



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:54 AM UTC

PDB ID : 1GUH / pdb_00001guh
Title : Structure determination and refinement of human alpha class glutathione transferase A1-1, and a comparison with the MU and PI class enzymes
Authors : Sinning, I.; Kleywegt, G.J.; Jones, T.A.
Deposited on : 1993-02-24
Resolution : 2.60 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

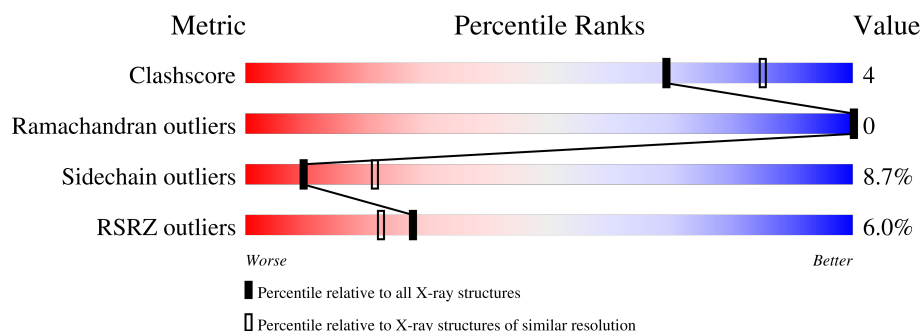
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	221	6% 78% 18% ..
1	B	221	5% 77% 19% ..
1	C	221	6% 78% 19% ..
1	D	221	7% 77% 19% ..

2 Entry composition [i](#)

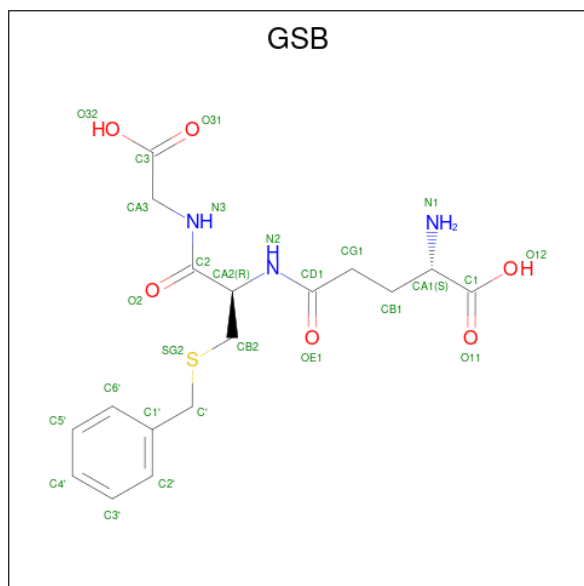
There are 2 unique types of molecules in this entry. The entry contains 7292 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 A1-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1796	1164	300	324	8			
1	B	221	Total	C	N	O	S	0	0	0
			1796	1164	300	324	8			
1	C	221	Total	C	N	O	S	0	0	0
			1796	1164	300	324	8			
1	D	221	Total	C	N	O	S	0	0	0
			1796	1164	300	324	8			

- Molecule 2 is S-BENZYL-GLUTATHIONE (CCD ID: GSB) (formula: $C_{17}H_{23}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	17	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			27	17	3	6	1		

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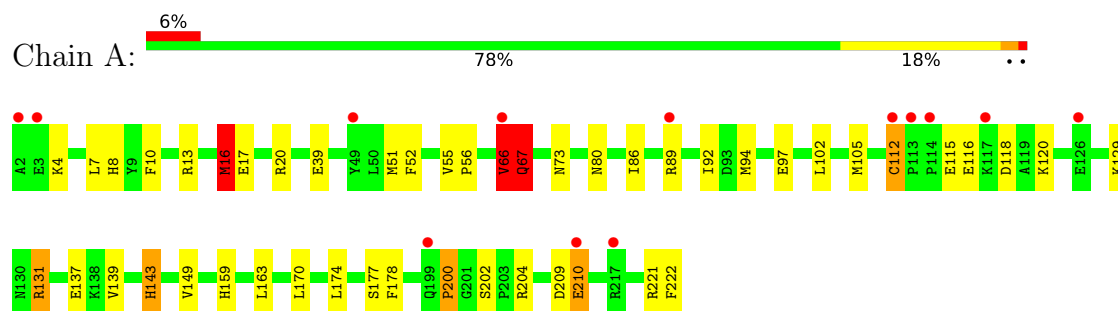
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			27	17	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			27	17	3	6	1		

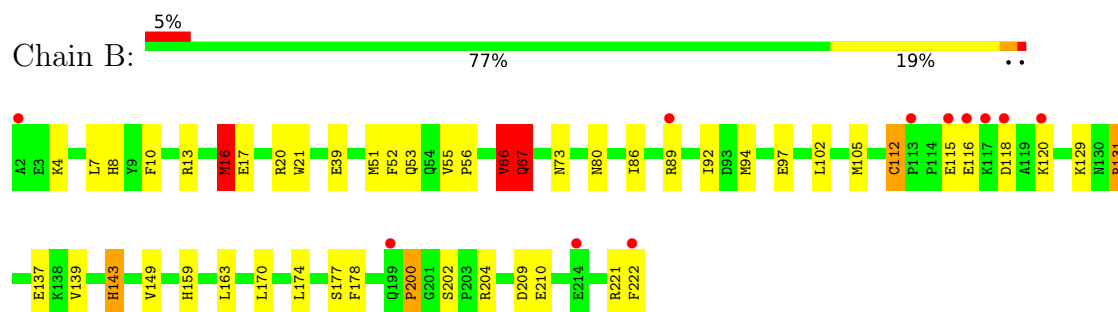
3 Residue-property plots

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.

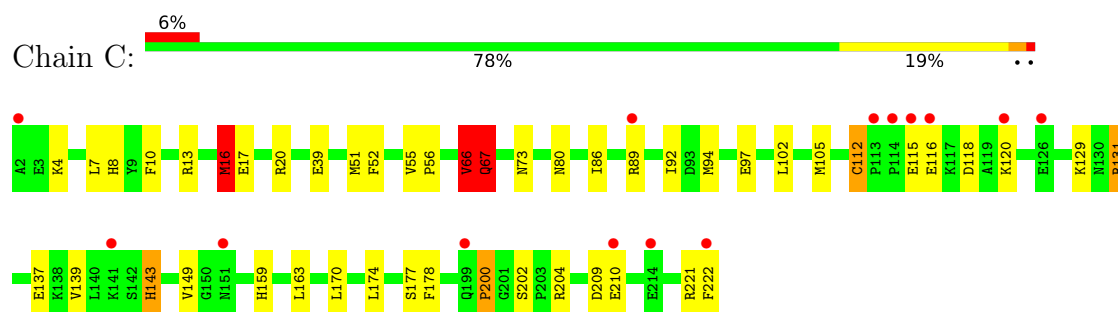
• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1



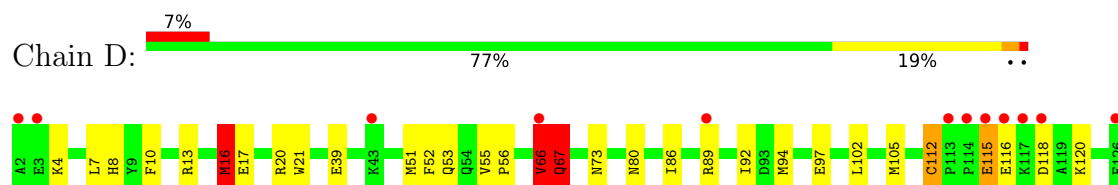
• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1



• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1



• Molecule 1: GLUTATHIONE S-TRANSFERASE A1-1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.80Å 95.40Å 105.20Å 90.00° 92.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60 105.11 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60) 80.9 (105.11-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.57Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.229 , (Not available) 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7292	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4225e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GSB

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	0.91	6/1832 (0.3%)	1.63	28/2461 (1.1%)
1	B	0.91	5/1832 (0.3%)	1.63	29/2461 (1.2%)
1	C	0.91	5/1832 (0.3%)	1.63	28/2461 (1.1%)
1	D	0.91	5/1832 (0.3%)	1.63	29/2461 (1.2%)
All	All	0.91	21/7328 (0.3%)	1.63	114/9844 (1.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	HIS	CD2-NE2	-7.16	1.29	1.37
1	C	143	HIS	CD2-NE2	-7.15	1.29	1.37
1	D	143	HIS	CD2-NE2	-7.12	1.30	1.37
1	B	143	HIS	CD2-NE2	-7.09	1.30	1.37
1	B	8	HIS	CD2-NE2	-6.49	1.30	1.37
1	C	8	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	8	HIS	CD2-NE2	-6.45	1.30	1.37
1	D	8	HIS	CD2-NE2	-6.44	1.30	1.37
1	C	159	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	159	HIS	CD2-NE2	-6.23	1.30	1.37
1	B	159	HIS	CD2-NE2	-6.16	1.31	1.37
1	D	159	HIS	CD2-NE2	-6.13	1.31	1.37
1	D	204	ARG	CA-CB	-5.38	1.44	1.53
1	B	204	ARG	CA-CB	-5.38	1.44	1.53
1	A	204	ARG	CA-CB	-5.36	1.44	1.53
1	C	204	ARG	CA-CB	-5.35	1.44	1.53
1	D	159	HIS	CG-ND1	-5.34	1.32	1.38
1	B	159	HIS	CG-ND1	-5.25	1.32	1.38
1	A	159	HIS	CG-ND1	-5.20	1.32	1.38
1	C	159	HIS	CG-ND1	-5.17	1.32	1.38
1	A	8	HIS	CG-ND1	-5.00	1.32	1.38

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	PHE	CA-CB-CG	9.78	123.58	113.80
1	C	10	PHE	CA-CB-CG	9.78	123.58	113.80
1	A	10	PHE	CA-CB-CG	9.76	123.56	113.80
1	D	10	PHE	CA-CB-CG	9.74	123.54	113.80
1	B	55	VAL	O-C-N	-8.40	114.43	121.40
1	A	55	VAL	O-C-N	-8.37	114.45	121.40
1	D	55	VAL	O-C-N	-8.37	114.45	121.40
1	C	55	VAL	O-C-N	-8.31	114.51	121.40
1	A	204	ARG	CB-CG-CD	-7.60	93.82	111.30
1	C	204	ARG	CB-CG-CD	-7.60	93.82	111.30
1	B	204	ARG	CB-CG-CD	-7.59	93.84	111.30
1	D	204	ARG	CB-CG-CD	-7.59	93.84	111.30
1	C	66	VAL	CA-C-O	-7.52	112.28	118.90
1	A	66	VAL	CA-C-O	-7.49	112.31	118.90
1	B	66	VAL	CA-C-O	-7.47	112.32	118.90
1	D	66	VAL	CA-C-O	-7.45	112.35	118.90
1	B	143	HIS	CB-CG-CD2	-6.82	122.34	131.20
1	D	143	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	A	143	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	C	143	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	A	80	ASN	N-CA-C	6.68	120.71	111.90
1	B	80	ASN	N-CA-C	6.67	120.70	111.90
1	C	80	ASN	N-CA-C	6.65	120.68	111.90
1	D	80	ASN	N-CA-C	6.65	120.68	111.90
1	D	116	GLU	N-CA-C	6.44	119.11	111.71
1	B	116	GLU	N-CA-C	6.41	119.08	111.71
1	A	116	GLU	N-CA-C	6.39	119.06	111.71
1	C	116	GLU	N-CA-C	6.38	119.05	111.71
1	C	67	GLN	CA-C-O	-6.19	113.81	120.92
1	D	16	MET	CG-SD-CE	-6.18	87.30	100.90
1	A	67	GLN	CA-C-O	-6.18	113.81	120.92
1	B	16	MET	CG-SD-CE	-6.17	87.32	100.90
1	D	67	GLN	CA-C-O	-6.17	113.82	120.92
1	A	16	MET	CG-SD-CE	-6.17	87.32	100.90
1	C	16	MET	CG-SD-CE	-6.17	87.33	100.90
1	B	67	GLN	CA-C-O	-6.17	113.83	120.92
1	D	4	LYS	CA-C-N	6.12	126.14	119.90
1	D	4	LYS	C-N-CA	6.12	126.14	119.90
1	B	4	LYS	CA-C-N	6.12	126.14	119.90
1	B	4	LYS	C-N-CA	6.12	126.14	119.90
1	B	202	SER	N-CA-C	6.11	119.77	109.87
1	D	202	SER	N-CA-C	6.10	119.75	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	CA-C-N	6.09	126.12	119.90
1	A	4	LYS	C-N-CA	6.09	126.12	119.90
1	A	202	SER	N-CA-C	6.09	119.73	109.87
1	C	202	SER	N-CA-C	6.08	119.72	109.87
1	A	67	GLN	O-C-N	-6.06	116.13	123.16
1	C	4	LYS	CA-C-N	6.06	126.08	119.90
1	C	4	LYS	C-N-CA	6.06	126.08	119.90
1	C	67	GLN	O-C-N	-6.05	116.14	123.16
1	B	67	GLN	O-C-N	-6.03	116.16	123.16
1	D	67	GLN	O-C-N	-6.03	116.17	123.16
1	A	222	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	222	PHE	CA-CB-CG	6.01	119.81	113.80
1	D	222	PHE	CA-CB-CG	6.00	119.80	113.80
1	C	222	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	200	PRO	N-CA-C	5.87	124.57	112.47
1	D	200	PRO	N-CA-C	5.86	124.54	112.47
1	B	200	PRO	N-CA-C	5.86	124.54	112.47
1	C	200	PRO	N-CA-C	5.85	124.53	112.47
1	C	20	ARG	CA-CB-CG	-5.83	102.43	114.10
1	A	20	ARG	CA-CB-CG	-5.83	102.45	114.10
1	D	20	ARG	CA-CB-CG	-5.81	102.48	114.10
1	B	20	ARG	CA-CB-CG	-5.80	102.49	114.10
1	C	149	VAL	CA-C-O	-5.76	113.58	120.78
1	D	149	VAL	CA-C-O	-5.76	113.58	120.78
1	A	149	VAL	CA-C-O	-5.76	113.58	120.78
1	B	149	VAL	CA-C-O	-5.74	113.60	120.78
1	C	17	GLU	N-CA-C	5.67	117.46	111.28
1	B	17	GLU	N-CA-C	5.66	117.45	111.28
1	A	17	GLU	N-CA-C	5.66	117.45	111.28
1	D	17	GLU	N-CA-C	5.65	117.44	111.28
1	D	51	MET	N-CA-C	5.60	117.38	111.28
1	B	51	MET	N-CA-C	5.58	117.37	111.28
1	A	51	MET	N-CA-C	5.58	117.36	111.28
1	C	51	MET	N-CA-C	5.58	117.36	111.28
1	A	80	ASN	CA-CB-CG	-5.54	107.06	112.60
1	B	80	ASN	CA-CB-CG	-5.53	107.08	112.60
1	C	80	ASN	CA-CB-CG	-5.51	107.09	112.60
1	D	80	ASN	CA-CB-CG	-5.49	107.11	112.60
1	D	86	ILE	CB-CA-C	-5.47	103.41	112.26
1	A	86	ILE	CB-CA-C	-5.46	103.42	112.26
1	B	86	ILE	CB-CA-C	-5.45	103.43	112.26
1	C	86	ILE	CB-CA-C	-5.44	103.45	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	209	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	115	GLU	N-CA-C	-5.37	105.11	110.97
1	C	209	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	209	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	209	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	115	GLU	N-CA-C	-5.33	105.17	110.97
1	D	115	GLU	N-CA-C	-5.32	105.17	110.97
1	B	115	GLU	N-CA-C	-5.31	105.18	110.97
1	C	143	HIS	CB-CG-ND1	5.31	130.66	122.70
1	B	143	HIS	CB-CG-ND1	5.29	130.64	122.70
1	A	143	HIS	CB-CG-ND1	5.29	130.63	122.70
1	D	143	HIS	CB-CG-ND1	5.28	130.62	122.70
1	B	204	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	D	204	ARG	NE-CZ-NH2	-5.26	114.46	119.20
1	A	204	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	C	204	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	D	112	CYS	CA-C-N	5.18	125.72	120.38
1	D	112	CYS	C-N-CA	5.18	125.72	120.38
1	B	112	CYS	CA-C-N	5.14	125.67	120.38
1	B	112	CYS	C-N-CA	5.14	125.67	120.38
1	B	92	ILE	CA-C-O	-5.12	115.75	121.17
1	A	92	ILE	CA-C-O	-5.10	115.77	121.17
1	C	112	CYS	CA-C-N	5.10	125.63	120.38
1	C	112	CYS	C-N-CA	5.10	125.63	120.38
1	C	92	ILE	CA-C-O	-5.10	115.77	121.17
1	A	112	CYS	CA-C-N	5.09	125.62	120.38
1	A	112	CYS	C-N-CA	5.09	125.62	120.38
1	D	92	ILE	CA-C-O	-5.09	115.77	121.17
1	D	21	TRP	CG-CD1-NE1	-5.03	103.67	110.20
1	B	21	TRP	CG-CD1-NE1	-5.02	103.67	110.20

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	1796	0	1863	20	1
1	B	1796	0	1863	20	0
1	C	1796	0	1863	20	0
1	D	1796	0	1863	20	1
2	A	27	0	21	0	0
2	B	27	0	21	0	0
2	C	27	0	21	0	0
2	D	27	0	21	0	0
All	All	7292	0	7536	52	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 4.

All (52) 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:67:GLN:HG2	1:B:97:GLU:HB3	1.73	0.70
1:A:97:GLU:HB3	1:B:67:GLN:HG2	1.75	0.68
1:C:67:GLN:HG2	1:D:97:GLU:HB3	1.73	0.68
1:C:97:GLU:HB3	1:D:67:GLN:HG2	1.75	0.68
1:A:73:ASN:HB3	1:B:89:ARG:HH21	1.59	0.66
1:C:73:ASN:HB3	1:D:89:ARG:HH21	1.59	0.66
1:A:66:VAL:HB	1:B:94:MET:HE3	1.79	0.65
1:C:66:VAL:HB	1:D:94:MET:HE3	1.79	0.64
1:C:89:ARG:HH21	1:D:73:ASN:HB3	1.68	0.59
1:D:129:LYS:HE3	1:D:174:LEU:HD23	1.86	0.58
1:A:129:LYS:HE3	1:A:174:LEU:HD23	1.86	0.58
1:A:89:ARG:HH21	1:B:73:ASN:HB3	1.68	0.58
1:C:129:LYS:HE3	1:C:174:LEU:HD23	1.86	0.58
1:B:129:LYS:HE3	1:B:174:LEU:HD23	1.86	0.57
1:A:67:GLN:HG2	1:B:97:GLU:CB	2.35	0.56
1:D:102:LEU:HD23	1:D:163:LEU:HD21	1.88	0.56
1:C:67:GLN:HG2	1:D:97:GLU:CB	2.35	0.56
1:A:102:LEU:HD23	1:A:163:LEU:HD21	1.88	0.55
1:C:102:LEU:HD23	1:C:163:LEU:HD21	1.88	0.55
1:B:102:LEU:HD23	1:B:163:LEU:HD21	1.88	0.55
1:A:102:LEU:HA	1:A:105:MET:HE3	1.90	0.53
1:C:131:ARG:HD2	1:D:52:PHE:O	2.08	0.53
1:B:102:LEU:HA	1:B:105:MET:HE3	1.90	0.53
1:D:102:LEU:HA	1:D:105:MET:HE3	1.90	0.53
1:A:131:ARG:HD2	1:B:52:PHE:O	2.08	0.53
1:C:102:LEU:HA	1:C:105:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:HE2	1:B:56:PRO:HB3	1.92	0.52
1:A:16:MET:HE2	1:A:56:PRO:HB3	1.92	0.52
1:C:16:MET:HE2	1:C:56:PRO:HB3	1.92	0.51
1:D:16:MET:HE2	1:D:56:PRO:HB3	1.92	0.51
1:C:89:ARG:NH1	1:D:89:ARG:NH1	2.60	0.50
1:B:137:GLU:HG3	1:B:178:PHE:HD1	1.77	0.50
1:A:89:ARG:NH1	1:B:89:ARG:NH1	2.60	0.50
1:A:137:GLU:HG3	1:A:178:PHE:HD1	1.77	0.49
1:C:94:MET:HE3	1:D:66:VAL:HB	1.94	0.49
1:C:97:GLU:CB	1:D:67:GLN:HG2	2.42	0.49
1:D:137:GLU:HG3	1:D:178:PHE:HD1	1.77	0.49
1:A:94:MET:HE3	1:B:66:VAL:HB	1.94	0.49
1:C:52:PHE:O	1:D:131:ARG:HD2	2.13	0.49
1:C:137:GLU:HG3	1:C:178:PHE:HD1	1.77	0.48
1:A:52:PHE:O	1:B:131:ARG:HD2	2.13	0.48
1:A:97:GLU:CB	1:B:67:GLN:HG2	2.42	0.47
1:C:131:ARG:NH1	1:D:53:GLN:HB2	2.31	0.46
1:A:131:ARG:NH1	1:B:53:GLN:HB2	2.31	0.46
1:A:89:ARG:HH12	1:B:89:ARG:NH1	2.14	0.46
1:D:129:LYS:HE3	1:D:174:LEU:CD2	2.46	0.46
1:C:89:ARG:HH12	1:D:89:ARG:NH1	2.14	0.45
1:B:129:LYS:HE3	1:B:174:LEU:CD2	2.46	0.45
1:C:129:LYS:HE3	1:C:174:LEU:CD2	2.46	0.45
1:A:129:LYS:HE3	1:A:174:LEU:CD2	2.46	0.44
1:C:89:ARG:NH1	1:D:89:ARG:HH12	2.18	0.42
1:A:89:ARG:NH1	1:B:89:ARG:HH12	2.18	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:A:210:GLU:OE2	1:D:115:GLU:OE2[2_756]	1.91	0.29

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	219/221 (99%)	211 (96%)	8 (4%)	0	100	100
1	B	219/221 (99%)	211 (96%)	8 (4%)	0	100	100
1	C	219/221 (99%)	211 (96%)	8 (4%)	0	100	100
1	D	219/221 (99%)	211 (96%)	8 (4%)	0	100	100
All	All	876/884 (99%)	844 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	195/195 (100%)	178 (91%)	17 (9%)	9	21
1	B	195/195 (100%)	178 (91%)	17 (9%)	9	21
1	C	195/195 (100%)	178 (91%)	17 (9%)	9	21
1	D	195/195 (100%)	178 (91%)	17 (9%)	9	21
All	All	780/780 (100%)	712 (91%)	68 (9%)	9	21

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	13	ARG
1	A	16	MET
1	A	39	GLU
1	A	66	VAL
1	A	67	GLN
1	A	112	CYS
1	A	118	ASP
1	A	120	LYS
1	A	131	ARG

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Mol	Chain	Res	Type
1	A	139	VAL
1	A	143	HIS
1	A	170	LEU
1	A	177	SER
1	A	200	PRO
1	A	210	GLU
1	A	221	ARG
1	B	7	LEU
1	B	13	ARG
1	B	16	MET
1	B	39	GLU
1	B	66	VAL
1	B	67	GLN
1	B	112	CYS
1	B	118	ASP
1	B	120	LYS
1	B	131	ARG
1	B	139	VAL
1	B	143	HIS
1	B	170	LEU
1	B	177	SER
1	B	200	PRO
1	B	210	GLU
1	B	221	ARG
1	C	7	LEU
1	C	13	ARG
1	C	16	MET
1	C	39	GLU
1	C	66	VAL
1	C	67	GLN
1	C	112	CYS
1	C	118	ASP
1	C	120	LYS
1	C	131	ARG
1	C	139	VAL
1	C	143	HIS
1	C	170	LEU
1	C	177	SER
1	C	200	PRO
1	C	210	GLU
1	C	221	ARG
1	D	7	LEU

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Mol	Chain	Res	Type
1	D	13	ARG
1	D	16	MET
1	D	39	GLU
1	D	66	VAL
1	D	67	GLN
1	D	112	CYS
1	D	118	ASP
1	D	120	LYS
1	D	131	ARG
1	D	139	VAL
1	D	143	HIS
1	D	170	LEU
1	D	177	SER
1	D	200	PRO
1	D	210	GLU
1	D	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	80	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](#)

4 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	GSB	A	223	-	26,27,27	0.84	2 (7%)	31,34,34	0.73	0
2	GSB	B	223	-	26,27,27	0.84	2 (7%)	31,34,34	0.72	0
2	GSB	D	223	-	26,27,27	0.84	2 (7%)	31,34,34	0.72	0
2	GSB	C	223	-	26,27,27	0.83	2 (7%)	31,34,34	0.72	0

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	GSB	A	223	-	-	2/28/28/28	0/1/1/1
2	GSB	B	223	-	-	2/28/28/28	0/1/1/1
2	GSB	D	223	-	-	2/28/28/28	0/1/1/1
2	GSB	C	223	-	-	2/28/28/28	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	223	GSB	O12-C1	-2.50	1.22	1.30
2	C	223	GSB	O12-C1	-2.48	1.22	1.30
2	B	223	GSB	O12-C1	-2.48	1.22	1.30
2	A	223	GSB	O12-C1	-2.47	1.22	1.30
2	D	223	GSB	O32-C3	-2.08	1.23	1.30
2	A	223	GSB	O32-C3	-2.06	1.24	1.30
2	B	223	GSB	O32-C3	-2.06	1.24	1.30
2	C	223	GSB	O32-C3	-2.05	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

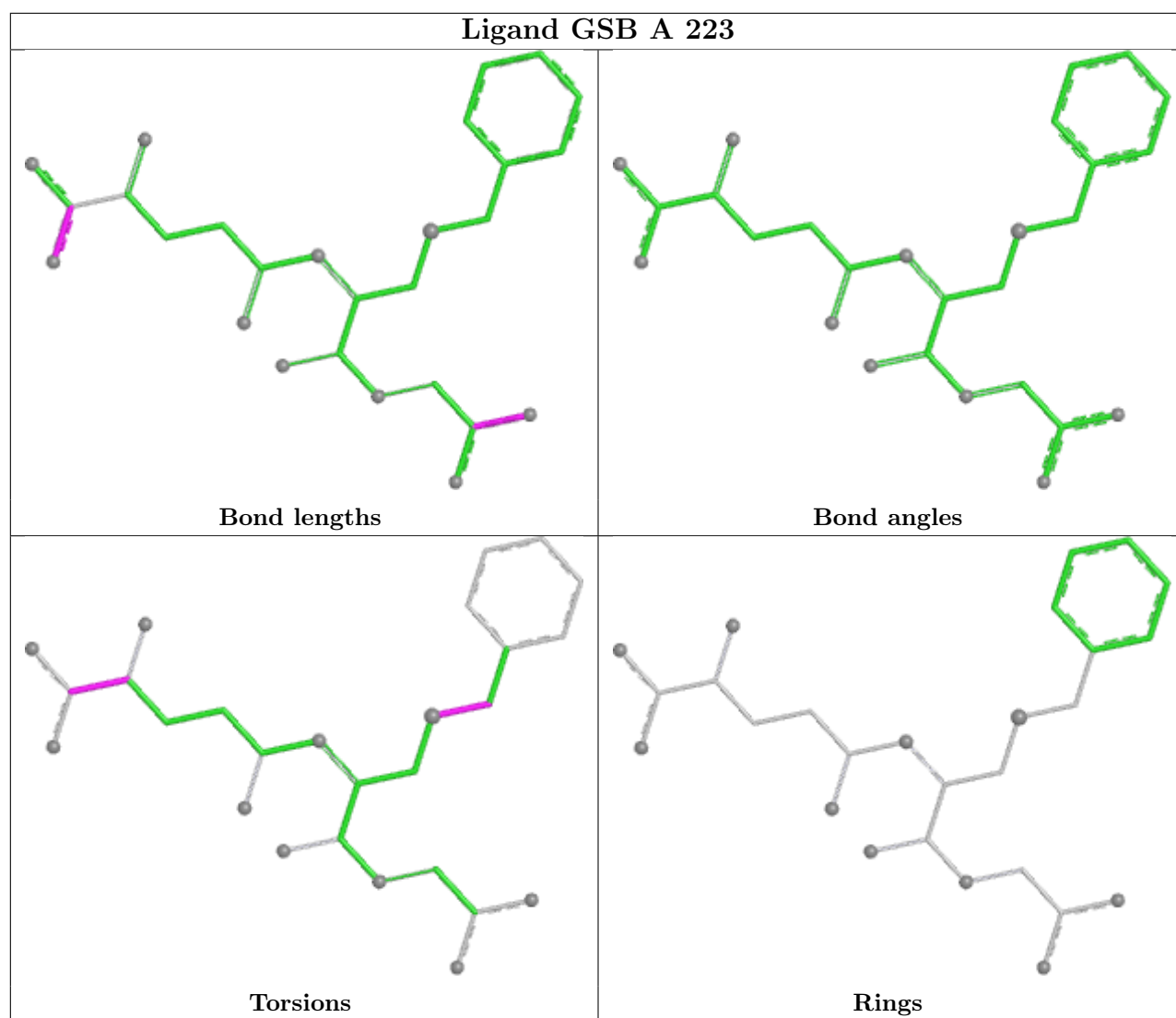
All (8) torsion outliers are listed below:

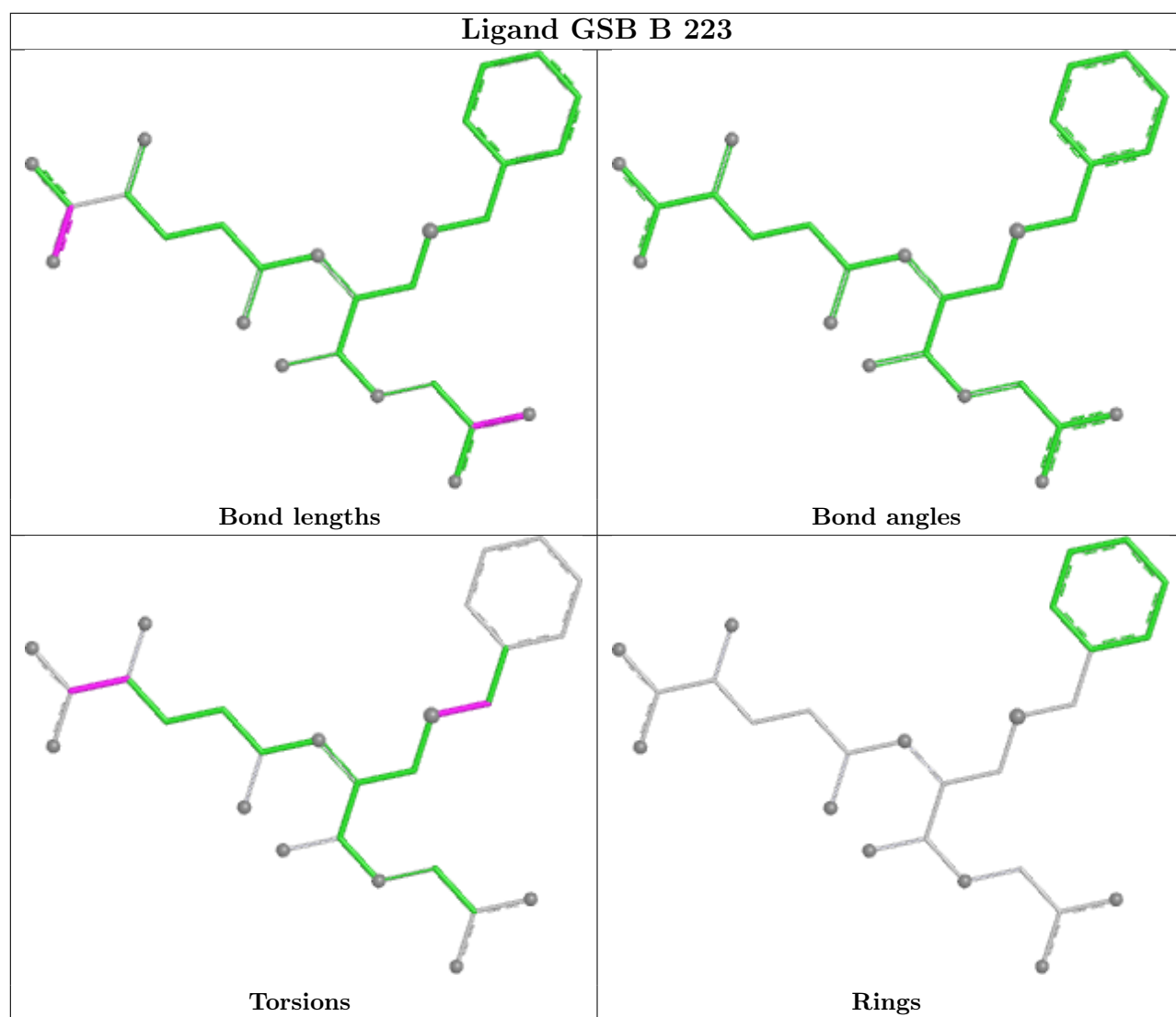
Mol	Chain	Res	Type	Atoms
2	A	223	GSB	C1'-C'-SG2-CB2
2	B	223	GSB	C1'-C'-SG2-CB2
2	C	223	GSB	C1'-C'-SG2-CB2
2	D	223	GSB	C1'-C'-SG2-CB2
2	A	223	GSB	O11-C1-CA1-N1
2	B	223	GSB	O11-C1-CA1-N1
2	C	223	GSB	O11-C1-CA1-N1
2	D	223	GSB	O11-C1-CA1-N1

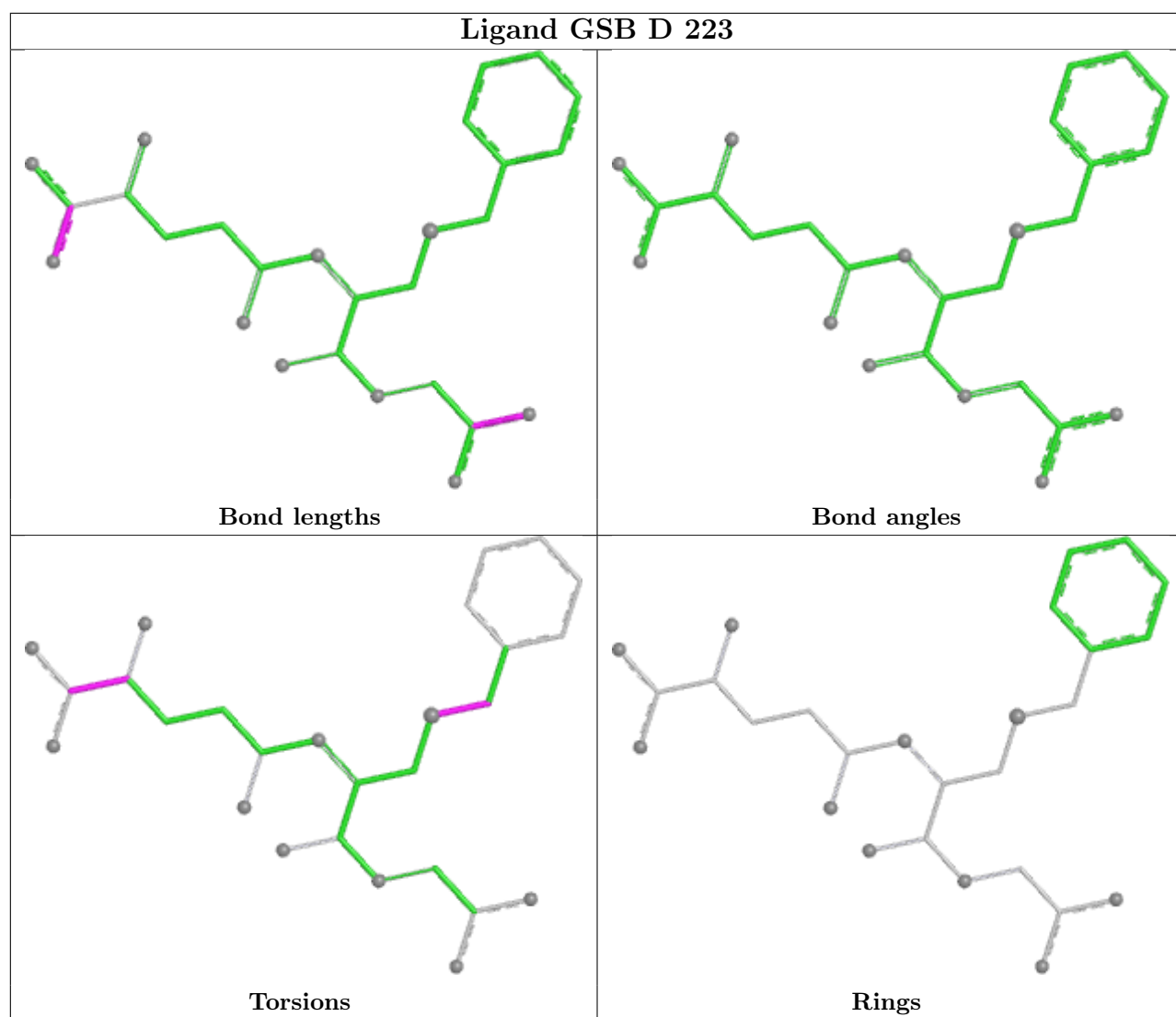
There are no ring outliers.

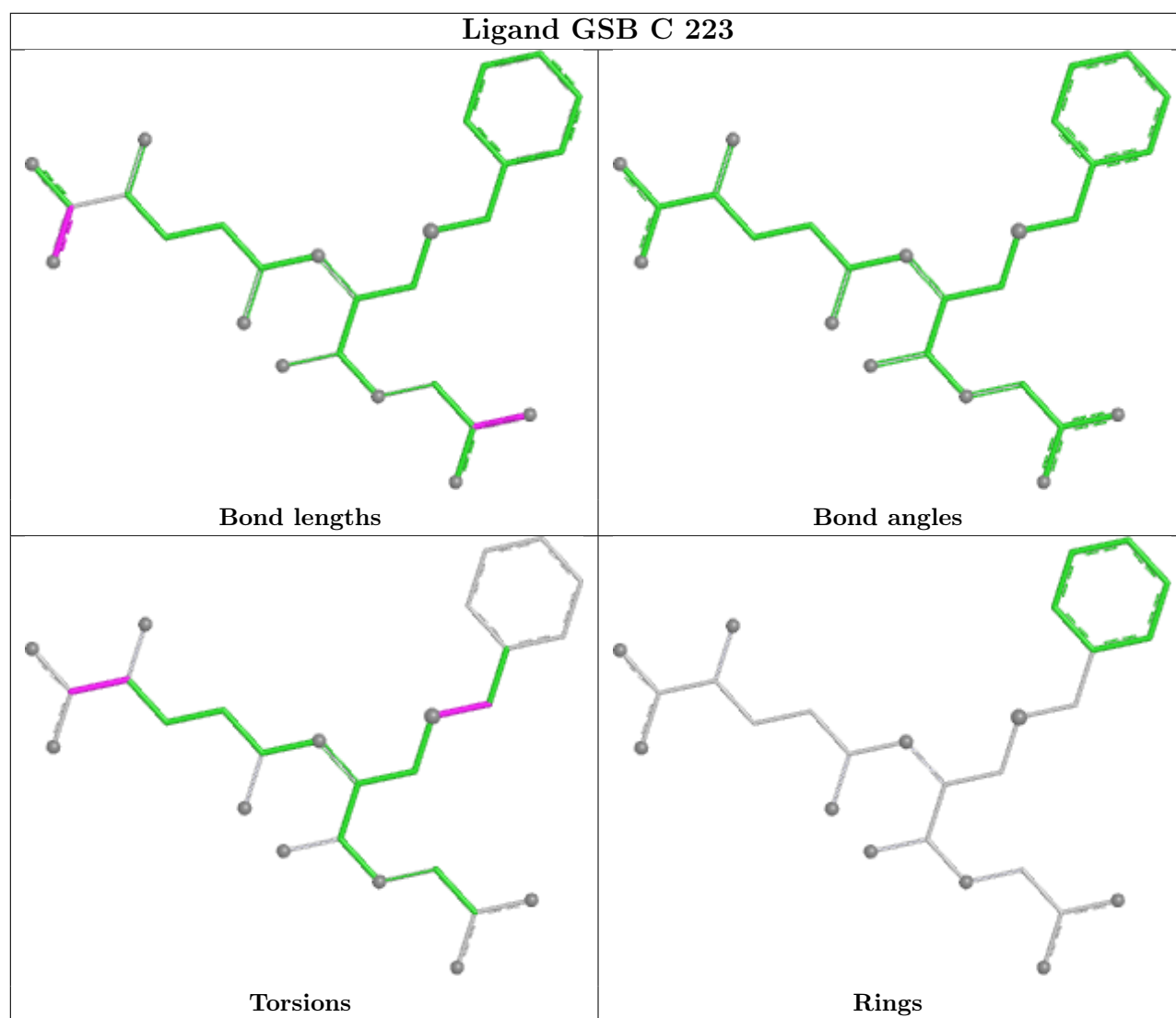
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	221/221 (100%)	0.18	13 (5%) 28 23	2, 27, 76, 132	0
1	B	221/221 (100%)	0.18	11 (4%) 34 28	2, 27, 76, 132	0
1	C	221/221 (100%)	0.29	14 (6%) 26 20	2, 27, 76, 132	0
1	D	221/221 (100%)	0.35	15 (6%) 23 19	2, 27, 76, 132	0
All	All	884/884 (100%)	0.25	53 (5%) 27 22	2, 28, 76, 132	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	PRO	4.2
1	B	116	GLU	3.7
1	D	113	PRO	3.6
1	C	89	ARG	3.4
1	D	43	LYS	3.3
1	A	113	PRO	3.2
1	C	199	GLN	3.2
1	D	66	VAL	3.2
1	A	2	ALA	3.2
1	D	126	GLU	3.2
1	B	89	ARG	2.9
1	D	200	PRO	2.9
1	D	117	LYS	2.9
1	D	2	ALA	2.9
1	B	2	ALA	2.8
1	B	115	GLU	2.8
1	A	199	GLN	2.8
1	B	118	ASP	2.8
1	C	115	GLU	2.8
1	A	117	LYS	2.8
1	C	2	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	211	LYS	2.7
1	D	3	GLU	2.7
1	B	117	LYS	2.6
1	D	199	GLN	2.5
1	D	89	ARG	2.5
1	A	3	GLU	2.5
1	C	126	GLU	2.5
1	C	222	PHE	2.5
1	D	116	GLU	2.5
1	B	199	GLN	2.5
1	D	115	GLU	2.4
1	C	151	ASN	2.4
1	A	112	CYS	2.4
1	C	116	GLU	2.4
1	A	66	VAL	2.4
1	B	120	LYS	2.4
1	B	113	PRO	2.3
1	A	89	ARG	2.3
1	A	114	PRO	2.3
1	A	49	TYR	2.3
1	D	118	ASP	2.3
1	A	210	GLU	2.3
1	C	214	GLU	2.3
1	A	126	GLU	2.2
1	A	217	ARG	2.2
1	B	214	GLU	2.2
1	C	114	PRO	2.2
1	D	114	PRO	2.1
1	B	222	PHE	2.0
1	C	210	GLU	2.0
1	C	120	LYS	2.0
1	C	141	LYS	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

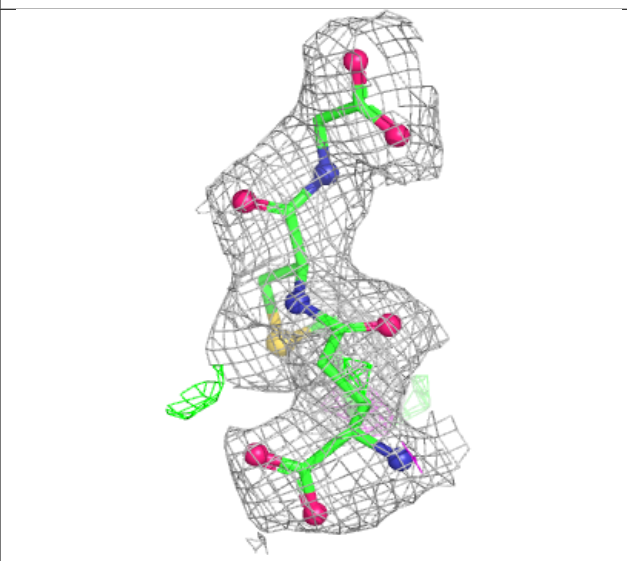
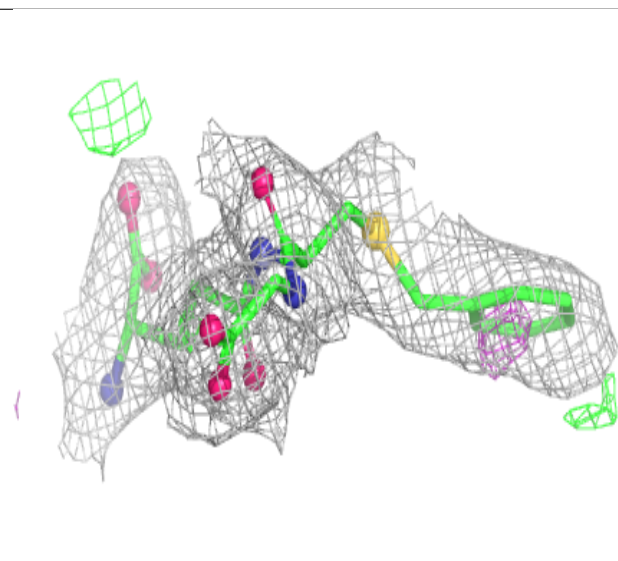
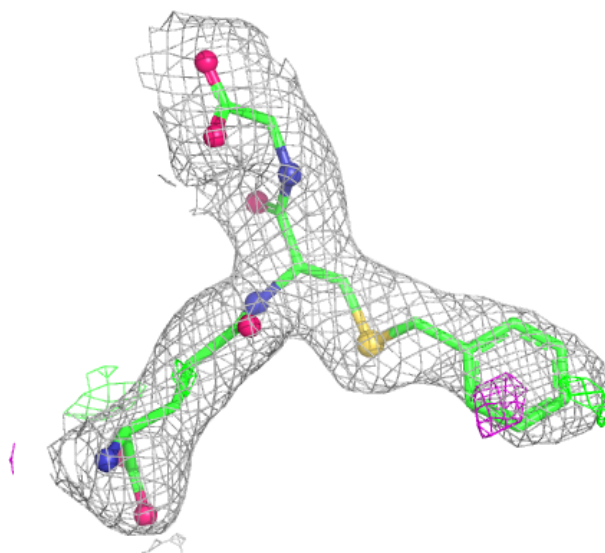
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GSB	A	223	27/27	0.90	0.10	21,21,25,25	0
2	GSB	D	223	27/27	0.92	0.09	21,21,25,25	0
2	GSB	C	223	27/27	0.93	0.08	21,21,25,25	0
2	GSB	B	223	27/27	0.93	0.09	21,21,25,25	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.

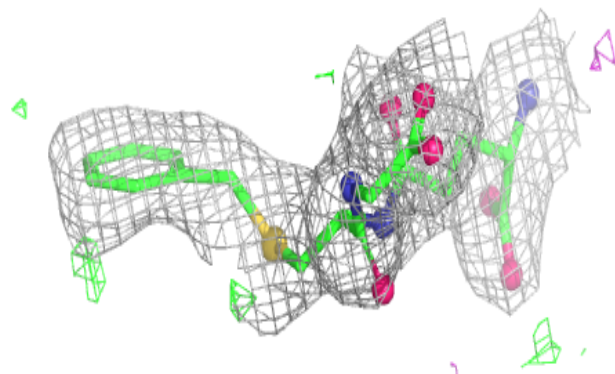
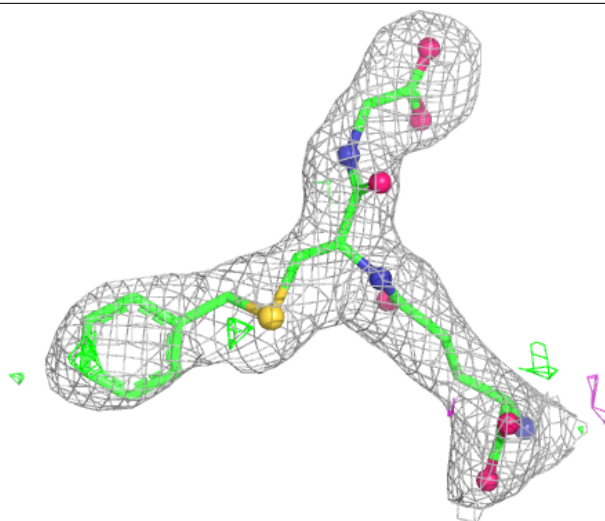
Electron density around GSB A 223:

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



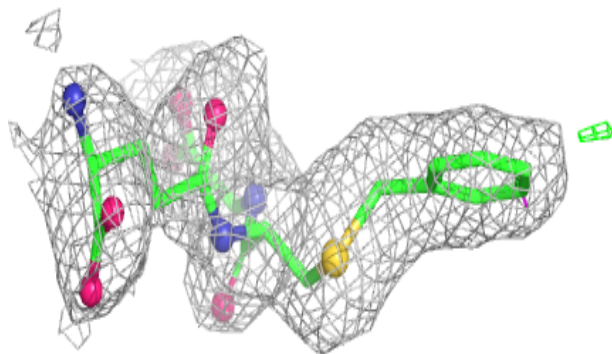
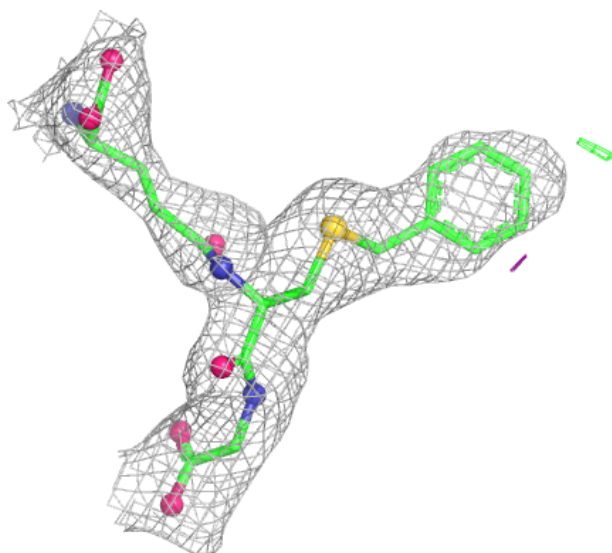
Electron density around GSB D 223:

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



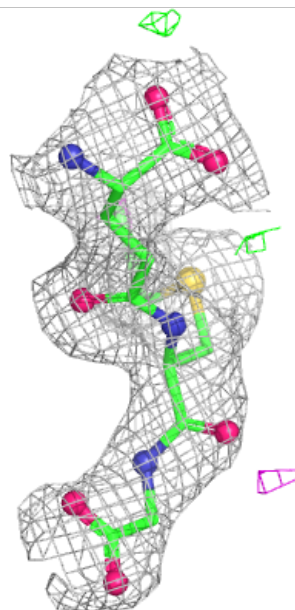
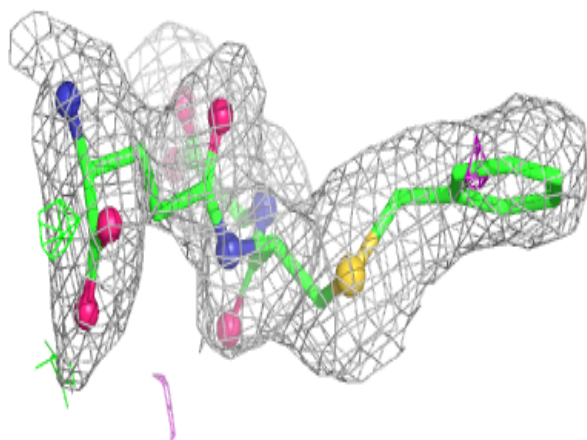
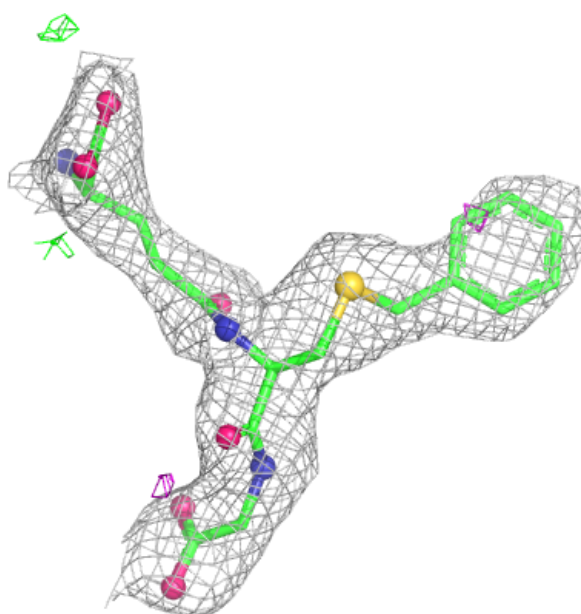
Electron density around GSB C 223:

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



Electron density around GSB B 223:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.