CB-CG	-7.08	106.72	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	PHE	CA-CB-CG	-7.08	106.72	113.80
1	F	180	PHE	CA-CB-CG	-7.08	106.72	113.80
1	G	180	PHE	CA-CB-CG	-7.07	106.73	113.80
1	H	180	PHE	CA-CB-CG	-7.05	106.75	113.80
1	G	124	MET	CB-CA-C	-6.97	99.22	110.79
1	C	124	MET	CB-CA-C	-6.96	99.23	110.79
1	A	124	MET	CB-CA-C	-6.96	99.25	110.79
1	E	124	MET	CB-CA-C	-6.95	99.25	110.79
1	H	124	MET	CB-CA-C	-6.95	99.25	110.79
1	F	124	MET	CB-CA-C	-6.95	99.26	110.79
1	B	124	MET	CB-CA-C	-6.95	99.26	110.79
1	D	124	MET	CB-CA-C	-6.94	99.27	110.79
1	A	113	LYS	CA-C-N	6.62	128.11	119.84
1	A	113	LYS	C-N-CA	6.62	128.11	119.84
1	H	113	LYS	CA-C-N	6.61	128.10	119.84
1	H	113	LYS	C-N-CA	6.61	128.10	119.84
1	C	113	LYS	CA-C-N	6.61	128.10	119.84
1	C	113	LYS	C-N-CA	6.61	128.10	119.84
1	B	113	LYS	CA-C-N	6.60	128.09	119.84
1	B	113	LYS	C-N-CA	6.60	128.09	119.84
1	D	113	LYS	CA-C-N	6.60	128.09	119.84
1	D	113	LYS	C-N-CA	6.60	128.09	119.84
1	E	113	LYS	CA-C-N	6.60	128.09	119.84
1	E	113	LYS	C-N-CA	6.60	128.09	119.84
1	G	113	LYS	CA-C-N	6.59	128.08	119.84
1	G	113	LYS	C-N-CA	6.59	128.08	119.84
1	F	113	LYS	CA-C-N	6.58	128.06	119.84
1	F	113	LYS	C-N-CA	6.58	128.06	119.84
1	E	15	ARG	CD-NE-CZ	-6.57	115.21	124.40
1	C	15	ARG	CD-NE-CZ	-6.53	115.25	124.40
1	G	15	ARG	CD-NE-CZ	-6.53	115.25	124.40
1	A	15	ARG	CD-NE-CZ	-6.53	115.26	124.40
1	D	15	ARG	CD-NE-CZ	-6.52	115.27	124.40
1	B	15	ARG	CD-NE-CZ	-6.52	115.27	124.40
1	F	15	ARG	CD-NE-CZ	-6.51	115.29	124.40
1	H	15	ARG	CD-NE-CZ	-6.49	115.31	124.40
1	B	207	PRO	CA-C-N	6.40	126.35	119.76
1	B	207	PRO	C-N-CA	6.40	126.35	119.76
1	G	207	PRO	CA-C-N	6.38	126.33	119.76
1	G	207	PRO	C-N-CA	6.38	126.33	119.76
1	F	207	PRO	CA-C-N	6.37	126.32	119.76
1	F	207	PRO	C-N-CA	6.37	126.32	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	207	PRO	CA-C-N	6.37	126.32	119.76
1	E	207	PRO	C-N-CA	6.37	126.32	119.76
1	A	207	PRO	CA-C-N	6.36	126.31	119.76
1	A	207	PRO	C-N-CA	6.36	126.31	119.76
1	C	207	PRO	CA-C-N	6.35	126.30	119.76
1	C	207	PRO	C-N-CA	6.35	126.30	119.76
1	D	207	PRO	CA-C-N	6.30	126.25	119.76
1	D	207	PRO	C-N-CA	6.30	126.25	119.76
1	H	207	PRO	CA-C-N	6.28	126.23	119.76
1	H	207	PRO	C-N-CA	6.28	126.23	119.76
1	H	120	GLU	N-CA-C	6.16	118.00	111.28
1	C	120	GLU	N-CA-C	6.15	117.98	111.28
1	D	120	GLU	N-CA-C	6.14	117.97	111.28
1	G	120	GLU	N-CA-C	6.13	117.97	111.28
1	A	120	GLU	N-CA-C	6.13	117.96	111.28
1	B	206	PRO	CB-CA-C	-6.12	103.46	110.92
1	E	120	GLU	N-CA-C	6.11	117.94	111.28
1	B	120	GLU	N-CA-C	6.09	117.92	111.28
1	A	206	PRO	CB-CA-C	-6.09	103.50	110.92
1	H	206	PRO	CB-CA-C	-6.08	103.50	110.92
1	F	120	GLU	N-CA-C	6.08	117.91	111.28
1	E	206	PRO	CB-CA-C	-6.07	103.51	110.92
1	G	206	PRO	CB-CA-C	-6.07	103.51	110.92
1	F	206	PRO	CB-CA-C	-6.07	103.52	110.92
1	C	206	PRO	CB-CA-C	-6.06	103.53	110.92
1	D	206	PRO	CB-CA-C	-6.05	103.53	110.92
1	C	216	VAL	N-CA-CB	6.04	118.75	110.54
1	E	216	VAL	N-CA-CB	6.02	118.73	110.54
1	A	216	VAL	N-CA-CB	6.00	118.70	110.54
1	G	216	VAL	N-CA-CB	5.99	118.69	110.54
1	B	216	VAL	N-CA-CB	5.99	118.69	110.54
1	H	216	VAL	N-CA-CB	5.97	118.67	110.54
1	B	109	HIS	CA-CB-CG	-5.96	107.83	113.80
1	D	109	HIS	CA-CB-CG	-5.96	107.84	113.80
1	F	216	VAL	N-CA-CB	5.96	118.65	110.54
1	D	216	VAL	N-CA-CB	5.95	118.64	110.54
1	H	109	HIS	CA-CB-CG	-5.95	107.85	113.80
1	F	109	HIS	CA-CB-CG	-5.95	107.85	113.80
1	A	109	HIS	CA-CB-CG	-5.94	107.86	113.80
1	G	109	HIS	CA-CB-CG	-5.93	107.86	113.80
1	F	136	PHE	CA-CB-CG	-5.92	107.88	113.80
1	E	109	HIS	CA-CB-CG	-5.91	107.89	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	136	PHE	CA-CB-CG	-5.91	107.89	113.80
1	C	109	HIS	CA-CB-CG	-5.90	107.90	113.80
1	C	136	PHE	CA-CB-CG	-5.90	107.90	113.80
1	A	136	PHE	CA-CB-CG	-5.90	107.90	113.80
1	E	136	PHE	CA-CB-CG	-5.90	107.90	113.80
1	B	136	PHE	CA-CB-CG	-5.88	107.92	113.80
1	D	136	PHE	CA-CB-CG	-5.87	107.93	113.80
1	H	136	PHE	CA-CB-CG	-5.87	107.93	113.80
1	D	141	ARG	N-CA-C	-5.87	105.02	111.82
1	C	93	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	141	ARG	N-CA-C	-5.86	105.03	111.82
1	G	141	ARG	N-CA-C	-5.86	105.03	111.82
1	H	130	ILE	CB-CA-C	-5.85	104.56	111.94
1	C	130	ILE	CB-CA-C	-5.85	104.57	111.94
1	B	141	ARG	N-CA-C	-5.85	105.03	111.82
1	B	130	ILE	CB-CA-C	-5.85	104.57	111.94
1	E	130	ILE	CB-CA-C	-5.84	104.58	111.94
1	F	93	ASP	CA-CB-CG	5.84	118.44	112.60
1	H	93	ASP	CA-CB-CG	5.84	118.44	112.60
1	E	141	ARG	N-CA-C	-5.84	105.04	111.82
1	A	93	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	130	ILE	CB-CA-C	-5.84	104.58	111.94
1	A	141	ARG	N-CA-C	-5.83	105.05	111.82
1	F	130	ILE	CB-CA-C	-5.83	104.59	111.94
1	D	93	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	130	ILE	CB-CA-C	-5.83	104.60	111.94
1	H	141	ARG	N-CA-C	-5.82	105.06	111.82
1	D	130	ILE	N-CA-C	5.82	117.75	111.58
1	F	141	ARG	N-CA-C	-5.82	105.07	111.82
1	E	93	ASP	CA-CB-CG	5.82	118.42	112.60
1	G	130	ILE	CB-CA-C	-5.82	104.61	111.94
1	G	130	ILE	N-CA-C	5.81	117.74	111.58
1	F	130	ILE	N-CA-C	5.81	117.74	111.58
1	B	93	ASP	CA-CB-CG	5.80	118.40	112.60
1	G	93	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	130	ILE	N-CA-C	5.80	117.73	111.58
1	B	130	ILE	N-CA-C	5.80	117.73	111.58
1	C	130	ILE	N-CA-C	5.79	117.71	111.58
1	E	130	ILE	N-CA-C	5.78	117.71	111.58
1	H	130	ILE	N-CA-C	5.78	117.71	111.58
1	C	44	LEU	N-CA-CB	-5.71	101.71	110.16
1	B	44	LEU	N-CA-CB	-5.70	101.72	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	44	LEU	N-CA-CB	-5.70	101.73	110.16
1	A	44	LEU	N-CA-CB	-5.69	101.73	110.16
1	E	44	LEU	N-CA-CB	-5.69	101.73	110.16
1	G	44	LEU	N-CA-CB	-5.69	101.74	110.16
1	H	44	LEU	N-CA-CB	-5.69	101.73	110.16
1	D	44	LEU	N-CA-CB	-5.68	101.75	110.16
1	D	129	ILE	CB-CG1-CD1	-5.60	102.03	113.80
1	G	129	ILE	CB-CG1-CD1	-5.59	102.06	113.80
1	B	129	ILE	CB-CG1-CD1	-5.59	102.06	113.80
1	C	129	ILE	CB-CG1-CD1	-5.59	102.06	113.80
1	F	129	ILE	CB-CG1-CD1	-5.59	102.06	113.80
1	A	129	ILE	CB-CG1-CD1	-5.58	102.07	113.80
1	H	129	ILE	CB-CG1-CD1	-5.58	102.08	113.80
1	E	129	ILE	CB-CG1-CD1	-5.57	102.10	113.80
1	D	205	LYS	CA-C-N	5.53	126.07	120.38
1	D	205	LYS	C-N-CA	5.53	126.07	120.38
1	F	205	LYS	CA-C-N	5.53	126.07	120.38
1	F	205	LYS	C-N-CA	5.53	126.07	120.38
1	E	205	LYS	CA-C-N	5.52	126.07	120.38
1	E	205	LYS	C-N-CA	5.52	126.07	120.38
1	G	132	TYR	N-CA-C	5.51	119.73	111.96
1	F	132	TYR	N-CA-C	5.51	119.73	111.96
1	A	132	TYR	N-CA-C	5.50	119.72	111.96
1	C	132	TYR	N-CA-C	5.50	119.72	111.96
1	A	205	LYS	CA-C-N	5.50	126.04	120.38
1	A	205	LYS	C-N-CA	5.50	126.04	120.38
1	C	205	LYS	CA-C-N	5.50	126.04	120.38
1	C	205	LYS	C-N-CA	5.50	126.04	120.38
1	E	132	TYR	N-CA-C	5.50	119.71	111.96
1	D	132	TYR	N-CA-C	5.49	119.71	111.96
1	B	205	LYS	CA-C-N	5.48	126.03	120.38
1	B	205	LYS	C-N-CA	5.48	126.03	120.38
1	G	205	LYS	CA-C-N	5.48	126.03	120.38
1	G	205	LYS	C-N-CA	5.48	126.03	120.38
1	H	132	TYR	N-CA-C	5.48	119.69	111.96
1	H	205	LYS	CA-C-N	5.48	126.02	120.38
1	H	205	LYS	C-N-CA	5.48	126.02	120.38
1	B	132	TYR	N-CA-C	5.47	119.67	111.96
1	F	71	ILE	CA-CB-CG2	-5.45	101.23	110.50
1	D	71	ILE	CA-CB-CG2	-5.45	101.24	110.50
1	H	71	ILE	CA-CB-CG2	-5.45	101.24	110.50
1	E	71	ILE	CA-CB-CG2	-5.44	101.25	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	ILE	CA-CB-CG2	-5.44	101.26	110.50
1	G	71	ILE	CA-CB-CG2	-5.43	101.26	110.50
1	A	71	ILE	CA-CB-CG2	-5.43	101.27	110.50
1	B	71	ILE	CA-CB-CG2	-5.41	101.30	110.50
1	D	184	TYR	N-CA-CB	-5.35	102.03	110.06
1	F	184	TYR	N-CA-CB	-5.35	102.04	110.06
1	G	184	TYR	N-CA-CB	-5.35	102.04	110.06
1	E	184	TYR	N-CA-CB	-5.34	102.06	110.06
1	A	184	TYR	N-CA-CB	-5.33	102.06	110.06
1	H	184	TYR	N-CA-CB	-5.33	102.06	110.06
1	C	184	TYR	N-CA-CB	-5.33	102.06	110.06
1	E	8	HIS	CA-CB-CG	-5.31	108.49	113.80
1	B	184	TYR	N-CA-CB	-5.30	102.11	110.06
1	F	8	HIS	CA-CB-CG	-5.29	108.51	113.80
1	H	8	HIS	CA-CB-CG	-5.29	108.52	113.80
1	G	94	MET	CG-SD-CE	-5.28	89.28	100.90
1	B	8	HIS	CA-CB-CG	-5.28	108.52	113.80
1	G	8	HIS	CA-CB-CG	-5.28	108.52	113.80
1	G	54	GLN	CB-CA-C	-5.28	99.86	110.30
1	E	94	MET	CG-SD-CE	-5.27	89.30	100.90
1	H	94	MET	CG-SD-CE	-5.27	89.30	100.90
1	E	54	GLN	CB-CA-C	-5.27	99.86	110.30
1	A	94	MET	CG-SD-CE	-5.27	89.31	100.90
1	C	94	MET	CG-SD-CE	-5.27	89.31	100.90
1	D	54	GLN	CB-CA-C	-5.27	99.86	110.30
1	F	54	GLN	CB-CA-C	-5.27	99.87	110.30
1	A	8	HIS	CA-CB-CG	-5.27	108.53	113.80
1	C	54	GLN	CB-CA-C	-5.27	99.87	110.30
1	D	94	MET	CG-SD-CE	-5.27	89.31	100.90
1	A	54	GLN	CB-CA-C	-5.26	99.88	110.30
1	C	8	HIS	CA-CB-CG	-5.26	108.54	113.80
1	B	54	GLN	CB-CA-C	-5.26	99.89	110.30
1	F	94	MET	CG-SD-CE	-5.26	89.33	100.90
1	D	8	HIS	CA-CB-CG	-5.25	108.55	113.80
1	B	94	MET	CG-SD-CE	-5.25	89.34	100.90
1	H	178	PHE	CA-CB-CG	-5.25	108.55	113.80
1	H	54	GLN	CB-CA-C	-5.24	99.92	110.30
1	G	61	ASP	CA-CB-CG	-5.24	107.36	112.60
1	C	178	PHE	CA-CB-CG	-5.22	108.58	113.80
1	E	61	ASP	CA-CB-CG	-5.22	107.38	112.60
1	H	61	ASP	CA-CB-CG	-5.22	107.38	112.60
1	C	61	ASP	CA-CB-CG	-5.21	107.39	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	178	PHE	CA-CB-CG	-5.21	108.59	113.80
1	D	178	PHE	CA-CB-CG	-5.21	108.59	113.80
1	B	178	PHE	CA-CB-CG	-5.20	108.60	113.80
1	F	61	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	61	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	178	PHE	CA-CB-CG	-5.20	108.60	113.80
1	G	178	PHE	CA-CB-CG	-5.20	108.61	113.80
1	B	61	ASP	CA-CB-CG	-5.17	107.43	112.60
1	E	178	PHE	CA-CB-CG	-5.17	108.63	113.80
1	D	61	ASP	CA-CB-CG	-5.15	107.45	112.60
1	B	145	GLN	CA-CB-CG	-5.13	103.84	114.10
1	G	145	GLN	CA-CB-CG	-5.12	103.85	114.10
1	D	145	GLN	CA-CB-CG	-5.12	103.87	114.10
1	H	145	GLN	CA-CB-CG	-5.11	103.87	114.10
1	F	145	GLN	CA-CB-CG	-5.11	103.88	114.10
1	A	145	GLN	CA-CB-CG	-5.10	103.90	114.10
1	E	145	GLN	CA-CB-CG	-5.10	103.90	114.10
1	C	145	GLN	CA-CB-CG	-5.09	103.92	114.10
1	C	113	LYS	C-N-CD	-5.08	104.16	125.00
1	A	113	LYS	C-N-CD	-5.07	104.21	125.00
1	B	113	LYS	C-N-CD	-5.07	104.21	125.00
1	G	113	LYS	C-N-CD	-5.07	104.21	125.00
1	D	113	LYS	C-N-CD	-5.07	104.23	125.00
1	E	113	LYS	C-N-CD	-5.06	104.24	125.00
1	F	113	LYS	C-N-CD	-5.06	104.24	125.00
1	H	113	LYS	C-N-CD	-5.06	104.26	125.00
1	G	171	ILE	O-C-N	5.04	126.84	121.10

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	1777	0	1829	76	0
1	B	1777	0	1829	78	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1777	0	1829	85	1
1	D	1777	0	1829	84	6
1	E	1777	0	1829	85	0
1	F	1777	0	1829	100	0
1	G	1777	0	1829	97	0
1	H	1777	0	1829	84	6
2	A	28	0	20	1	0
2	B	28	0	20	1	0
2	C	28	0	20	1	0
2	D	28	0	20	1	0
2	E	28	0	20	1	0
2	F	28	0	20	1	0
2	G	28	0	20	1	0
2	H	28	0	20	1	0
3	A	27	0	0	1	0
3	B	27	0	0	1	0
3	C	27	0	0	1	0
3	D	27	0	0	1	0
3	E	27	0	0	1	0
3	F	27	0	0	1	0
3	G	27	0	0	1	0
3	H	27	0	0	1	0
All	All	14656	0	14792	603	7

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 21.

All (603) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:VAL:H	1:F:94:MET:CE	1.51	1.23
1:C:94:MET:CE	1:D:66:VAL:H	1.51	1.20
1:E:94:MET:CE	1:F:66:VAL:H	1.58	1.16
1:A:94:MET:CE	1:B:66:VAL:H	1.66	1.08
1:E:66:VAL:H	1:F:94:MET:HE1	1.17	1.07
1:C:94:MET:HE1	1:D:66:VAL:H	1.18	1.07
1:G:66:VAL:H	1:H:94:MET:CE	1.71	1.04
1:A:66:VAL:H	1:B:94:MET:CE	1.71	1.03
1:E:94:MET:HE1	1:F:66:VAL:H	1.24	1.03
1:C:66:VAL:H	1:D:94:MET:CE	1.75	0.98
1:G:94:MET:CE	1:H:66:VAL:H	1.78	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:MET:HE1	1:B:66:VAL:H	1.32	0.95
1:A:113:LYS:HE2	1:A:113:LYS:H	1.32	0.94
1:B:113:LYS:H	1:B:113:LYS:HE2	1.32	0.94
1:F:113:LYS:HE2	1:F:113:LYS:H	1.33	0.94
1:E:113:LYS:HE2	1:E:113:LYS:H	1.32	0.94
1:H:113:LYS:HE2	1:H:113:LYS:H	1.32	0.93
1:D:113:LYS:HE2	1:D:113:LYS:H	1.32	0.93
1:C:113:LYS:HE2	1:C:113:LYS:H	1.33	0.92
1:G:113:LYS:H	1:G:113:LYS:HE2	1.32	0.91
1:B:119:LYS:NZ	1:B:123:ASN:HB2	1.88	0.89
1:G:66:VAL:H	1:H:94:MET:HE1	1.37	0.89
1:C:119:LYS:NZ	1:C:123:ASN:HB2	1.88	0.89
1:D:119:LYS:NZ	1:D:123:ASN:HB2	1.88	0.89
1:F:118:GLN:HG2	1:G:118:GLN:HG2	1.52	0.89
1:H:119:LYS:NZ	1:H:123:ASN:HB2	1.88	0.89
1:G:119:LYS:NZ	1:G:123:ASN:HB2	1.88	0.88
1:A:119:LYS:NZ	1:A:123:ASN:HB2	1.88	0.88
1:E:119:LYS:NZ	1:E:123:ASN:HB2	1.88	0.87
1:F:119:LYS:NZ	1:F:123:ASN:HB2	1.88	0.87
1:C:94:MET:CE	1:D:66:VAL:N	2.37	0.87
1:E:66:VAL:N	1:F:94:MET:HE1	1.90	0.86
1:E:66:VAL:N	1:F:94:MET:CE	2.37	0.86
1:G:119:LYS:HZ3	1:G:123:ASN:HB2	1.42	0.84
1:A:66:VAL:H	1:B:94:MET:HE1	1.39	0.83
1:F:118:GLN:CG	1:G:118:GLN:HG2	2.08	0.83
1:C:94:MET:HE1	1:D:66:VAL:N	1.91	0.82
1:C:66:VAL:H	1:D:94:MET:HE1	1.43	0.82
1:G:94:MET:HE1	1:H:66:VAL:H	1.44	0.81
1:C:59:GLU:OE1	1:G:211:ILE:HD11	1.80	0.81
1:E:66:VAL:H	1:F:94:MET:HE3	1.42	0.81
1:A:119:LYS:HZ3	1:A:123:ASN:HB2	1.47	0.80
1:E:119:LYS:HZ3	1:E:123:ASN:HB2	1.46	0.80
1:B:119:LYS:HZ3	1:B:123:ASN:HB2	1.45	0.80
1:C:119:LYS:HZ3	1:C:123:ASN:HB2	1.47	0.78
1:E:94:MET:HE1	1:F:66:VAL:N	1.98	0.78
1:H:119:LYS:HZ3	1:H:123:ASN:HB2	1.46	0.78
1:C:94:MET:HE3	1:D:66:VAL:H	1.45	0.78
1:E:94:MET:HE3	1:F:66:VAL:H	1.47	0.78
1:F:119:LYS:HZ3	1:F:123:ASN:HB2	1.46	0.78
1:A:94:MET:HE3	1:B:66:VAL:H	1.48	0.77
1:F:37:THR:OG1	1:F:40:GLN:HG3	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:THR:OG1	1:B:40:GLN:HG3	1.85	0.77
1:C:37:THR:OG1	1:C:40:GLN:HG3	1.85	0.76
1:E:37:THR:OG1	1:E:40:GLN:HG3	1.85	0.76
1:D:37:THR:OG1	1:D:40:GLN:HG3	1.85	0.76
1:D:119:LYS:HZ3	1:D:123:ASN:HB2	1.50	0.76
1:A:37:THR:OG1	1:A:40:GLN:HG3	1.85	0.75
1:H:37:THR:OG1	1:H:40:GLN:HG3	1.85	0.75
1:G:37:THR:OG1	1:G:40:GLN:HG3	1.85	0.75
1:F:118:GLN:HE21	1:G:118:GLN:HG3	1.50	0.75
1:F:118:GLN:NE2	1:G:118:GLN:HG3	2.02	0.74
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.53	0.73
1:A:214:ARG:HG2	1:A:214:ARG:HH11	1.53	0.73
1:E:94:MET:CE	1:F:66:VAL:N	2.44	0.73
1:H:214:ARG:HG2	1:H:214:ARG:HH11	1.53	0.73
1:G:214:ARG:HG2	1:G:214:ARG:HH11	1.53	0.72
1:F:214:ARG:HG2	1:F:214:ARG:HH11	1.53	0.72
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.53	0.72
1:E:214:ARG:HG2	1:E:214:ARG:HH11	1.53	0.72
1:D:214:ARG:HH11	1:D:214:ARG:HG2	1.53	0.72
1:A:94:MET:HE1	1:B:66:VAL:N	2.06	0.70
1:G:205:LYS:HB3	1:G:206:PRO:HD2	1.75	0.69
1:B:205:LYS:HB3	1:B:206:PRO:HD2	1.74	0.69
1:G:66:VAL:H	1:H:94:MET:HE3	1.55	0.69
1:E:205:LYS:HB3	1:E:206:PRO:HD2	1.74	0.69
1:A:205:LYS:HB3	1:A:206:PRO:HD2	1.74	0.68
1:H:205:LYS:HB3	1:H:206:PRO:HD2	1.74	0.68
1:D:205:LYS:HB3	1:D:206:PRO:HD2	1.74	0.68
1:C:205:LYS:HB3	1:C:206:PRO:HD2	1.75	0.68
1:C:113:LYS:H	1:C:113:LYS:CE	2.07	0.68
1:F:205:LYS:HB3	1:F:206:PRO:HD2	1.75	0.68
1:E:112:LEU:HB2	1:E:117:GLN:HG2	1.76	0.67
1:H:112:LEU:HB2	1:H:117:GLN:HG2	1.76	0.67
1:A:112:LEU:HB2	1:A:117:GLN:HG2	1.76	0.67
1:F:113:LYS:H	1:F:113:LYS:CE	2.07	0.67
1:F:118:GLN:CG	1:G:118:GLN:CG	2.72	0.67
1:B:112:LEU:HB2	1:B:117:GLN:HG2	1.76	0.67
1:C:112:LEU:HB2	1:C:117:GLN:HG2	1.76	0.67
1:D:9:TYR:CG	1:D:10:PRO:HD2	2.30	0.67
1:E:113:LYS:H	1:E:113:LYS:CE	2.07	0.66
1:B:113:LYS:H	1:B:113:LYS:CE	2.07	0.66
1:F:9:TYR:CG	1:F:10:PRO:HD2	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:TYR:CG	1:G:10:PRO:HD2	2.30	0.66
1:G:112:LEU:HB2	1:G:117:GLN:HG2	1.76	0.66
1:H:9:TYR:CG	1:H:10:PRO:HD2	2.30	0.66
1:F:112:LEU:HB2	1:F:117:GLN:HG2	1.76	0.66
1:A:9:TYR:CG	1:A:10:PRO:HD2	2.30	0.66
1:B:9:TYR:CG	1:B:10:PRO:HD2	2.30	0.66
1:A:113:LYS:H	1:A:113:LYS:CE	2.07	0.66
1:C:9:TYR:CG	1:C:10:PRO:HD2	2.30	0.66
1:G:94:MET:HE3	1:H:66:VAL:H	1.61	0.66
1:G:113:LYS:H	1:G:113:LYS:CE	2.07	0.66
1:D:112:LEU:HB2	1:D:117:GLN:HG2	1.76	0.65
1:E:9:TYR:CG	1:E:10:PRO:HD2	2.30	0.65
1:F:118:GLN:HG2	1:G:118:GLN:CG	2.25	0.65
1:C:66:VAL:H	1:D:94:MET:HE3	1.62	0.64
1:H:113:LYS:H	1:H:113:LYS:CE	2.07	0.64
1:D:113:LYS:H	1:D:113:LYS:CE	2.07	0.64
1:A:66:VAL:H	1:B:94:MET:HE3	1.60	0.64
1:H:141:ARG:HH11	1:H:141:ARG:HG2	1.63	0.64
1:C:141:ARG:HG2	1:C:141:ARG:HH11	1.63	0.63
1:B:141:ARG:HG2	1:B:141:ARG:HH11	1.63	0.63
1:E:141:ARG:HG2	1:E:141:ARG:HH11	1.63	0.63
1:D:141:ARG:HG2	1:D:141:ARG:HH11	1.63	0.63
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.63	0.63
1:F:141:ARG:HH11	1:F:141:ARG:HG2	1.63	0.63
1:F:215:THR:O	1:F:219:ILE:HG13	2.00	0.62
1:A:215:THR:O	1:A:219:ILE:HG13	2.00	0.62
1:E:215:THR:O	1:E:219:ILE:HG13	2.00	0.62
1:G:141:ARG:HG2	1:G:141:ARG:HH11	1.63	0.62
1:F:109:HIS:HB3	1:F:110:PRO:HD3	1.82	0.62
1:A:109:HIS:HB3	1:A:110:PRO:HD3	1.82	0.62
1:G:109:HIS:HB3	1:G:110:PRO:HD3	1.82	0.61
1:H:109:HIS:HB3	1:H:110:PRO:HD3	1.82	0.61
1:H:215:THR:O	1:H:219:ILE:HG13	2.00	0.61
1:C:113:LYS:O	1:C:116:ASP:N	2.33	0.61
1:F:113:LYS:O	1:F:116:ASP:N	2.33	0.61
1:A:94:MET:HE2	1:B:66:VAL:HG22	1.81	0.61
1:C:215:THR:O	1:C:219:ILE:HG13	2.00	0.61
1:A:94:MET:CE	1:B:66:VAL:HG22	2.31	0.61
1:D:215:THR:O	1:D:219:ILE:HG13	2.00	0.61
1:F:118:GLN:CD	1:G:118:GLN:HG2	2.25	0.61
1:D:109:HIS:HB3	1:D:110:PRO:HD3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:VAL:HG22	1:F:94:MET:HE2	1.81	0.61
1:E:109:HIS:HB3	1:E:110:PRO:HD3	1.82	0.60
1:A:113:LYS:O	1:A:116:ASP:N	2.33	0.60
1:B:215:THR:O	1:B:219:ILE:HG13	2.00	0.60
1:D:113:LYS:O	1:D:116:ASP:N	2.33	0.60
1:H:113:LYS:O	1:H:116:ASP:N	2.33	0.60
1:A:65:LEU:HA	1:B:94:MET:HE1	1.82	0.60
1:B:109:HIS:HB3	1:B:110:PRO:HD3	1.82	0.60
1:B:113:LYS:O	1:B:116:ASP:N	2.34	0.60
1:C:94:MET:HE1	1:D:65:LEU:HA	1.84	0.60
1:E:113:LYS:O	1:E:116:ASP:N	2.34	0.60
1:A:66:VAL:N	1:B:94:MET:HE1	2.13	0.60
1:G:113:LYS:O	1:G:116:ASP:N	2.34	0.60
1:G:212:TYR:O	1:G:216:VAL:HG13	2.02	0.60
1:G:215:THR:O	1:G:219:ILE:HG13	2.00	0.60
1:G:66:VAL:N	1:H:94:MET:HE1	2.11	0.60
1:F:212:TYR:O	1:F:216:VAL:HG13	2.02	0.59
1:C:212:TYR:O	1:C:216:VAL:HG13	2.02	0.59
1:E:212:TYR:O	1:E:216:VAL:HG13	2.02	0.59
1:H:212:TYR:O	1:H:216:VAL:HG13	2.02	0.59
1:B:212:TYR:O	1:B:216:VAL:HG13	2.02	0.59
1:C:109:HIS:HB3	1:C:110:PRO:HD3	1.82	0.59
1:D:212:TYR:O	1:D:216:VAL:HG13	2.02	0.59
1:A:94:MET:CE	1:B:66:VAL:N	2.51	0.59
1:C:133:PHE:HB2	1:C:134:PRO:HD3	1.85	0.59
1:F:133:PHE:HB2	1:F:134:PRO:HD3	1.85	0.59
1:A:133:PHE:HB2	1:A:134:PRO:HD3	1.85	0.59
1:B:133:PHE:HB2	1:B:134:PRO:HD3	1.85	0.59
1:G:133:PHE:HB2	1:G:134:PRO:HD3	1.85	0.59
1:H:133:PHE:HB2	1:H:134:PRO:HD3	1.85	0.59
1:A:212:TYR:O	1:A:216:VAL:HG13	2.02	0.58
1:C:65:LEU:HA	1:D:94:MET:HE1	1.84	0.58
1:D:129:ILE:N	1:D:129:ILE:HD13	2.18	0.58
1:C:129:ILE:HD13	1:C:129:ILE:N	2.18	0.58
1:F:191:ILE:O	1:F:195:LYS:N	2.29	0.58
1:E:133:PHE:HB2	1:E:134:PRO:HD3	1.85	0.58
1:F:118:GLN:NE2	1:G:118:GLN:CG	2.65	0.58
1:H:129:ILE:HD13	1:H:129:ILE:N	2.18	0.57
1:D:133:PHE:HB2	1:D:134:PRO:HD3	1.85	0.57
1:E:66:VAL:HG22	1:F:94:MET:CE	2.35	0.57
1:C:66:VAL:N	1:D:94:MET:HE1	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:O	1:C:195:LYS:N	2.29	0.57
1:G:94:MET:HE1	1:H:66:VAL:N	2.19	0.57
1:A:94:MET:HE2	1:B:66:VAL:CG2	2.35	0.57
1:F:129:ILE:HD13	1:F:129:ILE:N	2.18	0.57
1:G:129:ILE:N	1:G:129:ILE:HD13	2.18	0.56
1:H:214:ARG:HH11	1:H:214:ARG:CG	2.18	0.56
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.18	0.56
1:A:214:ARG:HH11	1:A:214:ARG:CG	2.18	0.56
1:C:94:MET:HE2	1:D:66:VAL:HG22	1.86	0.56
1:G:66:VAL:HG22	1:H:94:MET:HE2	1.87	0.56
1:H:39:GLU:O	1:H:43:LYS:HG3	2.06	0.56
1:E:39:GLU:O	1:E:43:LYS:HG3	2.06	0.56
1:G:214:ARG:HH11	1:G:214:ARG:CG	2.18	0.56
1:B:39:GLU:O	1:B:43:LYS:HG3	2.06	0.56
1:D:214:ARG:HH11	1:D:214:ARG:CG	2.18	0.56
1:F:214:ARG:HH11	1:F:214:ARG:CG	2.18	0.56
1:B:119:LYS:HD3	1:B:119:LYS:C	2.32	0.55
1:E:66:VAL:CG2	1:F:94:MET:HE2	2.35	0.55
1:A:119:LYS:HD3	1:A:119:LYS:C	2.32	0.55
1:D:92:ILE:HD13	1:D:154:SER:HB2	1.88	0.55
1:E:214:ARG:HH11	1:E:214:ARG:CG	2.18	0.55
1:F:118:GLN:HG3	1:G:118:GLN:NE2	2.21	0.55
1:D:39:GLU:O	1:D:43:LYS:HG3	2.06	0.55
1:G:119:LYS:HD3	1:G:119:LYS:C	2.32	0.55
1:A:129:ILE:HD13	1:A:129:ILE:N	2.18	0.55
1:C:92:ILE:HD13	1:C:154:SER:HB2	1.88	0.55
1:C:119:LYS:C	1:C:119:LYS:HD3	2.32	0.55
1:E:66:VAL:O	1:F:94:MET:HE3	2.06	0.55
1:F:92:ILE:HD13	1:F:154:SER:HB2	1.88	0.55
1:A:92:ILE:HD13	1:A:154:SER:HB2	1.88	0.55
1:C:39:GLU:O	1:C:43:LYS:HG3	2.06	0.55
1:A:39:GLU:O	1:A:43:LYS:HG3	2.06	0.55
1:F:119:LYS:HD3	1:F:119:LYS:C	2.32	0.55
1:E:129:ILE:HD13	1:E:129:ILE:N	2.18	0.55
1:F:39:GLU:O	1:F:43:LYS:HG3	2.06	0.55
1:D:119:LYS:HD3	1:D:119:LYS:C	2.32	0.55
1:E:137:GLU:CD	1:E:180:PHE:HB2	2.32	0.55
1:B:137:GLU:CD	1:B:180:PHE:HB2	2.32	0.55
1:E:92:ILE:HD13	1:E:154:SER:HB2	1.88	0.55
1:H:92:ILE:HD13	1:H:154:SER:HB2	1.88	0.55
1:H:119:LYS:HD3	1:H:119:LYS:C	2.32	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:GLU:CD	1:G:180:PHE:HB2	2.32	0.55
1:D:137:GLU:CD	1:D:180:PHE:HB2	2.32	0.54
1:G:39:GLU:O	1:G:43:LYS:HG3	2.06	0.54
1:B:92:ILE:HD13	1:B:154:SER:HB2	1.88	0.54
1:B:214:ARG:HH11	1:B:214:ARG:CG	2.18	0.54
1:B:129:ILE:N	1:B:129:ILE:HD13	2.18	0.54
1:A:137:GLU:CD	1:A:180:PHE:HB2	2.32	0.54
1:E:94:MET:HE2	1:F:66:VAL:HG22	1.87	0.54
1:E:119:LYS:C	1:E:119:LYS:HD3	2.32	0.54
1:C:137:GLU:CD	1:C:180:PHE:HB2	2.32	0.54
1:F:137:GLU:CD	1:F:180:PHE:HB2	2.32	0.54
1:H:137:GLU:CD	1:H:180:PHE:HB2	2.32	0.53
1:G:66:VAL:N	1:H:94:MET:CE	2.56	0.53
1:B:191:ILE:O	1:B:195:LYS:N	2.29	0.53
1:E:94:MET:HE1	1:F:65:LEU:HA	1.90	0.53
1:G:92:ILE:HD13	1:G:154:SER:HB2	1.88	0.53
1:C:129:ILE:O	1:C:129:ILE:HG22	2.09	0.52
1:H:129:ILE:O	1:H:129:ILE:HG22	2.09	0.52
1:G:94:MET:HE2	1:H:66:VAL:HG22	1.92	0.51
1:B:129:ILE:O	1:B:129:ILE:HG22	2.09	0.51
1:D:191:ILE:O	1:D:195:LYS:N	2.29	0.51
1:G:66:VAL:HG22	1:H:94:MET:CE	2.40	0.51
1:A:171:ILE:N	1:A:172:PRO:HD3	2.26	0.51
1:E:94:MET:CE	1:F:66:VAL:HG22	2.41	0.51
1:E:171:ILE:N	1:E:172:PRO:HD3	2.26	0.51
1:F:129:ILE:O	1:F:129:ILE:HG22	2.09	0.51
1:D:171:ILE:N	1:D:172:PRO:HD3	2.26	0.50
1:A:129:ILE:O	1:A:129:ILE:HG22	2.09	0.50
1:C:51:LEU:HB3	1:C:66:VAL:HG21	1.94	0.50
1:H:51:LEU:HB3	1:H:66:VAL:HG21	1.94	0.50
1:C:94:MET:HE3	1:D:66:VAL:O	2.11	0.49
1:E:51:LEU:HB3	1:E:66:VAL:HG21	1.94	0.49
1:F:51:LEU:HB3	1:F:66:VAL:HG21	1.94	0.49
1:C:94:MET:HE2	1:D:66:VAL:CG2	2.42	0.49
1:D:51:LEU:HB3	1:D:66:VAL:HG21	1.94	0.49
1:E:65:LEU:HA	1:F:94:MET:HE1	1.93	0.49
1:A:94:MET:HE3	1:B:66:VAL:O	2.11	0.49
1:B:177:ALA:C	1:B:179:PRO:HD3	2.38	0.49
1:E:177:ALA:C	1:E:179:PRO:HD3	2.38	0.49
1:D:177:ALA:C	1:D:179:PRO:HD3	2.38	0.49
1:E:94:MET:HE2	1:F:66:VAL:CG2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:ALA:C	1:F:179:PRO:HD3	2.38	0.49
1:A:177:ALA:C	1:A:179:PRO:HD3	2.38	0.49
1:C:171:ILE:N	1:C:172:PRO:HD3	2.26	0.49
1:G:129:ILE:O	1:G:129:ILE:HG22	2.09	0.48
1:G:171:ILE:N	1:G:172:PRO:HD3	2.26	0.48
1:B:51:LEU:HB3	1:B:66:VAL:HG21	1.94	0.48
1:C:94:MET:CE	1:D:66:VAL:HG22	2.43	0.48
1:C:177:ALA:C	1:C:179:PRO:HD3	2.38	0.48
1:A:51:LEU:HB3	1:A:66:VAL:HG21	1.94	0.48
1:B:171:ILE:N	1:B:172:PRO:HD3	2.26	0.48
1:D:129:ILE:O	1:D:129:ILE:HG22	2.09	0.48
1:G:177:ALA:C	1:G:179:PRO:HD3	2.38	0.48
1:G:51:LEU:HB3	1:G:66:VAL:HG21	1.94	0.48
1:H:177:ALA:C	1:H:179:PRO:HD3	2.38	0.48
1:E:191:ILE:O	1:E:195:LYS:N	2.29	0.48
1:H:191:ILE:O	1:H:195:LYS:N	2.29	0.48
1:E:66:VAL:O	1:E:67:GLN:HB2	2.14	0.48
1:H:171:ILE:N	1:H:172:PRO:HD3	2.26	0.48
1:A:113:LYS:HA	1:A:114:PRO:HD3	1.50	0.47
1:E:129:ILE:O	1:E:129:ILE:HG22	2.09	0.47
1:B:66:VAL:O	1:B:67:GLN:HB2	2.14	0.47
1:E:94:MET:HE3	1:F:66:VAL:O	2.14	0.47
1:F:171:ILE:N	1:F:172:PRO:HD3	2.26	0.47
1:G:113:LYS:HA	1:G:114:PRO:HD3	1.50	0.47
1:A:191:ILE:O	1:A:195:LYS:N	2.29	0.47
1:F:214:ARG:HD2	1:F:214:ARG:HA	1.64	0.47
1:A:66:VAL:O	1:A:67:GLN:HB2	2.14	0.47
1:D:66:VAL:O	1:D:67:GLN:HB2	2.14	0.47
1:D:133:PHE:N	1:D:134:PRO:CD	2.78	0.47
1:B:133:PHE:N	1:B:134:PRO:CD	2.78	0.47
1:D:178:PHE:HA	1:D:179:PRO:HD2	1.66	0.47
1:G:94:MET:HE1	1:H:65:LEU:HA	1.97	0.47
1:H:66:VAL:O	1:H:67:GLN:HB2	2.14	0.47
1:A:170:LYS:C	1:A:172:PRO:HD3	2.40	0.47
1:E:66:VAL:N	1:F:94:MET:HE3	2.18	0.47
1:D:214:ARG:HD2	1:D:214:ARG:HA	1.65	0.46
1:G:66:VAL:CG2	1:H:94:MET:HE2	2.44	0.46
1:G:66:VAL:O	1:G:67:GLN:HB2	2.14	0.46
1:G:133:PHE:N	1:G:134:PRO:CD	2.78	0.46
1:B:170:LYS:C	1:B:172:PRO:HD3	2.40	0.46
1:A:120:GLU:O	1:A:124:MET:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:O	1:C:67:GLN:HB2	2.14	0.46
1:C:78:LYS:HD2	1:C:78:LYS:HA	1.73	0.46
1:C:170:LYS:C	1:C:172:PRO:HD3	2.40	0.46
1:D:170:LYS:C	1:D:172:PRO:HD3	2.41	0.46
1:F:66:VAL:O	1:F:67:GLN:HB2	2.14	0.46
1:G:94:MET:CE	1:H:66:VAL:HG22	2.46	0.46
1:G:120:GLU:O	1:G:124:MET:HG3	2.16	0.46
1:H:60:ILE:HG23	1:H:60:ILE:O	2.16	0.46
1:B:120:GLU:O	1:B:124:MET:HG3	2.16	0.46
1:C:120:GLU:O	1:C:124:MET:HG3	2.16	0.46
1:E:60:ILE:O	1:E:60:ILE:HG23	2.15	0.46
1:E:94:MET:HE3	1:F:66:VAL:N	2.25	0.46
1:A:214:ARG:CG	1:A:214:ARG:NH1	2.79	0.46
1:C:94:MET:HE3	1:D:66:VAL:N	2.21	0.46
1:C:113:LYS:HA	1:C:114:PRO:HD3	1.50	0.46
1:D:113:LYS:HA	1:D:114:PRO:HD3	1.50	0.46
1:E:120:GLU:O	1:E:124:MET:HG3	2.16	0.46
1:A:60:ILE:HG23	1:A:60:ILE:O	2.15	0.46
1:C:133:PHE:N	1:C:134:PRO:CD	2.78	0.46
1:D:191:ILE:HA	1:D:192:PRO:HD3	1.68	0.46
1:E:211:ILE:HD12	1:E:211:ILE:N	2.31	0.46
1:F:120:GLU:O	1:F:124:MET:HG3	2.16	0.46
1:H:170:LYS:C	1:H:172:PRO:HD3	2.41	0.46
1:H:211:ILE:HD12	1:H:211:ILE:N	2.31	0.46
1:A:133:PHE:N	1:A:134:PRO:CD	2.78	0.46
1:D:113:LYS:N	1:D:113:LYS:CD	2.79	0.46
1:G:65:LEU:HA	1:H:94:MET:HE1	1.97	0.46
1:G:211:ILE:N	1:G:211:ILE:HD12	2.31	0.46
1:H:120:GLU:O	1:H:124:MET:HG3	2.16	0.46
1:H:133:PHE:N	1:H:134:PRO:CD	2.78	0.46
1:B:211:ILE:N	1:B:211:ILE:HD12	2.31	0.46
1:C:178:PHE:HA	1:C:179:PRO:HD2	1.66	0.46
1:E:214:ARG:CG	1:E:214:ARG:NH1	2.79	0.46
1:F:133:PHE:N	1:F:134:PRO:CD	2.78	0.46
1:F:170:LYS:C	1:F:172:PRO:HD3	2.40	0.46
1:F:211:ILE:HD12	1:F:211:ILE:N	2.31	0.46
1:H:131:ARG:HE	1:H:131:ARG:HB2	1.54	0.46
1:D:60:ILE:O	1:D:60:ILE:HG23	2.15	0.46
1:D:120:GLU:O	1:D:124:MET:HG3	2.16	0.46
1:E:113:LYS:HA	1:E:114:PRO:HD3	1.50	0.46
1:F:55:VAL:HA	1:F:56:PRO:C	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:LYS:CD	1:F:113:LYS:N	2.79	0.46
1:G:55:VAL:HA	1:G:56:PRO:C	2.41	0.46
1:G:170:LYS:C	1:G:172:PRO:HD3	2.40	0.46
1:E:113:LYS:N	1:E:113:LYS:CD	2.79	0.45
1:E:133:PHE:N	1:E:134:PRO:CD	2.78	0.45
1:G:113:LYS:N	1:G:113:LYS:CD	2.79	0.45
1:C:55:VAL:HA	1:C:56:PRO:C	2.41	0.45
1:E:170:LYS:C	1:E:172:PRO:HD3	2.40	0.45
1:C:214:ARG:CG	1:C:214:ARG:NH1	2.79	0.45
1:D:30:PHE:O	1:D:203:LYS:HE2	2.17	0.45
1:D:211:ILE:N	1:D:211:ILE:HD12	2.31	0.45
1:F:60:ILE:HG23	1:F:60:ILE:O	2.15	0.45
1:F:112:LEU:HD23	1:F:112:LEU:HA	1.61	0.45
1:G:214:ARG:CG	1:G:214:ARG:NH1	2.79	0.45
1:C:59:GLU:CD	1:G:211:ILE:HD11	2.41	0.45
1:F:118:GLN:CD	1:G:118:GLN:CG	2.89	0.45
1:G:60:ILE:HG23	1:G:60:ILE:O	2.15	0.45
1:A:66:VAL:HG22	1:B:94:MET:HE2	1.98	0.45
1:B:113:LYS:N	1:B:113:LYS:CD	2.79	0.45
1:C:30:PHE:O	1:C:203:LYS:HE2	2.16	0.45
1:C:113:LYS:CD	1:C:113:LYS:N	2.79	0.45
1:F:30:PHE:O	1:F:203:LYS:HE2	2.16	0.45
1:H:178:PHE:N	1:H:179:PRO:CD	2.79	0.45
1:E:30:PHE:O	1:E:203:LYS:HE2	2.17	0.45
1:G:30:PHE:O	1:G:203:LYS:HE2	2.16	0.45
1:A:55:VAL:HA	1:A:56:PRO:C	2.41	0.45
1:A:211:ILE:HD12	1:A:211:ILE:N	2.31	0.45
1:B:55:VAL:HA	1:B:56:PRO:C	2.41	0.45
1:B:214:ARG:CG	1:B:214:ARG:NH1	2.79	0.45
1:D:55:VAL:HA	1:D:56:PRO:C	2.41	0.45
1:H:30:PHE:O	1:H:203:LYS:HE2	2.16	0.45
1:H:113:LYS:CD	1:H:113:LYS:N	2.79	0.45
1:A:113:LYS:CD	1:A:113:LYS:N	2.79	0.45
1:C:211:ILE:HD12	1:C:211:ILE:N	2.31	0.45
1:B:60:ILE:HG23	1:B:60:ILE:O	2.15	0.45
1:G:48:ASN:HA	3:G:406:HOH:O	2.17	0.45
1:C:60:ILE:HG23	1:C:60:ILE:O	2.15	0.44
1:D:48:ASN:HA	3:D:406:HOH:O	2.17	0.44
1:E:197:PHE:CZ	1:E:204:LYS:HB2	2.53	0.44
1:H:55:VAL:HA	1:H:56:PRO:C	2.41	0.44
1:H:178:PHE:HA	1:H:179:PRO:HD2	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:ASN:HA	3:F:406:HOH:O	2.17	0.44
1:F:197:PHE:CZ	1:F:204:LYS:HB2	2.53	0.44
1:H:48:ASN:HA	3:H:406:HOH:O	2.17	0.44
1:H:214:ARG:HD2	1:H:214:ARG:HA	1.65	0.44
1:B:30:PHE:O	1:B:203:LYS:HE2	2.17	0.44
1:B:113:LYS:HA	1:B:114:PRO:HD3	1.50	0.44
1:E:48:ASN:HA	3:E:406:HOH:O	2.17	0.44
1:A:30:PHE:O	1:A:203:LYS:HE2	2.16	0.44
1:B:178:PHE:HA	1:B:179:PRO:HD2	1.66	0.44
1:C:48:ASN:HA	3:C:406:HOH:O	2.17	0.44
1:E:78:LYS:HA	1:E:78:LYS:HD2	1.73	0.44
1:G:191:ILE:O	1:G:195:LYS:N	2.29	0.44
1:B:145:GLN:HB3	1:B:151:ASN:OD1	2.18	0.44
1:E:55:VAL:HA	1:E:56:PRO:C	2.41	0.44
1:G:178:PHE:N	1:G:179:PRO:CD	2.79	0.44
1:A:48:ASN:HA	3:A:406:HOH:O	2.17	0.44
1:A:197:PHE:CZ	1:A:204:LYS:HB2	2.52	0.44
1:B:78:LYS:HA	1:B:78:LYS:HD2	1.73	0.44
1:B:178:PHE:N	1:B:179:PRO:CD	2.79	0.44
1:C:197:PHE:CZ	1:C:204:LYS:HB2	2.52	0.44
1:G:197:PHE:CZ	1:G:204:LYS:HB2	2.53	0.44
1:B:197:PHE:CZ	1:B:204:LYS:HB2	2.52	0.44
1:D:145:GLN:HB3	1:D:151:ASN:OD1	2.18	0.44
1:D:171:ILE:HA	1:D:172:PRO:HD2	1.82	0.44
1:H:205:LYS:HA	1:H:206:PRO:HD3	1.79	0.44
1:D:197:PHE:CZ	1:D:204:LYS:HB2	2.52	0.43
1:E:205:LYS:HA	1:E:206:PRO:HD3	1.79	0.43
1:H:145:GLN:HB3	1:H:151:ASN:OD1	2.18	0.43
1:H:207:PRO:HA	1:H:208:PRO:HD3	1.81	0.43
1:D:78:LYS:HD2	1:D:78:LYS:HA	1.73	0.43
1:B:48:ASN:HA	3:B:406:HOH:O	2.17	0.43
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.61	0.43
1:H:113:LYS:HB3	1:H:114:PRO:HD2	2.01	0.43
1:H:197:PHE:CZ	1:H:204:LYS:HB2	2.52	0.43
1:F:78:LYS:HD2	1:F:78:LYS:HA	1.73	0.43
1:F:145:GLN:HB3	1:F:151:ASN:OD1	2.18	0.43
1:G:131:ARG:HE	1:G:131:ARG:HB2	1.54	0.43
1:B:111:PHE:CZ	1:B:216:VAL:HG21	2.54	0.43
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.61	0.43
1:C:214:ARG:HA	1:C:214:ARG:HD2	1.65	0.43
1:E:111:PHE:CZ	1:E:216:VAL:HG21	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ARG:HD2	1:E:214:ARG:HA	1.65	0.43
1:D:207:PRO:HA	1:D:208:PRO:HD3	1.81	0.43
1:F:113:LYS:HB3	1:F:114:PRO:HD2	2.01	0.43
1:G:55:VAL:HB	1:G:56:PRO:HA	2.01	0.43
1:G:107:ILE:HG22	2:G:301:IBG:H3S	2.01	0.43
1:H:107:ILE:HG22	2:H:301:IBG:H3S	2.01	0.43
1:H:112:LEU:HB2	1:H:117:GLN:CG	2.48	0.43
1:A:9:TYR:HE1	1:A:56:PRO:HD3	1.84	0.43
1:B:113:LYS:HB3	1:B:114:PRO:HD2	2.01	0.43
1:C:107:ILE:HG22	2:C:301:IBG:H3S	2.01	0.43
1:D:107:ILE:HG22	2:D:301:IBG:H3S	2.01	0.43
1:F:107:ILE:HG22	2:F:301:IBG:H3S	2.01	0.43
1:G:145:GLN:HB3	1:G:151:ASN:OD1	2.18	0.43
1:G:178:PHE:HA	1:G:179:PRO:HD2	1.67	0.43
1:A:145:GLN:HB3	1:A:151:ASN:OD1	2.18	0.43
1:F:205:LYS:HA	1:F:206:PRO:HD3	1.79	0.43
1:G:111:PHE:CZ	1:G:216:VAL:HG21	2.54	0.43
1:G:170:LYS:C	1:G:171:ILE:HG13	2.44	0.43
1:C:113:LYS:HB3	1:C:114:PRO:HD2	2.01	0.42
1:D:9:TYR:CD1	1:D:10:PRO:HD2	2.54	0.42
1:E:113:LYS:HB3	1:E:114:PRO:HD2	2.01	0.42
1:E:133:PHE:CB	1:E:134:PRO:HD3	2.49	0.42
1:F:9:TYR:HE1	1:F:56:PRO:HD3	1.84	0.42
1:F:42:TYR:HD1	1:F:42:TYR:HA	1.72	0.42
1:G:9:TYR:CD1	1:G:10:PRO:HD2	2.54	0.42
1:B:9:TYR:HE1	1:B:56:PRO:HD3	1.84	0.42
1:C:205:LYS:HA	1:C:206:PRO:HD3	1.79	0.42
1:E:145:GLN:HB3	1:E:151:ASN:OD1	2.18	0.42
1:E:181:LEU:HD23	1:E:181:LEU:HA	1.89	0.42
1:E:9:TYR:HE1	1:E:56:PRO:HD3	1.84	0.42
1:F:214:ARG:CG	1:F:214:ARG:NH1	2.79	0.42
1:A:112:LEU:HB2	1:A:117:GLN:CG	2.48	0.42
1:C:111:PHE:CZ	1:C:216:VAL:HG21	2.54	0.42
1:F:181:LEU:HD23	1:F:181:LEU:HA	1.89	0.42
1:G:185:THR:O	1:G:189:SER:OG	2.35	0.42
1:H:111:PHE:CZ	1:H:216:VAL:HG21	2.54	0.42
1:H:112:LEU:HD23	1:H:112:LEU:HA	1.61	0.42
1:A:38:LYS:O	1:A:41:LEU:HB3	2.19	0.42
1:C:145:GLN:HB3	1:C:151:ASN:OD1	2.18	0.42
1:G:9:TYR:HE1	1:G:56:PRO:HD3	1.84	0.42
1:G:38:LYS:O	1:G:41:LEU:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:PHE:CB	1:H:134:PRO:HD3	2.49	0.42
1:A:9:TYR:CD1	1:A:10:PRO:HD2	2.54	0.42
1:A:37:THR:HG1	1:A:40:GLN:HG3	1.82	0.42
1:A:107:ILE:HG22	2:A:301:IBG:H3S	2.01	0.42
1:A:111:PHE:CZ	1:A:216:VAL:HG21	2.54	0.42
1:B:178:PHE:N	1:B:179:PRO:HD3	2.35	0.42
1:C:38:LYS:O	1:C:41:LEU:HB3	2.19	0.42
1:C:66:VAL:HG22	1:D:94:MET:HE2	2.01	0.42
1:D:9:TYR:HE1	1:D:56:PRO:HD3	1.84	0.42
1:D:111:PHE:CZ	1:D:216:VAL:HG21	2.54	0.42
1:D:133:PHE:CB	1:D:134:PRO:HD3	2.49	0.42
1:A:113:LYS:HB3	1:A:114:PRO:HD2	2.01	0.42
1:D:170:LYS:C	1:D:171:ILE:HG13	2.44	0.42
1:E:38:LYS:O	1:E:41:LEU:HB3	2.19	0.42
1:F:9:TYR:CD1	1:F:10:PRO:HD2	2.54	0.42
1:F:38:LYS:O	1:F:41:LEU:HB3	2.19	0.42
1:F:170:LYS:C	1:F:171:ILE:HG13	2.44	0.42
1:G:113:LYS:HB3	1:G:114:PRO:HD2	2.01	0.42
1:G:178:PHE:N	1:G:179:PRO:HD3	2.35	0.42
1:C:9:TYR:CD1	1:C:10:PRO:HD2	2.54	0.42
1:D:38:LYS:O	1:D:41:LEU:HB3	2.19	0.42
1:H:9:TYR:HE1	1:H:56:PRO:HD3	1.84	0.42
1:H:170:LYS:C	1:H:171:ILE:HG13	2.44	0.42
1:A:178:PHE:N	1:A:179:PRO:HD3	2.35	0.42
1:B:55:VAL:HB	1:B:56:PRO:HA	2.01	0.42
1:B:191:ILE:HA	1:B:192:PRO:HD3	1.68	0.42
1:C:9:TYR:HE1	1:C:56:PRO:HD3	1.84	0.42
1:C:170:LYS:C	1:C:171:ILE:HG13	2.44	0.42
1:G:78:LYS:HD2	1:G:78:LYS:HA	1.73	0.42
1:G:112:LEU:HB2	1:G:117:GLN:CG	2.48	0.42
1:H:55:VAL:HB	1:H:56:PRO:HA	2.01	0.42
1:A:55:VAL:HB	1:A:56:PRO:HA	2.01	0.42
1:C:111:PHE:CE1	1:C:216:VAL:CG2	3.03	0.42
1:C:206:PRO:HA	1:C:207:PRO:HD3	1.88	0.42
1:D:205:LYS:HB3	1:D:206:PRO:CD	2.48	0.42
1:E:178:PHE:N	1:E:179:PRO:HD3	2.35	0.42
1:F:111:PHE:CZ	1:F:216:VAL:HG21	2.54	0.42
1:F:113:LYS:HA	1:F:114:PRO:HD3	1.50	0.42
1:F:178:PHE:N	1:F:179:PRO:HD3	2.35	0.42
1:G:133:PHE:CB	1:G:134:PRO:HD3	2.49	0.42
1:H:9:TYR:CD1	1:H:10:PRO:HD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:O	1:A:34:PHE:HA	2.20	0.41
1:B:9:TYR:CD1	1:B:10:PRO:HD2	2.54	0.41
1:B:36:GLU:N	1:B:40:GLN:OE1	2.49	0.41
1:D:205:LYS:HA	1:D:206:PRO:HD3	1.79	0.41
1:E:9:TYR:CD1	1:E:10:PRO:HD2	2.54	0.41
1:G:9:TYR:O	1:G:34:PHE:HA	2.20	0.41
1:H:214:ARG:CG	1:H:214:ARG:NH1	2.79	0.41
1:A:209:ASP:OD1	1:A:211:ILE:HB	2.21	0.41
1:B:38:LYS:O	1:B:41:LEU:HB3	2.19	0.41
1:B:107:ILE:HG22	2:B:301:IBG:H3S	2.01	0.41
1:C:55:VAL:HB	1:C:56:PRO:HA	2.01	0.41
1:C:112:LEU:HB2	1:C:117:GLN:CG	2.48	0.41
1:C:185:THR:O	1:C:189:SER:OG	2.35	0.41
1:D:119:LYS:HZ2	1:D:123:ASN:HB2	1.79	0.41
1:E:55:VAL:HB	1:E:56:PRO:HA	2.01	0.41
1:E:66:VAL:O	1:F:94:MET:CE	2.68	0.41
1:F:9:TYR:O	1:F:34:PHE:HA	2.20	0.41
1:H:38:LYS:O	1:H:41:LEU:HB3	2.19	0.41
1:B:133:PHE:CB	1:B:134:PRO:HD3	2.49	0.41
1:C:42:TYR:HD1	1:C:42:TYR:HA	1.72	0.41
1:C:57:MET:HG2	1:C:65:LEU:O	2.21	0.41
1:D:214:ARG:CG	1:D:214:ARG:NH1	2.79	0.41
1:E:107:ILE:HG22	2:E:301:IBG:H3S	2.01	0.41
1:E:111:PHE:CE1	1:E:216:VAL:CG2	3.03	0.41
1:F:133:PHE:CB	1:F:134:PRO:HD3	2.49	0.41
1:F:178:PHE:N	1:F:179:PRO:CD	2.79	0.41
1:F:179:PRO:HB3	1:H:42:TYR:CE2	2.55	0.41
1:F:209:ASP:OD1	1:F:211:ILE:HB	2.21	0.41
1:H:7:LEU:HD12	1:H:7:LEU:N	2.36	0.41
1:H:80:ASN:HD21	1:H:84:LYS:HE3	1.85	0.41
1:A:7:LEU:HD12	1:A:7:LEU:N	2.36	0.41
1:B:9:TYR:O	1:B:34:PHE:HA	2.20	0.41
1:C:178:PHE:N	1:C:179:PRO:CD	2.79	0.41
1:D:7:LEU:HD12	1:D:7:LEU:N	2.36	0.41
1:D:113:LYS:HB3	1:D:114:PRO:HD2	2.01	0.41
1:F:80:ASN:HD21	1:F:84:LYS:HE3	1.85	0.41
1:F:111:PHE:CE1	1:F:216:VAL:CG2	3.03	0.41
1:G:80:ASN:HD21	1:G:84:LYS:HE3	1.86	0.41
1:B:7:LEU:N	1:B:7:LEU:HD12	2.36	0.41
1:B:209:ASP:OD1	1:B:211:ILE:HB	2.21	0.41
1:C:9:TYR:O	1:C:34:PHE:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:MET:HG2	1:D:65:LEU:O	2.21	0.41
1:D:80:ASN:HD21	1:D:84:LYS:HE3	1.85	0.41
1:F:55:VAL:HB	1:F:56:PRO:HA	2.01	0.41
1:G:171:ILE:HA	1:G:172:PRO:HD2	1.82	0.41
1:H:111:PHE:CE1	1:H:216:VAL:CG2	3.03	0.41
1:A:111:PHE:CE1	1:A:216:VAL:CG2	3.03	0.41
1:B:112:LEU:HB2	1:B:117:GLN:CG	2.48	0.41
1:C:7:LEU:N	1:C:7:LEU:HD12	2.36	0.41
1:C:80:ASN:HD21	1:C:84:LYS:HE3	1.86	0.41
1:C:191:ILE:HA	1:C:192:PRO:HD3	1.68	0.41
1:D:178:PHE:N	1:D:179:PRO:HD3	2.35	0.41
1:E:57:MET:HG2	1:E:65:LEU:O	2.20	0.41
1:E:178:PHE:HA	1:E:179:PRO:HD2	1.66	0.41
1:F:7:LEU:HD12	1:F:7:LEU:N	2.36	0.41
1:G:111:PHE:CE1	1:G:216:VAL:CG2	3.03	0.41
1:H:57:MET:HG2	1:H:65:LEU:O	2.21	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.61	0.41
1:D:209:ASP:OD1	1:D:211:ILE:HB	2.21	0.41
1:H:209:ASP:OD1	1:H:211:ILE:HB	2.21	0.41
1:A:80:ASN:HD21	1:A:84:LYS:HE3	1.85	0.41
1:B:111:PHE:CE1	1:B:216:VAL:CG2	3.03	0.41
1:C:209:ASP:OD1	1:C:211:ILE:HB	2.21	0.41
1:F:43:LYS:HG3	1:F:43:LYS:H	1.75	0.41
1:G:17:GLU:OE1	1:G:20:ARG:NH1	2.52	0.41
1:B:112:LEU:CD1	1:B:120:GLU:HG3	2.51	0.41
1:C:178:PHE:N	1:C:179:PRO:HD3	2.35	0.41
1:D:9:TYR:O	1:D:34:PHE:HA	2.20	0.41
1:D:55:VAL:HB	1:D:56:PRO:HA	2.01	0.41
1:D:111:PHE:CE1	1:D:216:VAL:CG2	3.03	0.41
1:E:170:LYS:C	1:E:171:ILE:HG13	2.44	0.41
1:F:57:MET:HG2	1:F:65:LEU:O	2.21	0.41
1:G:66:VAL:O	1:H:94:MET:HE3	2.20	0.41
1:G:181:LEU:HD23	1:G:181:LEU:HA	1.89	0.41
1:H:181:LEU:HA	1:H:181:LEU:HD23	1.89	0.41
1:A:178:PHE:N	1:A:179:PRO:CD	2.79	0.41
1:B:205:LYS:HB3	1:B:206:PRO:CD	2.48	0.41
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.87	0.40
1:A:170:LYS:C	1:A:171:ILE:HG13	2.44	0.40
1:E:9:TYR:O	1:E:34:PHE:HA	2.20	0.40
1:E:17:GLU:OE1	1:E:20:ARG:NH1	2.52	0.40
1:E:209:ASP:OD1	1:E:211:ILE:HB	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:ASP:OD1	1:G:211:ILE:HB	2.21	0.40
1:H:130:ILE:HG21	1:H:130:ILE:HD13	1.87	0.40
1:B:170:LYS:C	1:B:171:ILE:HG13	2.44	0.40
1:C:207:PRO:HA	1:C:208:PRO:HD3	1.82	0.40
1:D:178:PHE:N	1:D:179:PRO:CD	2.79	0.40
1:G:205:LYS:HB3	1:G:206:PRO:CD	2.49	0.40
1:A:78:LYS:HA	1:A:78:LYS:HD2	1.73	0.40
1:F:112:LEU:HB2	1:F:117:GLN:CG	2.48	0.40
1:F:118:GLN:HG3	1:G:118:GLN:HE21	1.85	0.40
1:G:57:MET:HG2	1:G:65:LEU:O	2.20	0.40
1:G:112:LEU:CD1	1:G:120:GLU:HG3	2.51	0.40
1:H:17:GLU:OE1	1:H:20:ARG:NH1	2.52	0.40
1:G:7:LEU:N	1:G:7:LEU:HD12	2.36	0.40
1:H:9:TYR:O	1:H:34:PHE:HA	2.20	0.40
1:H:178:PHE:N	1:H:179:PRO:HD3	2.35	0.40
1:A:57:MET:HG2	1:A:65:LEU:O	2.20	0.40
1:D:112:LEU:CD1	1:D:120:GLU:HG3	2.51	0.40
1:E:112:LEU:HB2	1:E:117:GLN:CG	2.48	0.40

All (7) 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:D:196:ARG:NH2	1:H:200:PRO:CG[4_455]	0.52	1.68
1:D:196:ARG:NH2	1:H:200:PRO:CB[4_455]	1.33	0.87
1:D:196:ARG:CZ	1:H:200:PRO:CB[4_455]	1.66	0.54
1:D:196:ARG:NH2	1:H:200:PRO:CD[4_455]	1.79	0.41
1:D:196:ARG:CZ	1:H:200:PRO:CG[4_455]	1.85	0.35
1:B:118:GLN:CG	1:C:118:GLN:CG[1_554]	2.00	0.20
1:D:196:ARG:NH1	1:H:200:PRO:CB[4_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
1	B	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
1	C	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
1	D	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
1	E	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
1	F	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
1	G	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
1	H	215/222 (97%)	208 (97%)	6 (3%)	1 (0%)	24	48
All	All	1720/1776 (97%)	1664 (97%)	48 (3%)	8 (0%)	24	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	B	114	PRO
1	C	114	PRO
1	D	114	PRO
1	E	114	PRO
1	F	114	PRO
1	G	114	PRO
1	H	114	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/200 (98%)	185 (94%)	12 (6%)	17	40
1	B	197/200 (98%)	185 (94%)	12 (6%)	17	40
1	C	197/200 (98%)	185 (94%)	12 (6%)	17	40
1	D	197/200 (98%)	185 (94%)	12 (6%)	17	40
1	E	197/200 (98%)	185 (94%)	12 (6%)	17	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	197/200 (98%)	185 (94%)	12 (6%)	17	40
1	G	197/200 (98%)	185 (94%)	12 (6%)	17	40
1	H	197/200 (98%)	185 (94%)	12 (6%)	17	40
All	All	1576/1600 (98%)	1480 (94%)	96 (6%)	17	40

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	PHE
1	A	106	LEU
1	A	113	LYS
1	A	115	ASP
1	A	119	LYS
1	A	129	ILE
1	A	141	ARG
1	A	143	HIS
1	A	146	SER
1	A	189	SER
1	A	214	ARG
1	A	216	VAL
1	B	82	PHE
1	B	106	LEU
1	B	113	LYS
1	B	115	ASP
1	B	119	LYS
1	B	129	ILE
1	B	141	ARG
1	B	143	HIS
1	B	146	SER
1	B	189	SER
1	B	214	ARG
1	B	216	VAL
1	C	82	PHE
1	C	106	LEU
1	C	113	LYS
1	C	115	ASP
1	C	119	LYS
1	C	129	ILE
1	C	141	ARG
1	C	143	HIS
1	C	146	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	189	SER
1	C	214	ARG
1	C	216	VAL
1	D	82	PHE
1	D	106	LEU
1	D	113	LYS
1	D	115	ASP
1	D	119	LYS
1	D	129	ILE
1	D	141	ARG
1	D	143	HIS
1	D	146	SER
1	D	189	SER
1	D	214	ARG
1	D	216	VAL
1	E	82	PHE
1	E	106	LEU
1	E	113	LYS
1	E	115	ASP
1	E	119	LYS
1	E	129	ILE
1	E	141	ARG
1	E	143	HIS
1	E	146	SER
1	E	189	SER
1	E	214	ARG
1	E	216	VAL
1	F	82	PHE
1	F	106	LEU
1	F	113	LYS
1	F	115	ASP
1	F	119	LYS
1	F	129	ILE
1	F	141	ARG
1	F	143	HIS
1	F	146	SER
1	F	189	SER
1	F	214	ARG
1	F	216	VAL
1	G	82	PHE
1	G	106	LEU
1	G	113	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	115	ASP
1	G	119	LYS
1	G	129	ILE
1	G	141	ARG
1	G	143	HIS
1	G	146	SER
1	G	189	SER
1	G	214	ARG
1	G	216	VAL
1	H	82	PHE
1	H	106	LEU
1	H	113	LYS
1	H	115	ASP
1	H	119	LYS
1	H	129	ILE
1	H	141	ARG
1	H	143	HIS
1	H	146	SER
1	H	189	SER
1	H	214	ARG
1	H	216	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	79	HIS
1	A	80	ASN
1	A	162	GLN
1	A	218	ASN
1	B	79	HIS
1	B	80	ASN
1	B	162	GLN
1	B	218	ASN
1	C	67	GLN
1	C	79	HIS
1	C	80	ASN
1	C	218	ASN
1	D	67	GLN
1	D	79	HIS
1	D	80	ASN
1	D	162	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	218	ASN
1	E	53	GLN
1	E	67	GLN
1	E	79	HIS
1	E	80	ASN
1	E	162	GLN
1	E	218	ASN
1	F	67	GLN
1	F	79	HIS
1	F	80	ASN
1	F	118	GLN
1	F	162	GLN
1	F	218	ASN
1	G	67	GLN
1	G	79	HIS
1	G	80	ASN
1	G	118	GLN
1	G	162	GLN
1	G	218	ASN
1	H	80	ASN
1	H	162	GLN
1	H	218	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	IBG	B	301	-	27,28,28	0.82	0	33,36,36	1.85	9 (27%)
2	IBG	F	301	-	27,28,28	0.82	0	33,36,36	1.85	9 (27%)
2	IBG	G	301	-	27,28,28	0.81	0	33,36,36	1.85	9 (27%)
2	IBG	A	301	-	27,28,28	0.82	0	33,36,36	1.85	9 (27%)
2	IBG	D	301	-	27,28,28	0.82	0	33,36,36	1.85	9 (27%)
2	IBG	C	301	-	27,28,28	0.81	0	33,36,36	1.85	9 (27%)
2	IBG	H	301	-	27,28,28	0.82	0	33,36,36	1.85	9 (27%)
2	IBG	E	301	-	27,28,28	0.82	0	33,36,36	1.85	9 (27%)

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	IBG	B	301	-	-	3/28/28/28	0/1/1/1
2	IBG	F	301	-	-	3/28/28/28	0/1/1/1
2	IBG	G	301	-	-	3/28/28/28	0/1/1/1
2	IBG	A	301	-	-	3/28/28/28	0/1/1/1
2	IBG	D	301	-	-	3/28/28/28	0/1/1/1
2	IBG	C	301	-	-	3/28/28/28	0/1/1/1
2	IBG	H	301	-	-	3/28/28/28	0/1/1/1
2	IBG	E	301	-	-	3/28/28/28	0/1/1/1

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	IBG	C3S-C2S-C1S	-4.63	116.54	121.66
2	B	301	IBG	C3S-C2S-C1S	-4.61	116.56	121.66
2	H	301	IBG	C3S-C2S-C1S	-4.61	116.57	121.66
2	A	301	IBG	C3S-C2S-C1S	-4.60	116.57	121.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	IBG	C3S-C2S-C1S	-4.60	116.58	121.66
2	C	301	IBG	C3S-C2S-C1S	-4.60	116.58	121.66
2	D	301	IBG	C3S-C2S-C1S	-4.59	116.58	121.66
2	G	301	IBG	C3S-C2S-C1S	-4.58	116.59	121.66
2	E	301	IBG	C6S-C1S-C2S	4.36	122.25	117.04
2	F	301	IBG	C6S-C1S-C2S	4.36	122.25	117.04
2	C	301	IBG	C6S-C1S-C2S	4.36	122.25	117.04
2	B	301	IBG	C6S-C1S-C2S	4.35	122.25	117.04
2	H	301	IBG	C6S-C1S-C2S	4.35	122.24	117.04
2	A	301	IBG	C6S-C1S-C2S	4.34	122.24	117.04
2	G	301	IBG	C6S-C1S-C2S	4.33	122.22	117.04
2	D	301	IBG	C6S-C1S-C2S	4.33	122.22	117.04
2	D	301	IBG	C1S-CS-SG2	-3.40	105.39	114.23
2	C	301	IBG	C1S-CS-SG2	-3.40	105.41	114.23
2	G	301	IBG	C1S-CS-SG2	-3.39	105.42	114.23
2	B	301	IBG	C1S-CS-SG2	-3.39	105.42	114.23
2	F	301	IBG	C1S-CS-SG2	-3.39	105.43	114.23
2	A	301	IBG	C1S-CS-SG2	-3.39	105.43	114.23
2	H	301	IBG	C1S-CS-SG2	-3.39	105.44	114.23
2	E	301	IBG	C1S-CS-SG2	-3.38	105.46	114.23
2	H	301	IBG	CS-C1S-C2S	-3.04	119.98	123.13
2	F	301	IBG	CS-C1S-C2S	-3.04	119.98	123.13
2	B	301	IBG	CS-C1S-C2S	-3.02	120.01	123.13
2	D	301	IBG	CS-C1S-C2S	-3.02	120.01	123.13
2	A	301	IBG	CS-C1S-C2S	-3.01	120.01	123.13
2	C	301	IBG	CS-C1S-C2S	-3.01	120.02	123.13
2	G	301	IBG	CS-C1S-C2S	-3.00	120.02	123.13
2	E	301	IBG	CS-C1S-C2S	-3.00	120.03	123.13
2	F	301	IBG	C3S-C2S-I2S	2.93	124.55	117.63
2	B	301	IBG	C3S-C2S-I2S	2.92	124.54	117.63
2	E	301	IBG	C3S-C2S-I2S	2.92	124.54	117.63
2	G	301	IBG	C3S-C2S-I2S	2.92	124.53	117.63
2	A	301	IBG	C3S-C2S-I2S	2.92	124.53	117.63
2	C	301	IBG	C3S-C2S-I2S	2.92	124.52	117.63
2	D	301	IBG	C3S-C2S-I2S	2.92	124.52	117.63
2	H	301	IBG	C3S-C2S-I2S	2.91	124.51	117.63
2	C	301	IBG	O31-C3-O32	2.74	130.37	123.33
2	F	301	IBG	O31-C3-O32	2.73	130.37	123.33
2	G	301	IBG	O31-C3-O32	2.73	130.36	123.33
2	H	301	IBG	O31-C3-O32	2.73	130.35	123.33
2	D	301	IBG	O31-C3-O32	2.73	130.35	123.33
2	B	301	IBG	O31-C3-O32	2.73	130.35	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	IBG	O31-C3-O32	2.73	130.35	123.33
2	A	301	IBG	O31-C3-O32	2.73	130.34	123.33
2	B	301	IBG	CB1-CG1-CD1	-2.39	107.73	113.06
2	C	301	IBG	CB1-CG1-CD1	-2.38	107.76	113.06
2	F	301	IBG	CB1-CG1-CD1	-2.38	107.76	113.06
2	G	301	IBG	CB1-CG1-CD1	-2.37	107.79	113.06
2	A	301	IBG	CB1-CG1-CD1	-2.36	107.79	113.06
2	D	301	IBG	CB1-CG1-CD1	-2.36	107.80	113.06
2	H	301	IBG	CB1-CG1-CD1	-2.36	107.80	113.06
2	E	301	IBG	CB1-CG1-CD1	-2.36	107.81	113.06
2	G	301	IBG	CB2-CA2-C2	2.08	114.14	109.46
2	D	301	IBG	CB2-CA2-C2	2.06	114.10	109.46
2	C	301	IBG	CB2-CA2-C2	2.06	114.10	109.46
2	A	301	IBG	CB2-CA2-C2	2.05	114.09	109.46
2	H	301	IBG	CB2-CA2-C2	2.04	114.07	109.46
2	E	301	IBG	CB2-CA2-C2	2.04	114.06	109.46
2	B	301	IBG	CB2-CA2-C2	2.04	114.06	109.46
2	F	301	IBG	CB2-CA2-C2	2.03	114.04	109.46
2	E	301	IBG	O32-C3-CA3	-2.01	114.31	122.66
2	F	301	IBG	O32-C3-CA3	-2.01	114.31	122.66
2	C	301	IBG	O32-C3-CA3	-2.01	114.32	122.66
2	B	301	IBG	O32-C3-CA3	-2.01	114.32	122.66
2	H	301	IBG	O32-C3-CA3	-2.01	114.32	122.66
2	G	301	IBG	O32-C3-CA3	-2.01	114.32	122.66
2	D	301	IBG	O32-C3-CA3	-2.01	114.33	122.66
2	A	301	IBG	O32-C3-CA3	-2.01	114.33	122.66

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	IBG	C1-CA1-CB1-CG1
2	B	301	IBG	C1-CA1-CB1-CG1
2	C	301	IBG	C1-CA1-CB1-CG1
2	D	301	IBG	C1-CA1-CB1-CG1
2	E	301	IBG	C1-CA1-CB1-CG1
2	F	301	IBG	C1-CA1-CB1-CG1
2	G	301	IBG	C1-CA1-CB1-CG1
2	H	301	IBG	C1-CA1-CB1-CG1
2	A	301	IBG	CA2-CB2-SG2-CS
2	B	301	IBG	CA2-CB2-SG2-CS
2	C	301	IBG	CA2-CB2-SG2-CS

Continued on next page...

Continued from previous page...

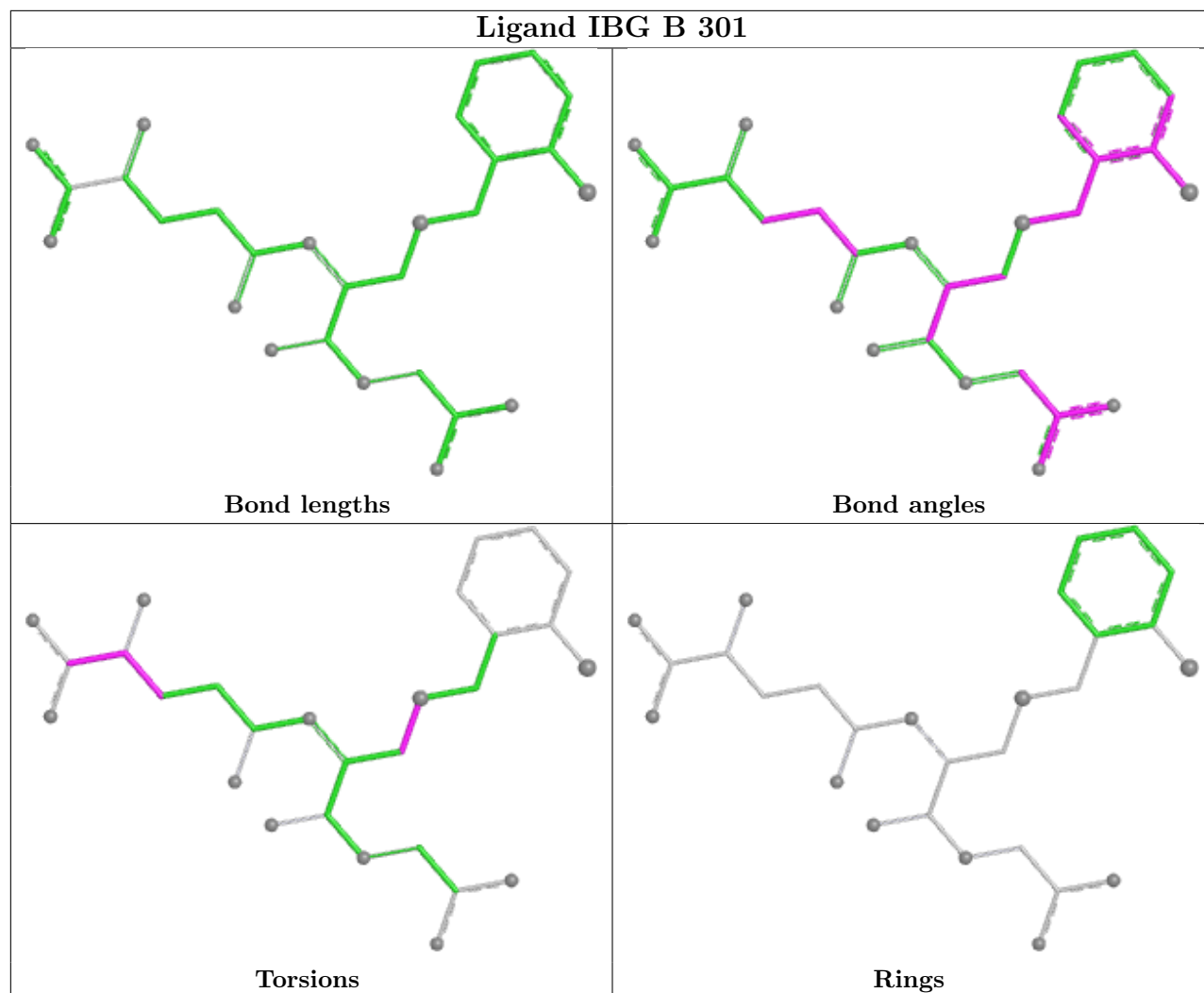
Mol	Chain	Res	Type	Atoms
2	D	301	IBG	CA2-CB2-SG2-CS
2	E	301	IBG	CA2-CB2-SG2-CS
2	F	301	IBG	CA2-CB2-SG2-CS
2	G	301	IBG	CA2-CB2-SG2-CS
2	H	301	IBG	CA2-CB2-SG2-CS
2	A	301	IBG	O12-C1-CA1-N1
2	B	301	IBG	O12-C1-CA1-N1
2	C	301	IBG	O12-C1-CA1-N1
2	D	301	IBG	O12-C1-CA1-N1
2	E	301	IBG	O12-C1-CA1-N1
2	F	301	IBG	O12-C1-CA1-N1
2	G	301	IBG	O12-C1-CA1-N1
2	H	301	IBG	O12-C1-CA1-N1

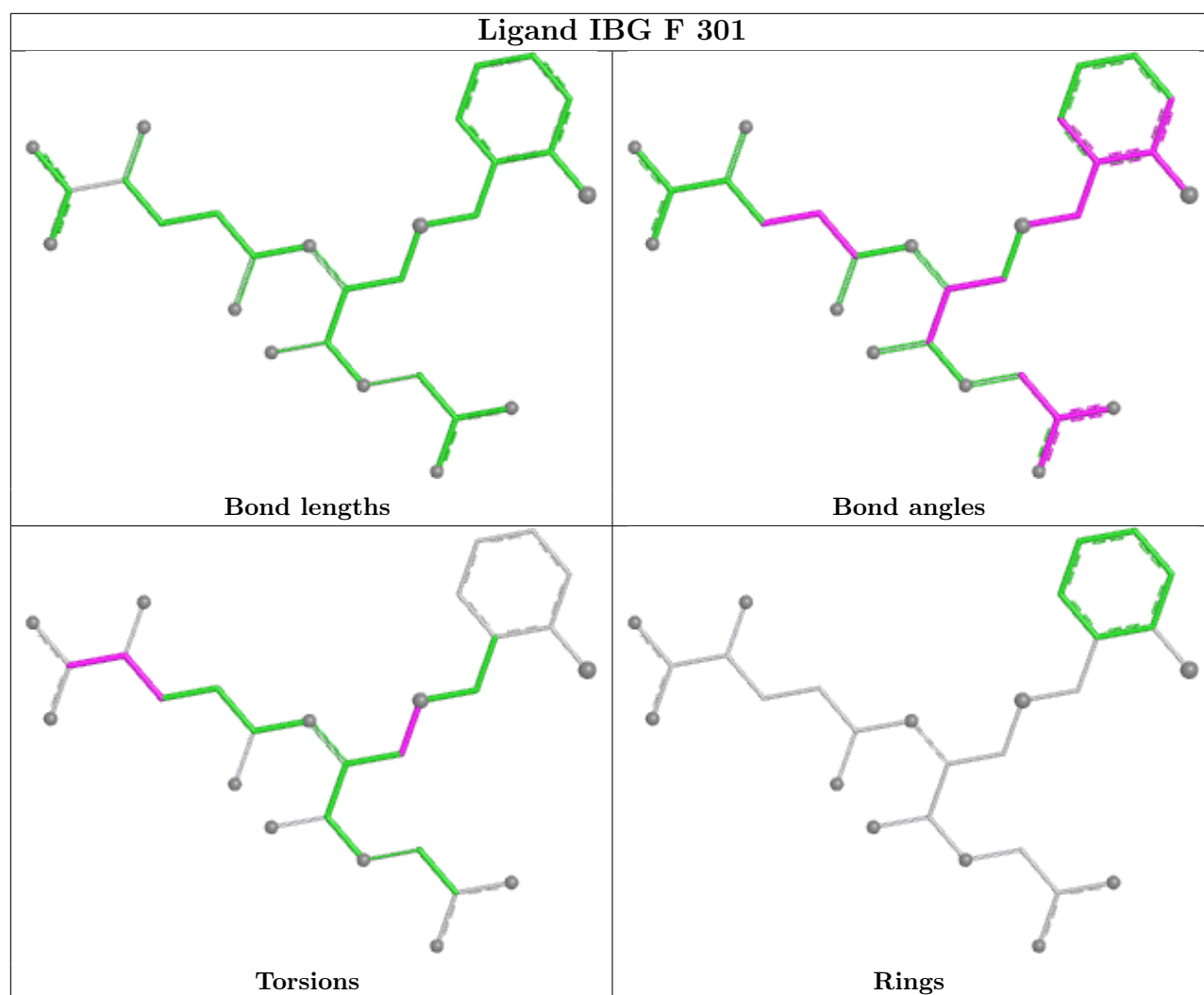
There are no ring outliers.

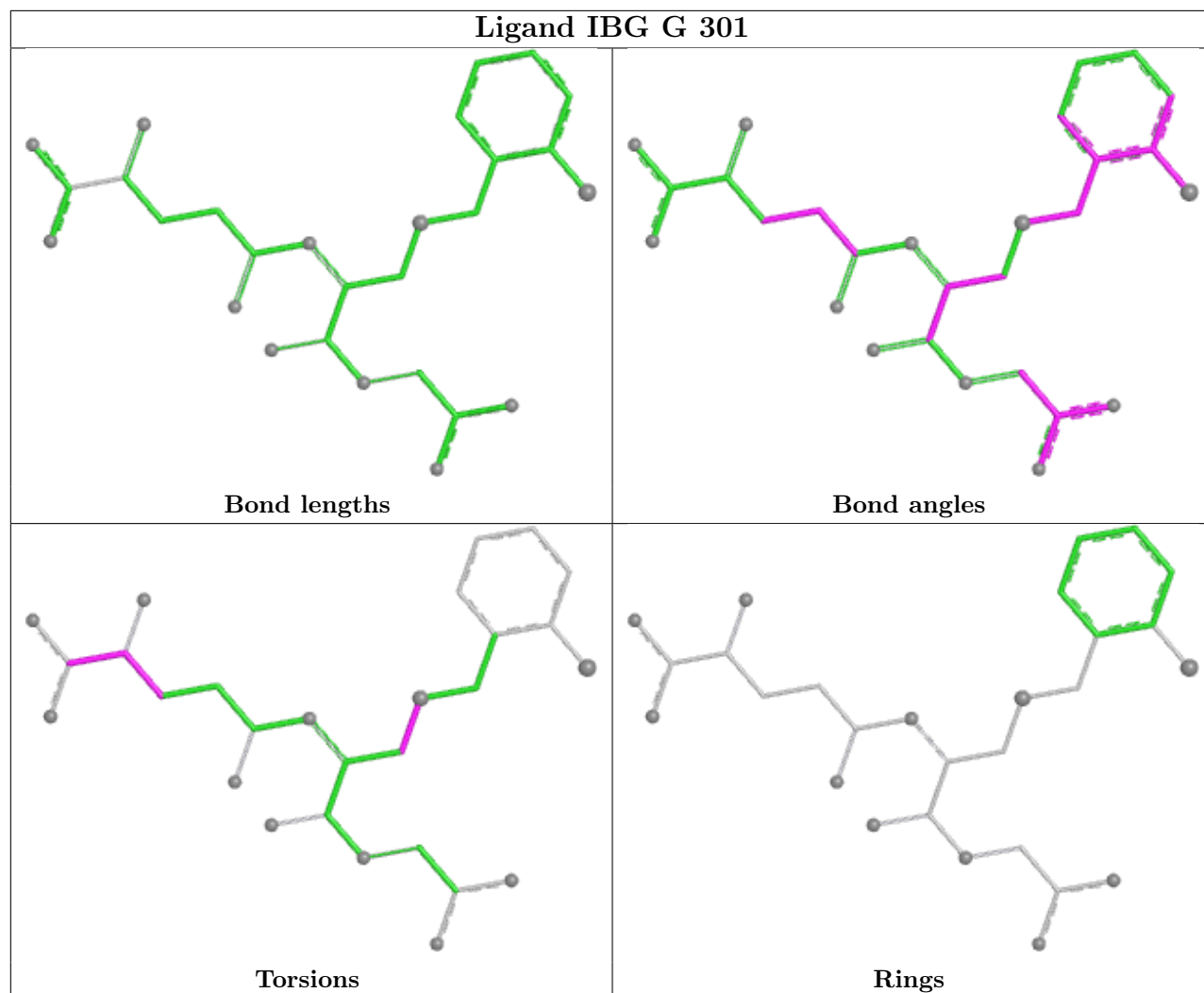
8 monomers are involved in 8 short contacts:

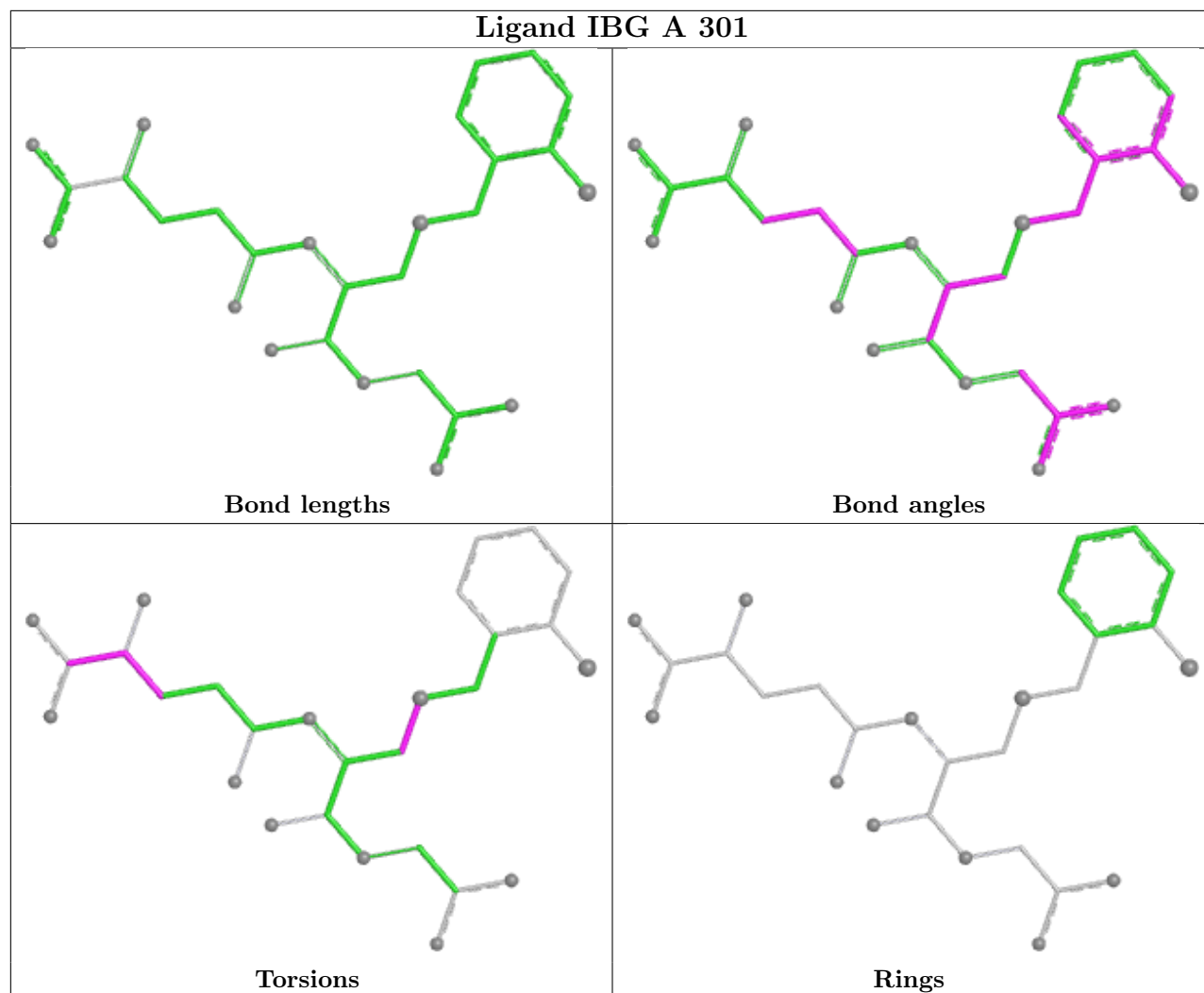
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	IBG	1	0
2	F	301	IBG	1	0
2	G	301	IBG	1	0
2	A	301	IBG	1	0
2	D	301	IBG	1	0
2	C	301	IBG	1	0
2	H	301	IBG	1	0
2	E	301	IBG	1	0

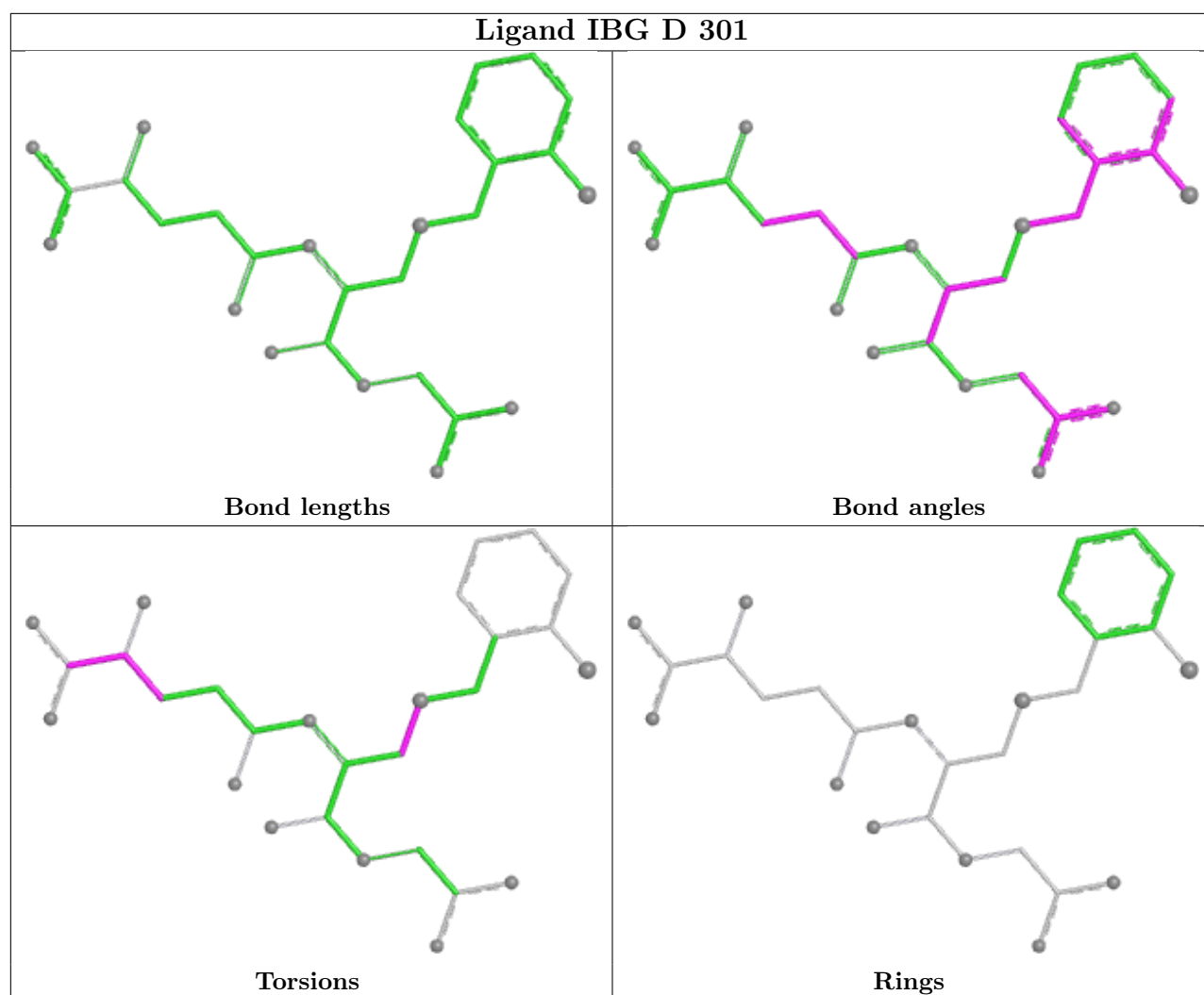
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

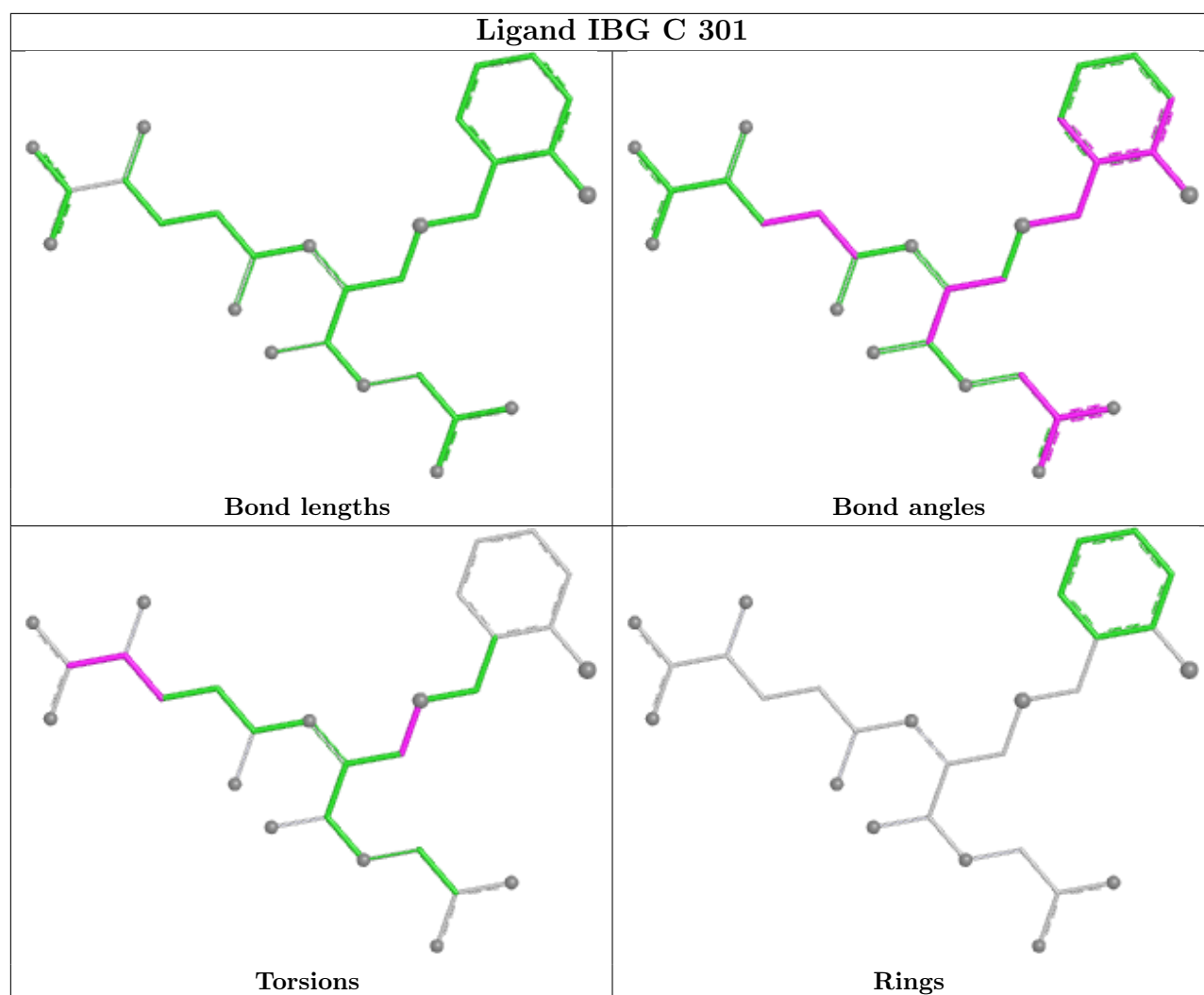




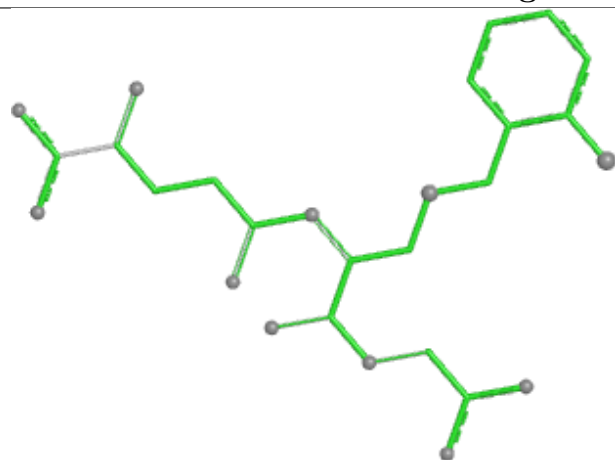




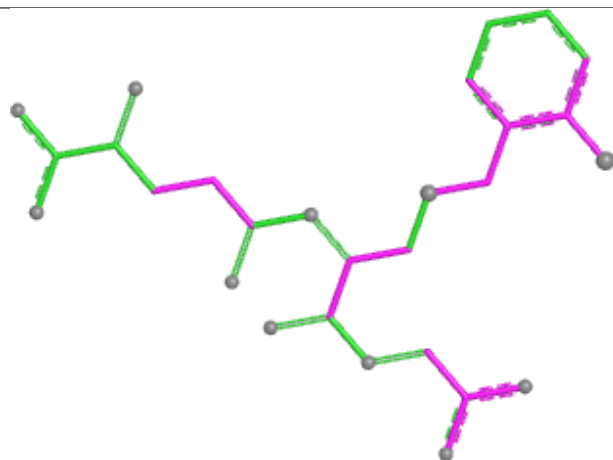




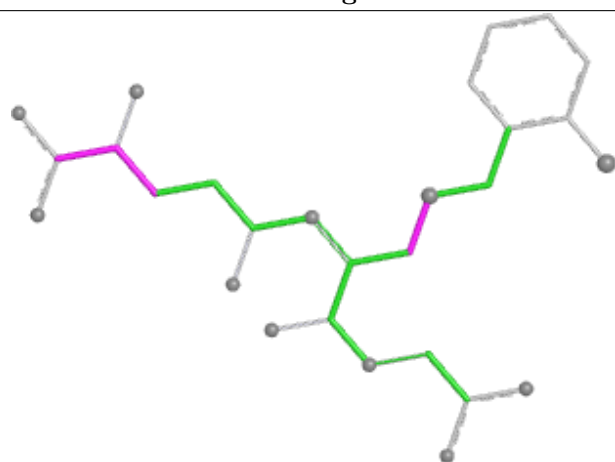
Ligand IBG H 301



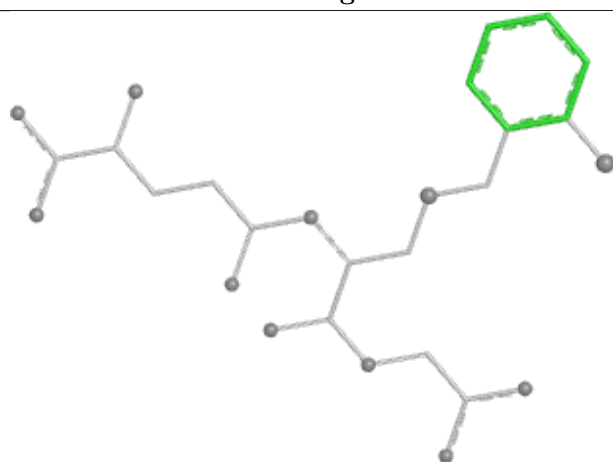
Bond lengths



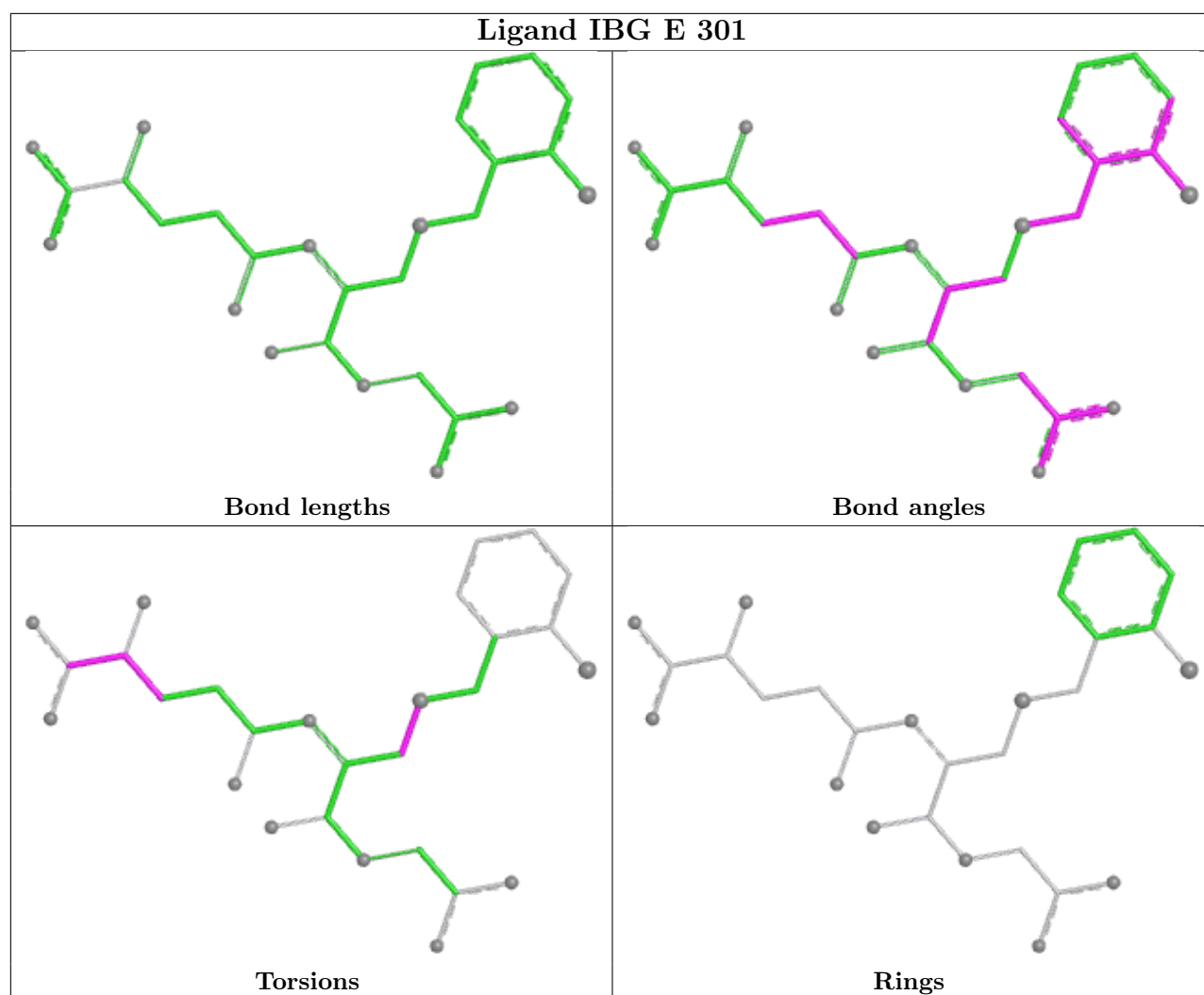
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/222 (97%)	0.49	24 (11%) 10 8	4, 14, 71, 147	0
1	B	217/222 (97%)	0.50	29 (13%) 7 6	4, 14, 71, 147	0
1	C	217/222 (97%)	0.55	27 (12%) 8 7	4, 14, 71, 147	0
1	D	217/222 (97%)	0.64	26 (11%) 9 7	4, 14, 71, 147	0
1	E	217/222 (97%)	0.61	26 (11%) 9 7	4, 14, 71, 147	0
1	F	217/222 (97%)	0.48	22 (10%) 12 10	4, 14, 71, 147	0
1	G	217/222 (97%)	0.55	31 (14%) 6 5	4, 14, 71, 147	0
1	H	217/222 (97%)	0.64	25 (11%) 9 8	4, 14, 71, 147	0
All	All	1736/1776 (97%)	0.56	210 (12%) 8 7	4, 15, 77, 147	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	201	GLY	8.0
1	G	210	GLU	7.4
1	F	196	ARG	6.5
1	E	200	PRO	6.3
1	A	183	GLU	6.1
1	G	196	ARG	6.1
1	G	214	ARG	6.1
1	H	118	GLN	5.7
1	C	39	GLU	5.5
1	E	196	ARG	5.5
1	A	196	ARG	5.5
1	E	118	GLN	5.3
1	G	39	GLU	5.2
1	G	209	ASP	5.2
1	E	183	GLU	5.1
1	B	183	GLU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	196	ARG	5.1
1	H	183	GLU	5.1
1	C	87	LYS	5.0
1	E	38	LYS	5.0
1	D	39	GLU	4.9
1	A	214	ARG	4.8
1	C	113	LYS	4.7
1	C	183	GLU	4.6
1	E	210	GLU	4.6
1	B	38	LYS	4.6
1	A	115	ASP	4.6
1	D	118	GLN	4.5
1	F	38	LYS	4.5
1	C	38	LYS	4.4
1	D	42	TYR	4.4
1	E	214	ARG	4.4
1	F	183	GLU	4.4
1	E	115	ASP	4.4
1	A	87	LYS	4.4
1	G	183	GLU	4.4
1	F	113	LYS	4.3
1	A	38	LYS	4.3
1	B	113	LYS	4.3
1	C	118	GLN	4.3
1	G	118	GLN	4.3
1	D	87	LYS	4.3
1	G	38	LYS	4.3
1	C	196	ARG	4.2
1	H	43	LYS	4.2
1	E	87	LYS	4.2
1	F	39	GLU	4.2
1	B	214	ARG	4.2
1	B	217	TYR	4.1
1	C	43	LYS	4.1
1	B	43	LYS	4.0
1	C	42	TYR	4.0
1	D	183	GLU	4.0
1	D	115	ASP	4.0
1	A	118	GLN	4.0
1	D	113	LYS	4.0
1	F	210	GLU	3.9
1	B	115	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	210	GLU	3.9
1	E	119	LYS	3.9
1	A	217	TYR	3.9
1	C	119	LYS	3.9
1	D	38	LYS	3.9
1	G	113	LYS	3.9
1	F	214	ARG	3.9
1	C	210	GLU	3.9
1	H	214	ARG	3.8
1	A	119	LYS	3.8
1	H	113	LYS	3.8
1	H	119	LYS	3.8
1	A	141	ARG	3.8
1	A	113	LYS	3.8
1	B	42	TYR	3.8
1	B	118	GLN	3.8
1	B	210	GLU	3.8
1	A	42	TYR	3.8
1	G	115	ASP	3.7
1	F	119	LYS	3.7
1	D	196	ARG	3.7
1	H	196	ARG	3.6
1	C	46	ASP	3.6
1	A	39	GLU	3.6
1	H	42	TYR	3.6
1	A	210	GLU	3.6
1	G	43	LYS	3.6
1	F	43	LYS	3.6
1	G	87	LYS	3.5
1	D	214	ARG	3.5
1	F	42	TYR	3.5
1	F	118	GLN	3.5
1	E	42	TYR	3.4
1	F	211	ILE	3.4
1	H	115	ASP	3.4
1	D	119	LYS	3.4
1	A	43	LYS	3.3
1	C	217	TYR	3.3
1	G	36	GLU	3.3
1	A	218	ASN	3.3
1	B	48	ASN	3.3
1	G	200	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	218	ASN	3.3
1	F	115	ASP	3.3
1	B	87	LYS	3.2
1	G	208	PRO	3.2
1	C	115	ASP	3.2
1	H	87	LYS	3.2
1	B	190	ASN	3.2
1	H	218	ASN	3.2
1	G	119	LYS	3.2
1	B	200	PRO	3.1
1	E	211	ILE	3.1
1	H	38	LYS	3.1
1	D	218	ASN	3.1
1	G	48	ASN	3.1
1	G	190	ASN	3.1
1	C	114	PRO	3.1
1	E	113	LYS	3.1
1	H	39	GLU	3.1
1	A	29	GLU	3.0
1	E	202	SER	3.0
1	D	190	ASN	3.0
1	A	4	ARG	3.0
1	D	29	GLU	3.0
1	H	48	ASN	3.0
1	B	119	LYS	3.0
1	B	36	GLU	3.0
1	C	48	ASN	3.0
1	D	114	PRO	2.9
1	F	87	LYS	2.9
1	G	195	LYS	2.9
1	A	48	ASN	2.9
1	C	190	ASN	2.9
1	C	214	ARG	2.9
1	D	4	ARG	2.9
1	D	217	TYR	2.9
1	B	201	GLY	2.9
1	H	195	LYS	2.9
1	H	114	PRO	2.9
1	D	210	GLU	2.8
1	G	42	TYR	2.8
1	G	211	ILE	2.8
1	G	29	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	36	GLU	2.8
1	D	211	ILE	2.7
1	D	43	LYS	2.7
1	D	36	GLU	2.7
1	F	114	PRO	2.6
1	E	141	ARG	2.6
1	E	29	GLU	2.6
1	B	39	GLU	2.6
1	E	43	LYS	2.5
1	E	217	TYR	2.5
1	C	123	ASN	2.5
1	G	218	ASN	2.5
1	C	36	GLU	2.5
1	F	217	TYR	2.5
1	E	48	ASN	2.5
1	F	190	ASN	2.5
1	A	190	ASN	2.4
1	B	141	ARG	2.4
1	H	190	ASN	2.4
1	H	217	TYR	2.4
1	F	53	GLN	2.4
1	C	220	PHE	2.4
1	D	220	PHE	2.4
1	B	218	ASN	2.4
1	C	200	PRO	2.4
1	C	141	ARG	2.4
1	A	114	PRO	2.4
1	E	138	LYS	2.4
1	B	220	PHE	2.4
1	F	203	LYS	2.4
1	B	114	PRO	2.4
1	C	4	ARG	2.3
1	E	190	ASN	2.3
1	F	48	ASN	2.3
1	B	29	GLU	2.3
1	C	29	GLU	2.3
1	G	141	ARG	2.3
1	G	201	GLY	2.3
1	E	195	LYS	2.3
1	E	36	GLU	2.3
1	E	218	ASN	2.3
1	A	220	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	36	GLU	2.2
1	H	29	GLU	2.2
1	B	138	LYS	2.2
1	H	209	ASP	2.2
1	H	212	TYR	2.2
1	G	6	LYS	2.1
1	C	211	ILE	2.1
1	G	120	GLU	2.1
1	B	4	ARG	2.1
1	G	4	ARG	2.1
1	D	192	PRO	2.1
1	G	114	PRO	2.1
1	B	176	SER	2.1
1	G	176	SER	2.1
1	D	195	LYS	2.1
1	E	199	GLU	2.1
1	H	120	GLU	2.1
1	C	218	ASN	2.1
1	A	209	ASP	2.0
1	F	141	ARG	2.0
1	G	199	GLU	2.0
1	H	141	ARG	2.0
1	D	209	ASP	2.0
1	B	216	VAL	2.0
1	D	141	ARG	2.0
1	B	212	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

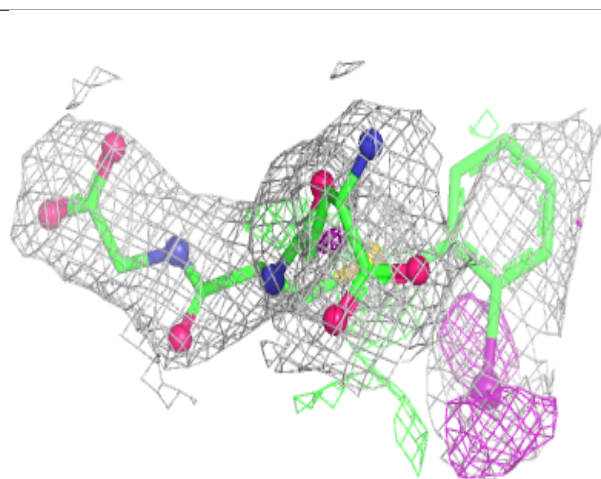
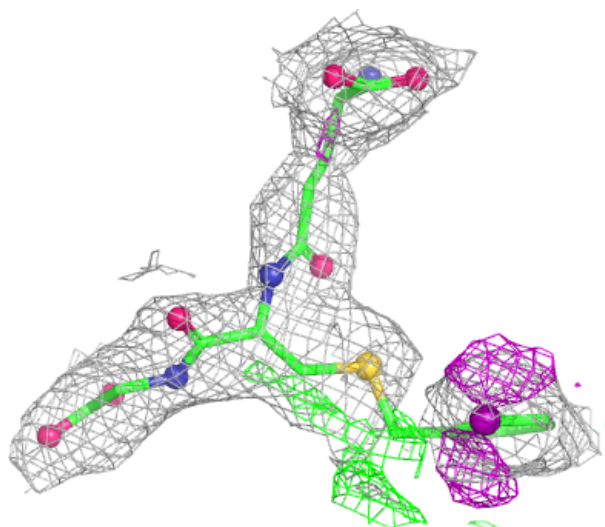
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IBG	G	301	28/28	0.82	0.27	5,31,300,300	0
2	IBG	A	301	28/28	0.88	0.23	5,31,300,300	0
2	IBG	C	301	28/28	0.90	0.21	5,31,300,300	0
2	IBG	B	301	28/28	0.90	0.21	5,31,300,300	0
2	IBG	E	301	28/28	0.91	0.20	5,31,300,300	0
2	IBG	D	301	28/28	0.91	0.22	5,31,300,300	0
2	IBG	F	301	28/28	0.92	0.19	5,31,300,300	0
2	IBG	H	301	28/28	0.92	0.20	5,31,300,300	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.

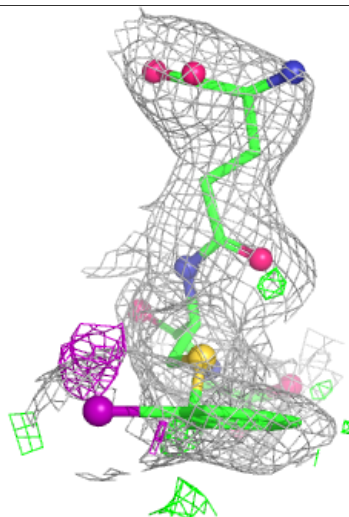
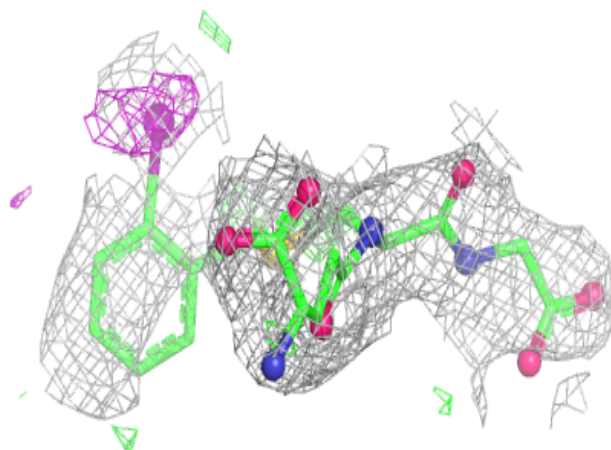
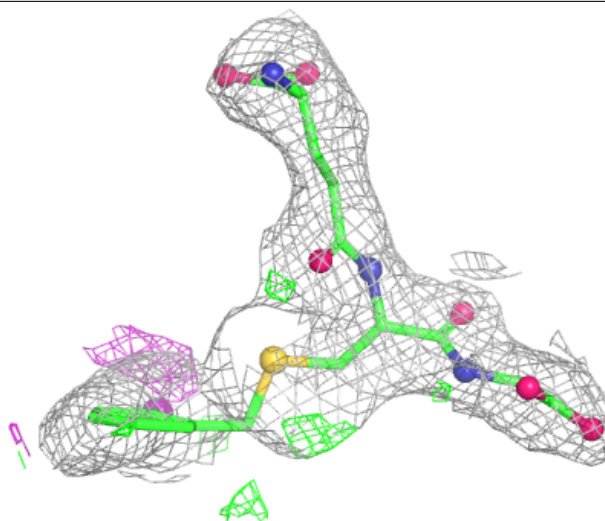
Electron density around IBG G 301:

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



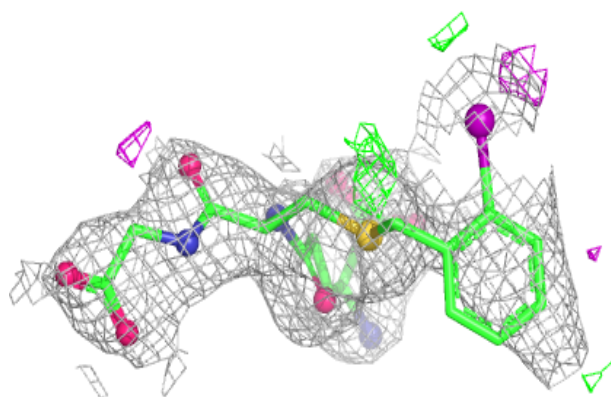
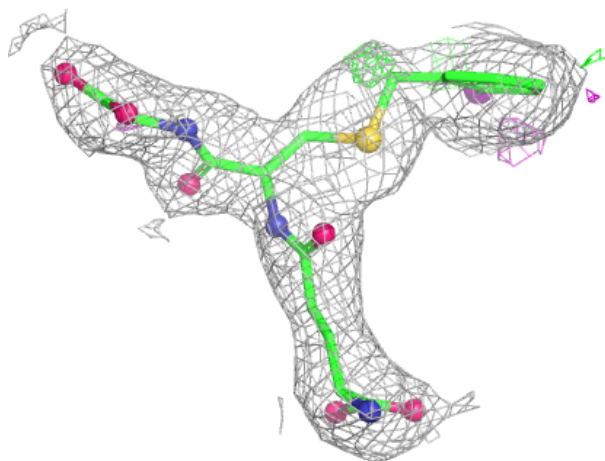
Electron density around IBG A 301:

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



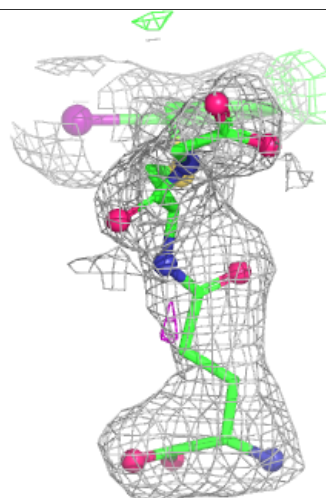
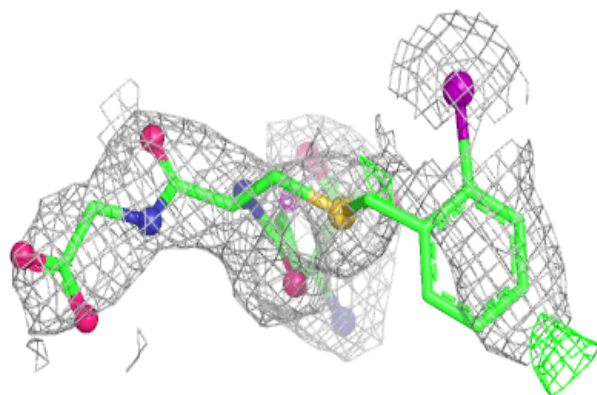
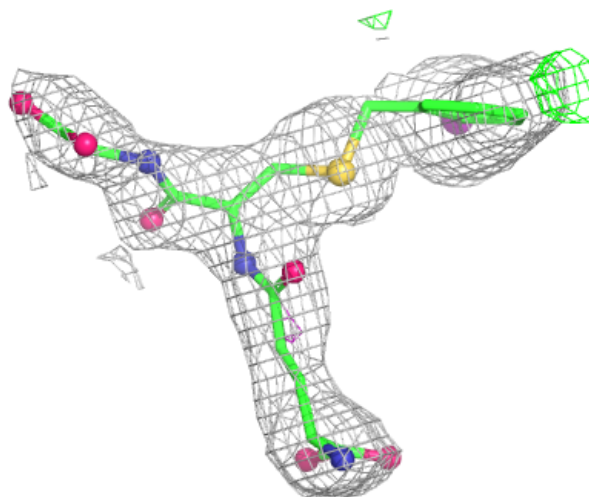
Electron density around IBG C 301:

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



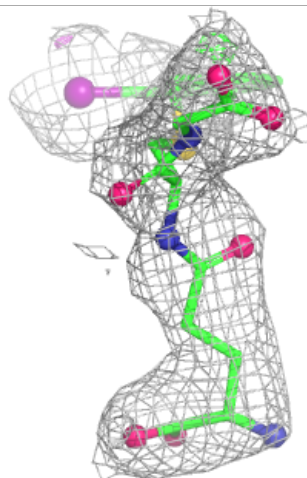
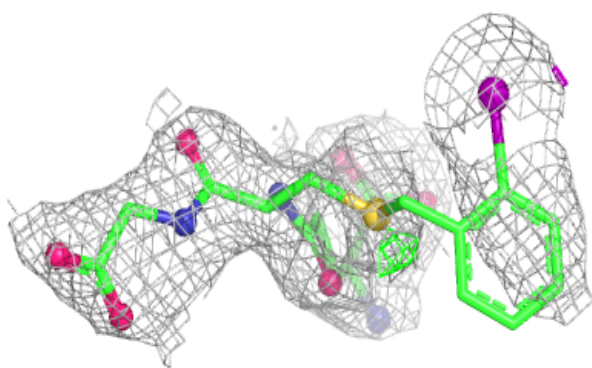
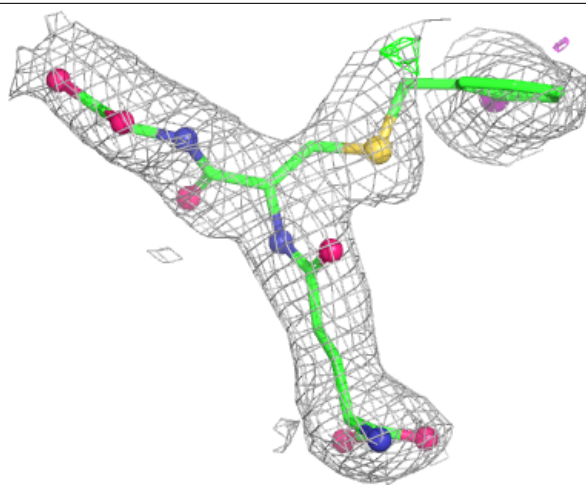
Electron density around IBG B 301:

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



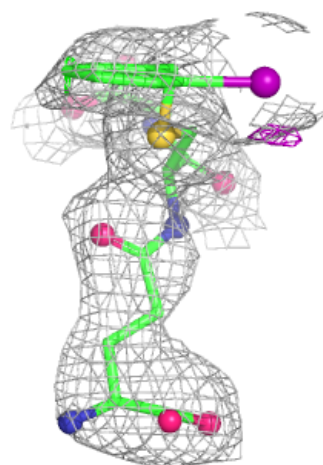
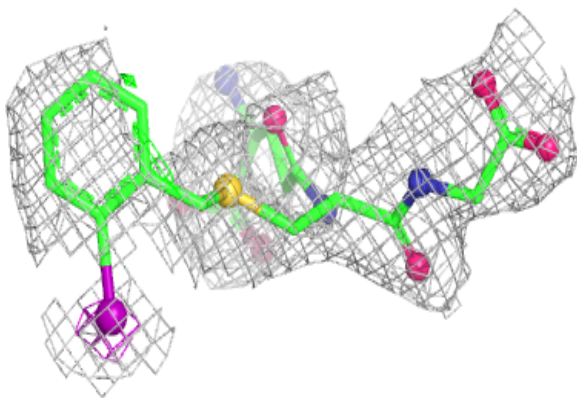
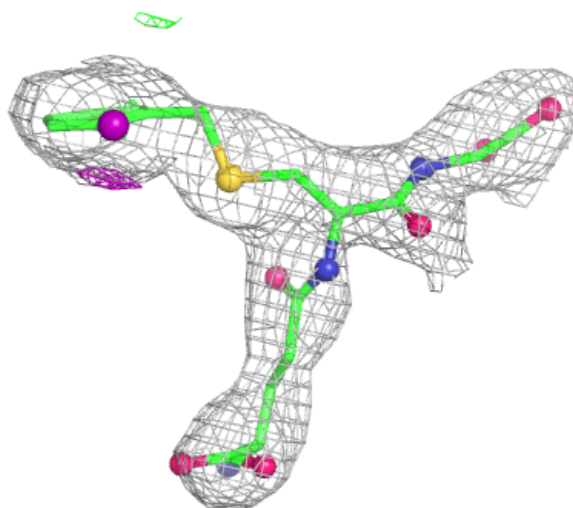
Electron density around IBG E 301:

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



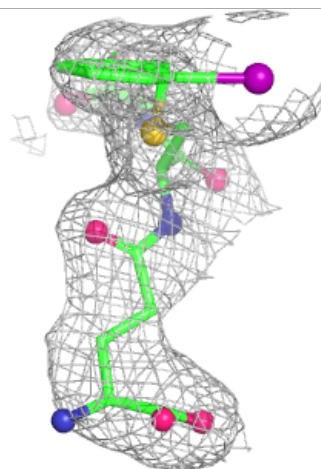
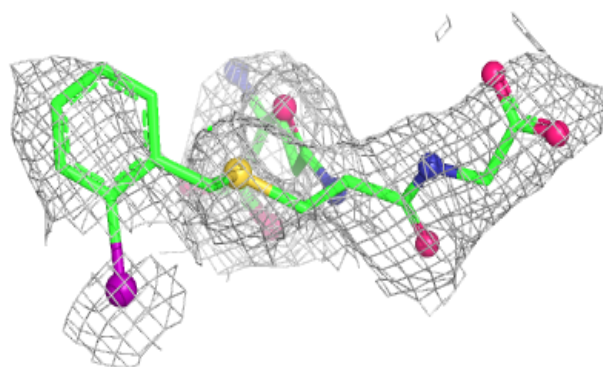
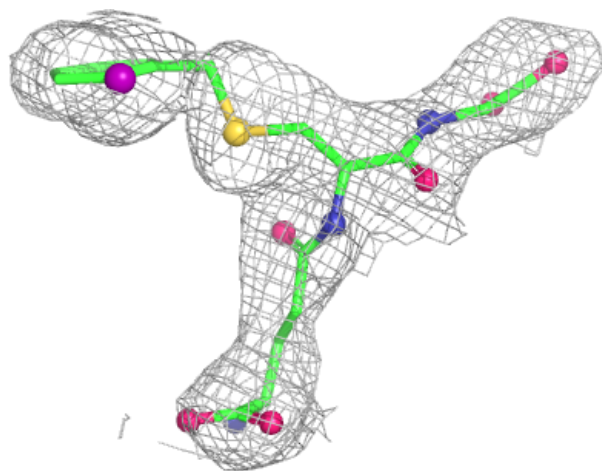
Electron density around IBG D 301:

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



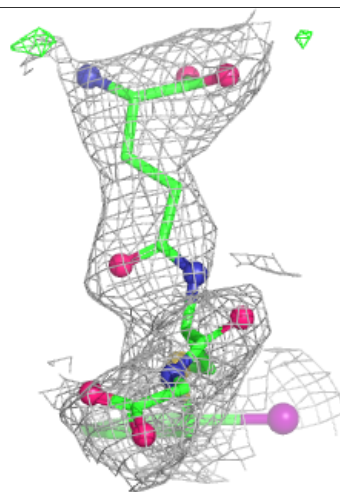
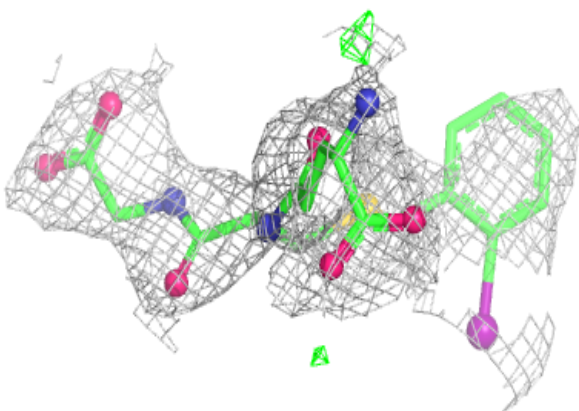
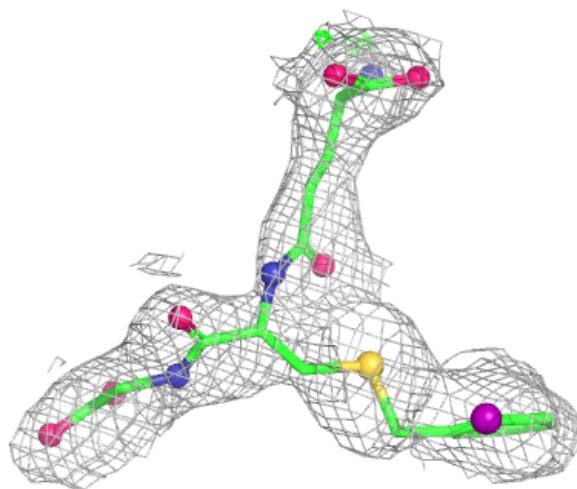
Electron density around IBG F 301:

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



Electron density around IBG H 301:

$2mF_o-DF_c$ (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.