



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:41 pm BST

PDB ID : 5HWL
Title : Human glutathione s-transferase Mu2 complexed with BDEA, monoclinic crystal form
Authors : Zhang, X.; Wei, J.; Wu, S.; Zhang, H.P.; Luo, M.; Yang, X.L.; Liao, F.; Wang, D.Q.
Deposited on : 2016-01-29
Resolution : 1.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

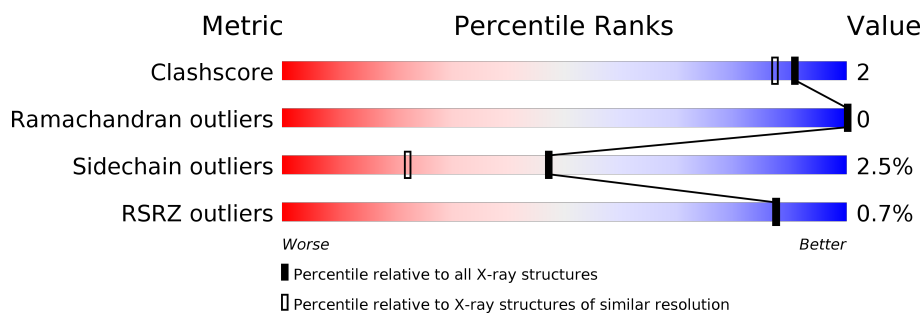
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.60 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	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	217	 28% 69% .
1	B	217	 % 27% 68% .

2 Entry composition [i](#)

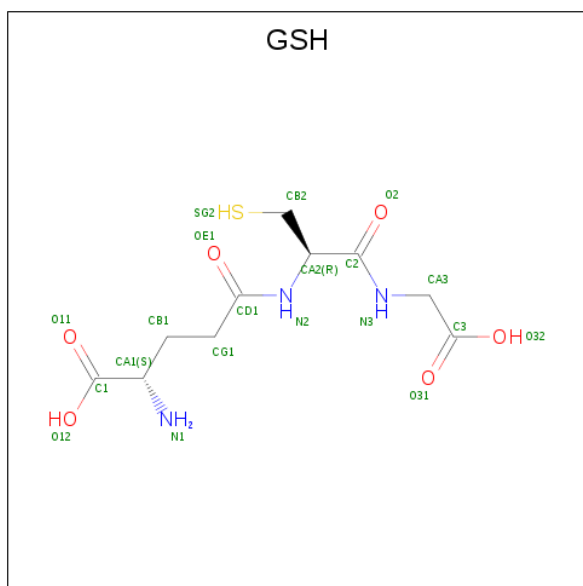
There are 4 unique types of molecules in this entry. The entry contains 3798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mu 2.

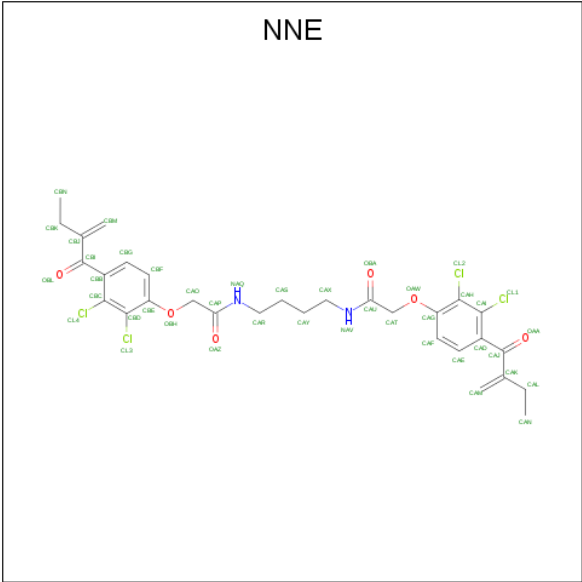
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1729	1128	273	318	10			
1	B	216	Total	C	N	O	S	110	0	0
			1764	1149	287	318	10			

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is N,N'-(butane-1,4-diyl)bis{2-[2,3-dichloro-4-(2-methylidenebutanoyl)phenoxy]acetamide} (three-letter code: NNE) (formula: $C_{30}H_{32}Cl_4N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			42	30	4	2	6		

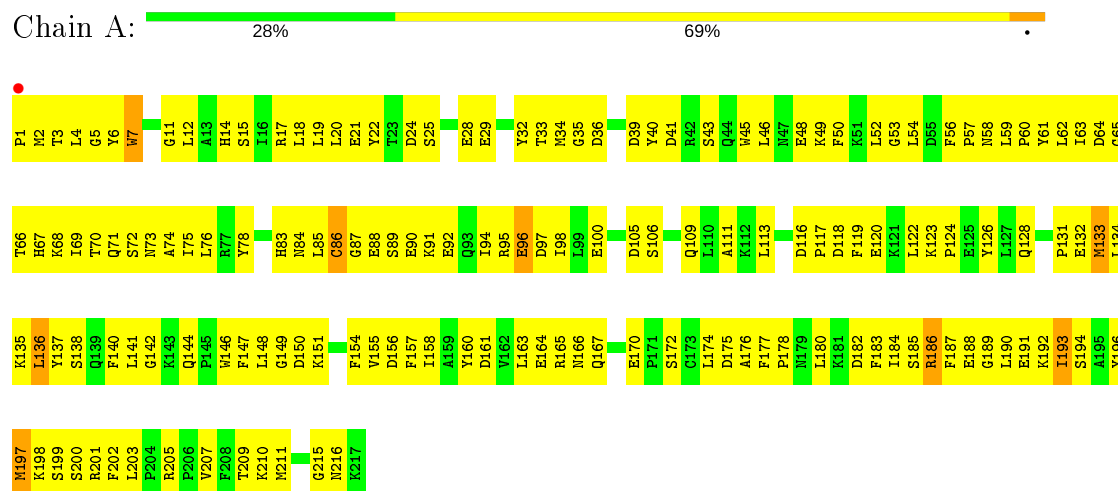
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	88	Total	O	0	0
			88	88		

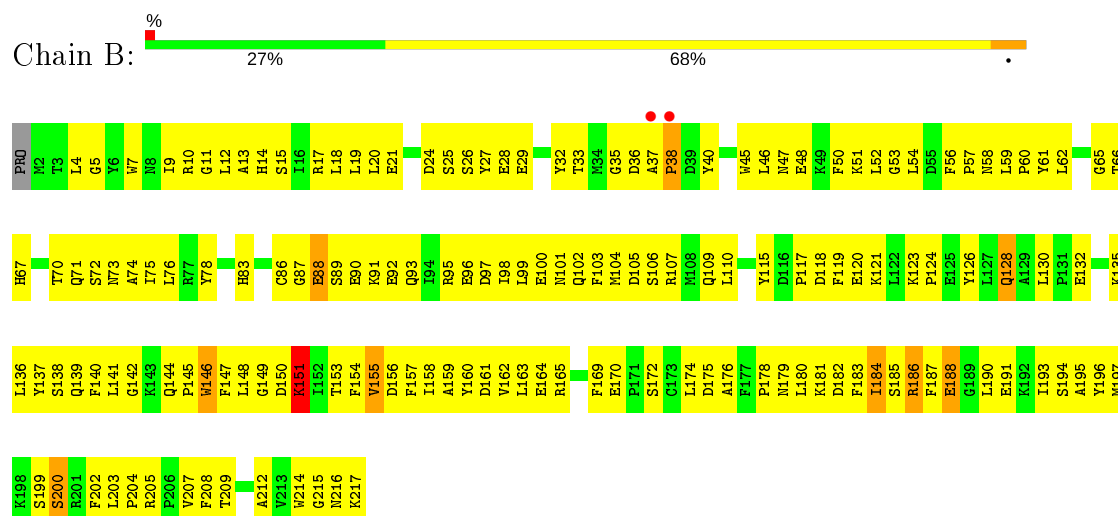
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 Mu 2



• Molecule 1: Glutathione S-transferase Mu 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.97Å 48.89Å 90.99Å 90.00° 93.38° 90.00°	Depositor
Resolution (Å)	45.55 – 1.60 45.55 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.6 (45.55-1.60) 98.8 (45.55-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.178 , 0.205 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3798	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% 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: GSH, NNE

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	3.17	203/1777 (11.4%)	1.51	24/2412 (1.0%)
1	B	3.18	223/1811 (12.3%)	1.51	22/2446 (0.9%)
All	All	3.18	426/3588 (11.9%)	1.51	46/4858 (0.9%)

All (426) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	GLU	CD-OE1	-13.65	1.10	1.25
1	B	92	GLU	CD-OE2	-13.51	1.10	1.25
1	A	45	TRP	CE3-CZ3	-12.90	1.16	1.38
1	A	40	TYR	CE2-CZ	-12.65	1.22	1.38
1	B	53	GLY	C-O	-12.41	1.03	1.23
1	B	21	GLU	CD-OE1	-12.22	1.12	1.25
1	A	40	TYR	CG-CD1	-12.17	1.23	1.39
1	A	100	GLU	CD-OE2	-12.04	1.12	1.25
1	B	21	GLU	CD-OE2	-12.00	1.12	1.25
1	B	164	GLU	CD-OE1	-11.81	1.12	1.25
1	B	48	GLU	CD-OE1	-11.81	1.12	1.25
1	B	40	TYR	CE2-CZ	-11.72	1.23	1.38
1	A	164	GLU	CD-OE1	-11.59	1.12	1.25
1	A	96	GLU	CD-OE2	-11.51	1.12	1.25
1	A	43	SER	CB-OG	-11.43	1.27	1.42
1	A	90	GLU	CD-OE2	-11.34	1.13	1.25
1	A	29	GLU	CD-OE2	-11.21	1.13	1.25
1	B	207	VAL	C-O	-11.18	1.02	1.23
1	A	149	GLY	C-O	-10.80	1.06	1.23
1	B	170	GLU	CD-OE1	-10.76	1.13	1.25
1	B	128	GLN	C-O	-10.71	1.03	1.23
1	A	188	GLU	CD-OE2	-10.47	1.14	1.25
1	A	87	GLY	C-O	-10.43	1.06	1.23
1	B	29	GLU	CD-OE1	-10.38	1.14	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	TYR	CG-CD1	-10.33	1.25	1.39
1	B	90	GLU	CD-OE2	-10.26	1.14	1.25
1	B	61	TYR	CE1-CZ	-10.20	1.25	1.38
1	A	61	TYR	CE1-CZ	-10.13	1.25	1.38
1	B	40	TYR	CG-CD1	-10.13	1.25	1.39
1	A	201	ARG	CZ-NH1	-10.12	1.19	1.33
1	A	199	SER	CB-OG	-10.10	1.29	1.42
1	B	188	GLU	CD-OE2	-10.07	1.14	1.25
1	B	87	GLY	C-O	-9.99	1.07	1.23
1	A	48	GLU	CD-OE2	-9.94	1.14	1.25
1	B	149	GLY	C-O	-9.90	1.07	1.23
1	B	90	GLU	CD-OE1	-9.83	1.14	1.25
1	A	155	VAL	CB-CG1	-9.77	1.32	1.52
1	A	56	PHE	C-O	-9.69	1.04	1.23
1	B	194	SER	CB-OG	-9.63	1.29	1.42
1	A	142	GLY	C-O	-9.49	1.08	1.23
1	A	92	GLU	CD-OE1	-9.47	1.15	1.25
1	B	96	GLU	CD-OE1	-9.44	1.15	1.25
1	A	60	PRO	C-O	-9.42	1.04	1.23
1	B	106	SER	CB-OG	-9.42	1.30	1.42
1	A	90	GLU	CD-OE1	-9.38	1.15	1.25
1	B	78	TYR	CE1-CZ	-9.37	1.26	1.38
1	A	61	TYR	CG-CD2	-9.27	1.27	1.39
1	B	172	SER	CB-OG	-9.24	1.30	1.42
1	A	73	ASN	C-O	-9.23	1.05	1.23
1	A	160	TYR	CG-CD2	-9.22	1.27	1.39
1	A	72	SER	C-O	-9.21	1.05	1.23
1	B	36	ASP	C-O	-9.20	1.05	1.23
1	A	53	GLY	C-O	-9.17	1.08	1.23
1	A	207	VAL	C-O	-9.15	1.05	1.23
1	A	98	ILE	C-O	-9.09	1.06	1.23
1	B	185	SER	CB-OG	-9.08	1.30	1.42
1	B	25	SER	CB-OG	-9.06	1.30	1.42
1	A	100	GLU	CD-OE1	-9.05	1.15	1.25
1	B	120	GLU	CD-OE1	-9.01	1.15	1.25
1	B	137	TYR	C-O	-8.99	1.06	1.23
1	B	163	LEU	C-O	-8.95	1.06	1.23
1	A	126	TYR	CG-CD2	-8.94	1.27	1.39
1	B	58	ASN	C-O	-8.94	1.06	1.23
1	B	124	PRO	C-O	-8.92	1.05	1.23
1	B	88	GLU	C-O	-8.92	1.06	1.23
1	B	205	ARG	C-O	-8.88	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLY	C-O	-8.81	1.09	1.23
1	A	184	ILE	C-O	-8.79	1.06	1.23
1	A	109	GLN	C-O	-8.79	1.06	1.23
1	A	203	LEU	C-O	-8.74	1.06	1.23
1	B	15	SER	C-O	-8.67	1.06	1.23
1	B	40	TYR	CZ-OH	-8.63	1.23	1.37
1	B	146	TRP	CE3-CZ3	-8.62	1.23	1.38
1	B	140	PHE	C-O	-8.59	1.07	1.23
1	B	74	ALA	C-O	-8.58	1.07	1.23
1	A	151	LYS	C-O	-8.53	1.07	1.23
1	B	73	ASN	C-O	-8.52	1.07	1.23
1	A	170	GLU	CD-OE2	-8.47	1.16	1.25
1	B	190	LEU	C-O	-8.47	1.07	1.23
1	A	72	SER	CB-OG	-8.45	1.31	1.42
1	B	100	GLU	CD-OE2	-8.44	1.16	1.25
1	B	100	GLU	CD-OE1	-8.44	1.16	1.25
1	A	1	PRO	C-O	-8.44	1.06	1.23
1	B	170	GLU	C-O	-8.35	1.07	1.23
1	A	205	ARG	C-O	-8.34	1.07	1.23
1	A	191	GLU	CD-OE1	-8.34	1.16	1.25
1	B	19	LEU	C-O	-8.33	1.07	1.23
1	A	96	GLU	CD-OE1	-8.32	1.16	1.25
1	B	56	PHE	C-O	-8.26	1.07	1.23
1	A	14	HIS	C-O	-8.25	1.07	1.23
1	A	209	THR	C-O	-8.25	1.07	1.23
1	B	29	GLU	CD-OE2	-8.23	1.16	1.25
1	B	144	GLN	C-O	-8.22	1.07	1.23
1	B	107	ARG	C-O	-8.22	1.07	1.23
1	B	105	ASP	C-O	-8.20	1.07	1.23
1	A	189	GLY	C-O	-8.16	1.10	1.23
1	B	188	GLU	CD-OE1	-8.13	1.16	1.25
1	A	177	PHE	C-O	-8.11	1.07	1.23
1	B	89	SER	CB-OG	-8.09	1.31	1.42
1	B	65	GLY	C-O	-8.07	1.10	1.23
1	B	157	PHE	C-O	-8.04	1.08	1.23
1	A	68	LYS	C-O	-7.99	1.08	1.23
1	B	52	LEU	C-O	-7.96	1.08	1.23
1	A	25	SER	C-O	-7.94	1.08	1.23
1	B	45	TRP	CE2-CZ2	-7.93	1.26	1.39
1	B	78	TYR	C-O	-7.93	1.08	1.23
1	A	78	TYR	CG-CD2	-7.92	1.28	1.39
1	A	134	LEU	C-O	-7.92	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	TYR	CG-CD2	-7.90	1.28	1.39
1	B	95	ARG	C-O	-7.89	1.08	1.23
1	B	184	ILE	C-O	-7.89	1.08	1.23
1	A	106	SER	CB-OG	-7.88	1.32	1.42
1	A	123	LYS	C-O	-7.87	1.08	1.23
1	A	146	TRP	CE3-CZ3	-7.85	1.25	1.38
1	B	174	LEU	C-O	-7.85	1.08	1.23
1	A	140	PHE	CD1-CE1	-7.83	1.23	1.39
1	B	72	SER	C-O	-7.83	1.08	1.23
1	B	102	GLN	C-O	-7.80	1.08	1.23
1	A	19	LEU	C-O	-7.80	1.08	1.23
1	B	54	LEU	C-O	-7.78	1.08	1.23
1	B	196	TYR	CG-CD2	-7.76	1.29	1.39
1	A	66	THR	C-O	-7.74	1.08	1.23
1	A	161	ASP	C-O	-7.73	1.08	1.23
1	A	190	LEU	C-O	-7.72	1.08	1.23
1	A	21	GLU	CD-OE1	-7.70	1.17	1.25
1	A	67	HIS	C-O	-7.68	1.08	1.23
1	B	191	GLU	C-O	-7.66	1.08	1.23
1	A	194	SER	CB-OG	-7.66	1.32	1.42
1	B	199	SER	CB-OG	-7.65	1.32	1.42
1	B	142	GLY	C-O	-7.65	1.11	1.23
1	B	209	THR	C-O	-7.63	1.08	1.23
1	B	180	LEU	C-O	-7.58	1.08	1.23
1	A	33	THR	C-O	-7.57	1.08	1.23
1	A	183	PHE	CG-CD2	-7.56	1.27	1.38
1	A	128	GLN	C-O	-7.55	1.09	1.23
1	B	109	GLN	C-O	-7.55	1.09	1.23
1	A	28	GLU	C-O	-7.55	1.09	1.23
1	A	111	ALA	C-O	-7.52	1.09	1.23
1	B	187	PHE	C-O	-7.52	1.09	1.23
1	B	135	LYS	C-O	-7.52	1.09	1.23
1	B	78	TYR	CG-CD2	-7.50	1.29	1.39
1	B	212	ALA	C-O	-7.50	1.09	1.23
1	A	216	ASN	CG-ND2	-7.48	1.14	1.32
1	A	120	GLU	CD-OE2	-7.48	1.17	1.25
1	B	132	GLU	C-O	-7.43	1.09	1.23
1	B	158	ILE	C-O	-7.43	1.09	1.23
1	A	83	HIS	C-O	-7.43	1.09	1.23
1	A	20	LEU	C-O	-7.42	1.09	1.23
1	B	25	SER	C-O	-7.41	1.09	1.23
1	A	15	SER	C-O	-7.41	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	TYR	C-O	-7.38	1.09	1.23
1	B	50	PHE	CG-CD2	-7.38	1.27	1.38
1	A	73	ASN	CG-OD1	-7.37	1.07	1.24
1	A	70	THR	C-O	-7.37	1.09	1.23
1	A	193	ILE	C-O	-7.36	1.09	1.23
1	A	95	ARG	C-O	-7.36	1.09	1.23
1	B	169	PHE	CG-CD1	-7.35	1.27	1.38
1	B	120	GLU	C-O	-7.34	1.09	1.23
1	B	45	TRP	CZ3-CH2	-7.34	1.28	1.40
1	B	216	ASN	C-O	-7.32	1.09	1.23
1	B	89	SER	C-O	-7.29	1.09	1.23
1	A	146	TRP	C-O	-7.25	1.09	1.23
1	A	116	ASP	C-O	-7.24	1.09	1.23
1	B	141	LEU	C-O	-7.22	1.09	1.23
1	A	137	TYR	C-O	-7.22	1.09	1.23
1	B	160	TYR	CG-CD2	-7.21	1.29	1.39
1	A	88	GLU	C-O	-7.20	1.09	1.23
1	A	63	ILE	C-O	-7.19	1.09	1.23
1	B	197	MET	C-O	-7.19	1.09	1.23
1	B	48	GLU	C-O	-7.18	1.09	1.23
1	A	5	GLY	C-O	-7.18	1.12	1.23
1	A	12	LEU	C-O	-7.15	1.09	1.23
1	A	76	LEU	C-O	-7.11	1.09	1.23
1	B	202	PHE	CG-CD1	-7.11	1.28	1.38
1	A	91	LYS	C-O	-7.10	1.09	1.23
1	A	50	PHE	C-O	-7.10	1.09	1.23
1	B	217	LYS	C-O	-7.09	1.09	1.23
1	B	67	HIS	C-O	-7.08	1.09	1.23
1	A	15	SER	CB-OG	-7.07	1.33	1.42
1	A	200	SER	C-O	-7.07	1.09	1.23
1	B	86	CYS	C-O	-7.04	1.09	1.23
1	A	180	LEU	C-O	-7.04	1.09	1.23
1	A	78	TYR	C-O	-7.02	1.10	1.23
1	B	138	SER	CB-OG	-7.02	1.33	1.42
1	B	139	GLN	C-O	-7.02	1.10	1.23
1	B	115	TYR	CE1-CZ	-6.99	1.29	1.38
1	B	193	ILE	C-O	-6.99	1.10	1.23
1	A	75	ILE	C-O	-6.96	1.10	1.23
1	B	151	LYS	C-O	-6.95	1.10	1.23
1	A	59	LEU	C-O	-6.93	1.10	1.23
1	B	73	ASN	CG-OD1	-6.90	1.08	1.24
1	A	191	GLU	CD-OE2	-6.88	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	TYR	CE1-CZ	-6.86	1.29	1.38
1	B	57	PRO	N-CD	6.86	1.57	1.47
1	A	172	SER	CB-OG	-6.85	1.33	1.42
1	A	120	GLU	C-O	-6.84	1.10	1.23
1	A	140	PHE	CG-CD1	-6.83	1.28	1.38
1	B	115	TYR	CG-CD2	-6.83	1.30	1.39
1	A	201	ARG	C-O	-6.82	1.10	1.23
1	A	32	TYR	CE1-CZ	-6.82	1.29	1.38
1	B	45	TRP	CD2-CE2	-6.80	1.33	1.41
1	B	14	HIS	C-O	-6.79	1.10	1.23
1	B	35	GLY	C-O	-6.79	1.12	1.23
1	B	12	LEU	C-O	-6.76	1.10	1.23
1	B	187	PHE	CG-CD2	-6.76	1.28	1.38
1	A	18	LEU	C-O	-6.76	1.10	1.23
1	B	96	GLU	C-O	-6.75	1.10	1.23
1	B	214	TRP	C-O	-6.75	1.10	1.23
1	A	170	GLU	C-O	-6.74	1.10	1.23
1	A	174	LEU	C-O	-6.72	1.10	1.23
1	B	154	PHE	C-O	-6.71	1.10	1.23
1	B	72	SER	CB-OG	-6.70	1.33	1.42
1	B	140	PHE	CB-CG	-6.70	1.40	1.51
1	A	4	LEU	C-O	-6.69	1.10	1.23
1	B	5	GLY	C-O	-6.68	1.12	1.23
1	A	138	SER	C-O	-6.68	1.10	1.23
1	A	182	ASP	CG-OD1	-6.68	1.09	1.25
1	A	45	TRP	C-O	-6.68	1.10	1.23
1	B	48	GLU	CD-OE2	-6.66	1.18	1.25
1	A	138	SER	CB-OG	-6.65	1.33	1.42
1	A	166	ASN	CG-OD1	-6.62	1.09	1.24
1	B	92	GLU	CD-OE1	-6.62	1.18	1.25
1	B	97	ASP	C-O	-6.60	1.10	1.23
1	B	96	GLU	CD-OE2	-6.60	1.18	1.25
1	A	96	GLU	C-O	-6.58	1.10	1.23
1	A	197	MET	C-O	-6.57	1.10	1.23
1	A	186	ARG	CZ-NH2	-6.56	1.24	1.33
1	A	64	ASP	CG-OD2	-6.54	1.10	1.25
1	B	58	ASN	CG-OD1	-6.53	1.09	1.24
1	A	40	TYR	CG-CD2	-6.53	1.30	1.39
1	B	45	TRP	C-O	-6.53	1.10	1.23
1	A	156	ASP	C-O	-6.50	1.11	1.23
1	B	50	PHE	CE2-CZ	-6.48	1.25	1.37
1	A	183	PHE	C-O	-6.47	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	GLU	C-O	-6.44	1.11	1.23
1	A	32	TYR	C-O	-6.43	1.11	1.23
1	B	36	ASP	CG-OD2	-6.43	1.10	1.25
1	A	187	PHE	C-O	-6.43	1.11	1.23
1	B	160	TYR	CE1-CZ	-6.42	1.30	1.38
1	B	61	TYR	CG-CD2	-6.41	1.30	1.39
1	B	17	ARG	C-O	-6.41	1.11	1.23
1	B	215	GLY	C-O	-6.40	1.13	1.23
1	B	48	GLU	CB-CG	-6.39	1.40	1.52
1	B	24	ASP	CG-OD2	-6.38	1.10	1.25
1	A	164	GLU	C-O	-6.36	1.11	1.23
1	B	204	PRO	N-CD	6.34	1.56	1.47
1	A	7	TRP	CZ3-CH2	-6.33	1.29	1.40
1	B	164	GLU	CD-OE2	-6.32	1.18	1.25
1	A	166	ASN	C-O	-6.28	1.11	1.23
1	A	188	GLU	CD-OE1	-6.27	1.18	1.25
1	A	28	GLU	CB-CG	-6.27	1.40	1.52
1	A	160	TYR	C-O	-6.27	1.11	1.23
1	B	46	LEU	C-O	-6.26	1.11	1.23
1	A	163	LEU	C-O	-6.26	1.11	1.23
1	A	202	PHE	C-O	-6.26	1.11	1.23
1	B	93	GLN	C-O	-6.25	1.11	1.23
1	B	202	PHE	C-O	-6.25	1.11	1.23
1	B	155	VAL	C-O	-6.21	1.11	1.23
1	A	161	ASP	CG-OD1	-6.21	1.11	1.25
1	A	210	LYS	C-O	-6.20	1.11	1.23
1	A	200	SER	CB-OG	-6.17	1.34	1.42
1	B	10	ARG	C-O	-6.16	1.11	1.23
1	B	151	LYS	N-CA	-6.16	1.34	1.46
1	A	22	TYR	C-O	-6.15	1.11	1.23
1	B	59	LEU	C-O	-6.14	1.11	1.23
1	B	155	VAL	CB-CG1	-6.12	1.40	1.52
1	B	119	PHE	C-O	-6.12	1.11	1.23
1	B	195	ALA	C-O	-6.12	1.11	1.23
1	B	179	ASN	C-O	-6.12	1.11	1.23
1	B	50	PHE	CG-CD1	-6.10	1.29	1.38
1	B	4	LEU	C-O	-6.08	1.11	1.23
1	A	86	CYS	C-O	-6.07	1.11	1.23
1	B	27	TYR	C-O	-6.06	1.11	1.23
1	A	3	THR	C-O	-6.06	1.11	1.23
1	B	186	ARG	C-O	-6.03	1.11	1.23
1	B	78	TYR	CG-CD1	-6.03	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	SER	C-O	-6.02	1.11	1.23
1	A	52	LEU	C-O	-6.02	1.11	1.23
1	B	103	PHE	C-O	-6.01	1.11	1.23
1	B	121	LYS	C-O	-6.00	1.11	1.23
1	B	17	ARG	CZ-NH1	-5.99	1.25	1.33
1	A	150	ASP	C-O	-5.98	1.11	1.23
1	A	58	ASN	C-O	-5.97	1.12	1.23
1	A	144	GLN	CD-NE2	-5.96	1.18	1.32
1	A	62	LEU	C-O	-5.95	1.12	1.23
1	B	159	ALA	C-O	-5.95	1.12	1.23
1	B	45	TRP	CG-CD1	-5.95	1.28	1.36
1	A	196	TYR	CZ-OH	-5.91	1.27	1.37
1	B	145	PRO	C-O	-5.91	1.11	1.23
1	A	140	PHE	C-O	-5.90	1.12	1.23
1	B	33	THR	C-O	-5.90	1.12	1.23
1	B	60	PRO	C-O	-5.89	1.11	1.23
1	A	135	LYS	C-O	-5.88	1.12	1.23
1	B	183	PHE	CG-CD2	-5.88	1.29	1.38
1	B	45	TRP	CE3-CZ3	-5.88	1.28	1.38
1	B	144	GLN	CD-NE2	-5.88	1.18	1.32
1	B	194	SER	C-O	-5.87	1.12	1.23
1	A	167	GLN	C-O	-5.86	1.12	1.23
1	A	157	PHE	CD2-CE2	-5.86	1.27	1.39
1	B	148	LEU	C-O	-5.85	1.12	1.23
1	B	146	TRP	C-O	-5.84	1.12	1.23
1	B	7	TRP	CZ3-CH2	-5.82	1.30	1.40
1	B	101	ASN	C-O	-5.81	1.12	1.23
1	B	98	ILE	C-O	-5.80	1.12	1.23
1	A	34	MET	C-O	-5.79	1.12	1.23
1	B	146	TRP	CD1-NE1	-5.79	1.28	1.38
1	A	183	PHE	CE1-CZ	-5.79	1.26	1.37
1	A	140	PHE	CG-CD2	-5.78	1.30	1.38
1	B	71	GLN	C-O	-5.78	1.12	1.23
1	B	97	ASP	CG-OD1	-5.78	1.12	1.25
1	B	176	ALA	C-O	-5.78	1.12	1.23
1	A	41	ASP	CG-OD2	-5.77	1.12	1.25
1	A	192	LYS	C-O	-5.77	1.12	1.23
1	A	78	TYR	CE1-CZ	-5.77	1.31	1.38
1	A	71	GLN	CD-OE1	-5.75	1.11	1.24
1	B	40	TYR	C-O	-5.75	1.12	1.23
1	A	11	GLY	C-O	-5.75	1.14	1.23
1	A	84	ASN	C-O	-5.75	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	HIS	CA-CB	-5.75	1.41	1.53
1	A	58	ASN	CG-OD1	-5.74	1.11	1.24
1	A	119	PHE	CG-CD2	-5.73	1.30	1.38
1	A	147	PHE	CG-CD1	-5.71	1.30	1.38
1	B	66	THR	C-O	-5.71	1.12	1.23
1	A	54	LEU	C-O	-5.69	1.12	1.23
1	B	161	ASP	C-O	-5.67	1.12	1.23
1	B	160	TYR	C-O	-5.67	1.12	1.23
1	B	100	GLU	C-O	-5.67	1.12	1.23
1	A	74	ALA	C-O	-5.67	1.12	1.23
1	B	91	LYS	C-O	-5.66	1.12	1.23
1	A	48	GLU	C-O	-5.66	1.12	1.23
1	A	118	ASP	CG-OD2	-5.66	1.12	1.25
1	A	36	ASP	C-O	-5.65	1.12	1.23
1	B	147	PHE	C-O	-5.65	1.12	1.23
1	A	35	GLY	C-O	-5.64	1.14	1.23
1	A	175	ASP	CG-OD2	-5.63	1.12	1.25
1	A	136	LEU	C-O	-5.63	1.12	1.23
1	B	9	ILE	C-O	-5.63	1.12	1.23
1	A	176	ALA	C-O	-5.61	1.12	1.23
1	A	158	ILE	C-O	-5.61	1.12	1.23
1	B	202	PHE	CD1-CE1	-5.60	1.28	1.39
1	A	131	PRO	C-O	-5.60	1.12	1.23
1	B	61	TYR	C-O	-5.57	1.12	1.23
1	B	200	SER	CB-OG	-5.57	1.35	1.42
1	B	11	GLY	C-O	-5.57	1.14	1.23
1	B	136	LEU	C-O	-5.54	1.12	1.23
1	A	124	PRO	N-CD	5.54	1.55	1.47
1	B	115	TYR	CG-CD1	-5.53	1.31	1.39
1	B	106	SER	C-O	-5.53	1.12	1.23
1	A	89	SER	CB-OG	-5.53	1.35	1.42
1	A	185	SER	CB-OG	-5.51	1.35	1.42
1	B	50	PHE	CD2-CE2	-5.50	1.28	1.39
1	B	102	GLN	CD-NE2	-5.50	1.19	1.32
1	B	178	PRO	C-O	-5.49	1.12	1.23
1	B	93	GLN	CD-OE1	-5.49	1.11	1.24
1	B	126	TYR	C-O	-5.49	1.12	1.23
1	B	197	MET	N-CA	-5.48	1.35	1.46
1	A	140	PHE	CB-CG	-5.47	1.42	1.51
1	B	99	LEU	C-O	-5.45	1.12	1.23
1	A	39	ASP	CG-OD1	-5.45	1.12	1.25
1	A	160	TYR	CD2-CE2	-5.45	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	MET	C-O	-5.44	1.13	1.23
1	A	89	SER	C-O	-5.44	1.13	1.23
1	A	40	TYR	CE1-CZ	-5.42	1.31	1.38
1	A	154	PHE	C-O	-5.41	1.13	1.23
1	B	70	THR	C-O	-5.41	1.13	1.23
1	A	215	GLY	C-O	-5.40	1.15	1.23
1	B	76	LEU	C-O	-5.39	1.13	1.23
1	B	13	ALA	C-O	-5.39	1.13	1.23
1	B	185	SER	C-O	-5.39	1.13	1.23
1	A	61	TYR	C-O	-5.38	1.13	1.23
1	B	172	SER	C-O	-5.37	1.13	1.23
1	A	78	TYR	CD2-CE2	-5.37	1.31	1.39
1	B	88	GLU	CA-CB	-5.37	1.42	1.53
1	A	198	LYS	CB-CG	-5.36	1.38	1.52
1	B	156	ASP	C-O	-5.36	1.13	1.23
1	A	49	LYS	C-O	-5.35	1.13	1.23
1	B	162	VAL	C-O	-5.34	1.13	1.23
1	B	26	SER	CB-OG	-5.34	1.35	1.42
1	B	7	TRP	CD2-CE2	-5.33	1.34	1.41
1	B	208	PHE	CG-CD2	-5.33	1.30	1.38
1	B	107	ARG	CZ-NH2	-5.31	1.26	1.33
1	A	41	ASP	C-O	-5.31	1.13	1.23
1	A	46	LEU	C-O	-5.30	1.13	1.23
1	B	75	ILE	C-O	-5.30	1.13	1.23
1	A	33	THR	CB-OG1	-5.29	1.32	1.43
1	B	28	GLU	N-CA	-5.28	1.35	1.46
1	A	69	ILE	C-O	-5.28	1.13	1.23
1	B	83	HIS	C-O	-5.27	1.13	1.23
1	B	21	GLU	CB-CG	-5.26	1.42	1.52
1	B	196	TYR	C-O	-5.26	1.13	1.23
1	A	71	GLN	C-O	-5.25	1.13	1.23
1	A	116	ASP	CG-OD2	-5.23	1.13	1.25
1	B	104	MET	C-O	-5.23	1.13	1.23
1	B	165	ARG	C-O	-5.22	1.13	1.23
1	B	57	PRO	C-O	-5.22	1.12	1.23
1	A	17	ARG	C-O	-5.21	1.13	1.23
1	B	140	PHE	CG-CD1	-5.20	1.30	1.38
1	A	36	ASP	CG-OD1	-5.19	1.13	1.25
1	A	64	ASP	C-O	-5.19	1.13	1.23
1	B	137	TYR	CG-CD2	-5.18	1.32	1.39
1	B	181	LYS	C-O	-5.17	1.13	1.23
1	A	41	ASP	CG-OD1	-5.16	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	PHE	CG-CD1	-5.15	1.31	1.38
1	A	94	ILE	C-O	-5.13	1.13	1.23
1	B	170	GLU	CD-OE2	-5.12	1.20	1.25
1	B	157	PHE	CD1-CE1	-5.11	1.29	1.39
1	B	203	LEU	C-O	-5.10	1.13	1.23
1	A	175	ASP	C-O	-5.10	1.13	1.23
1	B	32	TYR	CD2-CE2	-5.09	1.31	1.39
1	A	216	ASN	CG-OD1	-5.09	1.12	1.24
1	B	182	ASP	C-O	-5.08	1.13	1.23
1	A	57	PRO	N-CD	5.08	1.54	1.47
1	B	92	GLU	C-O	-5.06	1.13	1.23
1	A	124	PRO	C-O	-5.06	1.13	1.23
1	B	28	GLU	C-O	-5.05	1.13	1.23
1	A	196	TYR	CG-CD2	-5.05	1.32	1.39
1	A	24	ASP	CG-OD1	-5.05	1.13	1.25
1	B	18	LEU	C-O	-5.04	1.13	1.23
1	B	153	THR	C-O	-5.04	1.13	1.23
1	B	147	PHE	CD2-CE2	-5.04	1.29	1.39
1	B	110	LEU	C-O	-5.03	1.13	1.23
1	B	62	LEU	C-O	-5.03	1.13	1.23
1	A	91	LYS	CA-CB	-5.02	1.43	1.53
1	A	141	LEU	C-O	-5.02	1.13	1.23
1	A	157	PHE	C-O	-5.00	1.13	1.23
1	B	216	ASN	CG-OD1	-5.00	1.12	1.24

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASP	CB-CG-OD1	11.82	128.94	118.30
1	A	36	ASP	CB-CG-OD1	11.66	128.80	118.30
1	A	133	MET	CG-SD-CE	-8.50	86.60	100.20
1	A	150	ASP	CB-CG-OD1	8.48	125.93	118.30
1	B	203	LEU	CB-CG-CD2	7.94	124.50	111.00
1	A	122	LEU	CB-CG-CD2	7.68	124.06	111.00
1	A	118	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	B	97	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	41	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	85	LEU	CB-CG-CD1	7.16	123.18	111.00
1	B	130	LEU	CB-CG-CD1	-6.74	99.55	111.00
1	B	151	LYS	CD-CE-NZ	-6.72	96.24	111.70
1	B	151	LYS	N-CA-CB	-6.69	98.55	110.60
1	B	165	ARG	NE-CZ-NH1	-6.69	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	A	48	GLU	OE1-CD-OE2	-6.51	115.48	123.30
1	A	119	PHE	CB-CG-CD1	6.37	125.26	120.80
1	B	36	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	150	ASP	CB-CG-OD1	6.17	123.86	118.30
1	B	123	LYS	CD-CE-NZ	6.13	125.80	111.70
1	A	140	PHE	CZ-CE2-CD2	-6.12	112.75	120.10
1	A	211	MET	CG-SD-CE	6.06	109.90	100.20
1	B	36	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	113	LEU	CB-CG-CD1	-6.03	100.74	111.00
1	B	20	LEU	CB-CG-CD1	5.84	120.93	111.00
1	B	203	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	186	ARG	CA-CB-CG	5.70	125.94	113.40
1	B	92	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	A	165	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	B	92	GLU	CG-CD-OE1	5.61	129.51	118.30
1	B	136	LEU	CB-CG-CD1	5.60	120.53	111.00
1	A	133	MET	CB-CG-SD	5.53	128.98	112.40
1	A	41	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	182	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	150	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	46	LEU	CB-CG-CD2	5.31	120.03	111.00
1	B	105	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	95	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	156	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	B	118	ASP	N-CA-C	5.14	124.89	111.00
1	B	205	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	97	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	105	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	161	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	A	2	MET	N-CA-CB	-5.03	101.54	110.60
1	A	36	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	1729	0	1618	5	0
1	B	1764	0	1715	6	0
2	A	20	0	14	0	0
2	B	20	0	14	0	0
3	B	42	0	0	0	0
4	A	135	0	0	1	0
4	B	88	0	0	2	0
All	All	3798	0	3361	11	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (11) 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:133:MET:HE3	1:A:136:LEU:HB2	1.89	0.55
1:A:193:ILE:O	1:A:197:MET:HG3	2.11	0.51
1:B:47:ASN:O	1:B:51:LYS:HE3	2.10	0.51
1:B:146:TRP:CH2	1:B:186:ARG:HG2	2.51	0.46
1:B:184:ILE:O	1:B:188:GLU:HG3	2.16	0.45
1:B:37:ALA:HA	1:B:38:PRO:HA	1.71	0.44
1:A:96:GLU:HB2	1:A:148:LEU:HD11	1.99	0.44
1:B:151:LYS:HB3	4:B:466:HOH:O	2.19	0.43
1:B:155:VAL:HG13	4:B:436:HOH:O	2.20	0.41
1:A:86:CYS:SG	4:A:527:HOH:O	2.55	0.41
1:A:6:TYR:CG	1:A:7:TRP:N	2.89	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
1	B	214/217 (99%)	206 (96%)	8 (4%)	0	100	100
All	All	429/434 (99%)	416 (97%)	13 (3%)	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	175/197 (89%)	172 (98%)	3 (2%)	60	38
1	B	186/197 (94%)	180 (97%)	6 (3%)	39	15
All	All	361/394 (92%)	352 (98%)	9 (2%)	47	22

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	PRO
1	A	178	PRO
1	A	186	ARG
1	B	38	PRO
1	B	88	GLU
1	B	117	PRO
1	B	128	GLN
1	B	151	LYS
1	B	200	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	B	144	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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$
3	NNE	B	302	2	39,43,43	3.23	12 (30%)	44,58,58	1.59	7 (15%)
2	GSH	A	301	3	12,19,19	1.07	1 (8%)	15,24,24	2.04	3 (20%)
2	GSH	B	301	3	12,19,19	0.96	0	15,24,24	1.39	2 (13%)

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
3	NNE	B	302	2	-	7/39/39/39	0/2/2/2
2	GSH	A	301	3	-	0/18/24/24	-
2	GSH	B	301	3	-	0/18/24/24	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	NNE	CAM-CAK	8.89	1.51	1.32
3	B	302	NNE	CAI-CL1	-7.89	1.55	1.72
3	B	302	NNE	CBM-CBJ	7.57	1.48	1.32
3	B	302	NNE	CAH-CL2	-7.10	1.57	1.72
3	B	302	NNE	CAD-CAI	-6.02	1.34	1.39
3	B	302	NNE	CBB-CBI	-5.74	1.38	1.49
3	B	302	NNE	CAD-CAJ	-4.70	1.40	1.49
3	B	302	NNE	CBC-CL4	-3.27	1.65	1.72
3	B	302	NNE	CAO-CAP	2.86	1.56	1.51
3	B	302	NNE	OAZ-CAP	-2.73	1.17	1.23
3	B	302	NNE	OBA-CAU	-2.48	1.18	1.23
2	A	301	GSH	CG1-CD1	2.41	1.55	1.51
3	B	302	NNE	CBD-CL3	-2.26	1.68	1.72

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GSH	C3-CA3-N3	5.24	120.54	110.43
3	B	302	NNE	CAG-CAH-CAI	4.65	122.94	119.86
2	A	301	GSH	CA2-CB2-SG2	-4.12	109.56	114.19
3	B	302	NNE	CAD-CAI-CAH	-3.99	118.05	120.89
3	B	302	NNE	CBE-CBD-CBC	3.83	122.40	119.86
2	B	301	GSH	C3-CA3-N3	3.24	116.68	110.43
2	B	301	GSH	CB2-CA2-C2	-3.03	103.52	109.76
3	B	302	NNE	CAT-CAU-NAV	-3.01	111.61	116.58
2	A	301	GSH	CB2-CA2-C2	-2.73	104.14	109.76
3	B	302	NNE	OAW-CAG-CAH	2.23	119.49	115.78
3	B	302	NNE	CAS-CAY-CAX	-2.11	103.55	113.56
3	B	302	NNE	CAH-CAI-CL1	2.02	123.86	119.98

There are no chirality outliers.

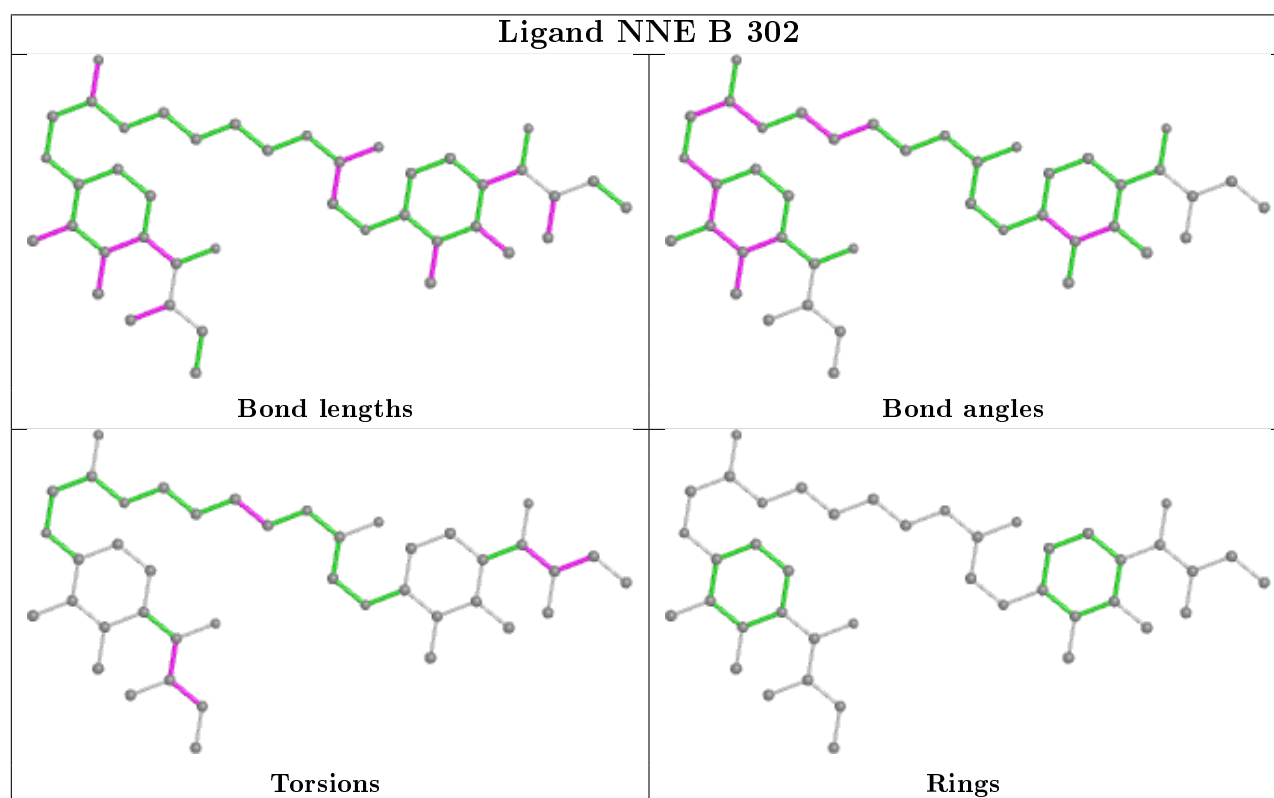
All (7) torsion outliers are listed below:

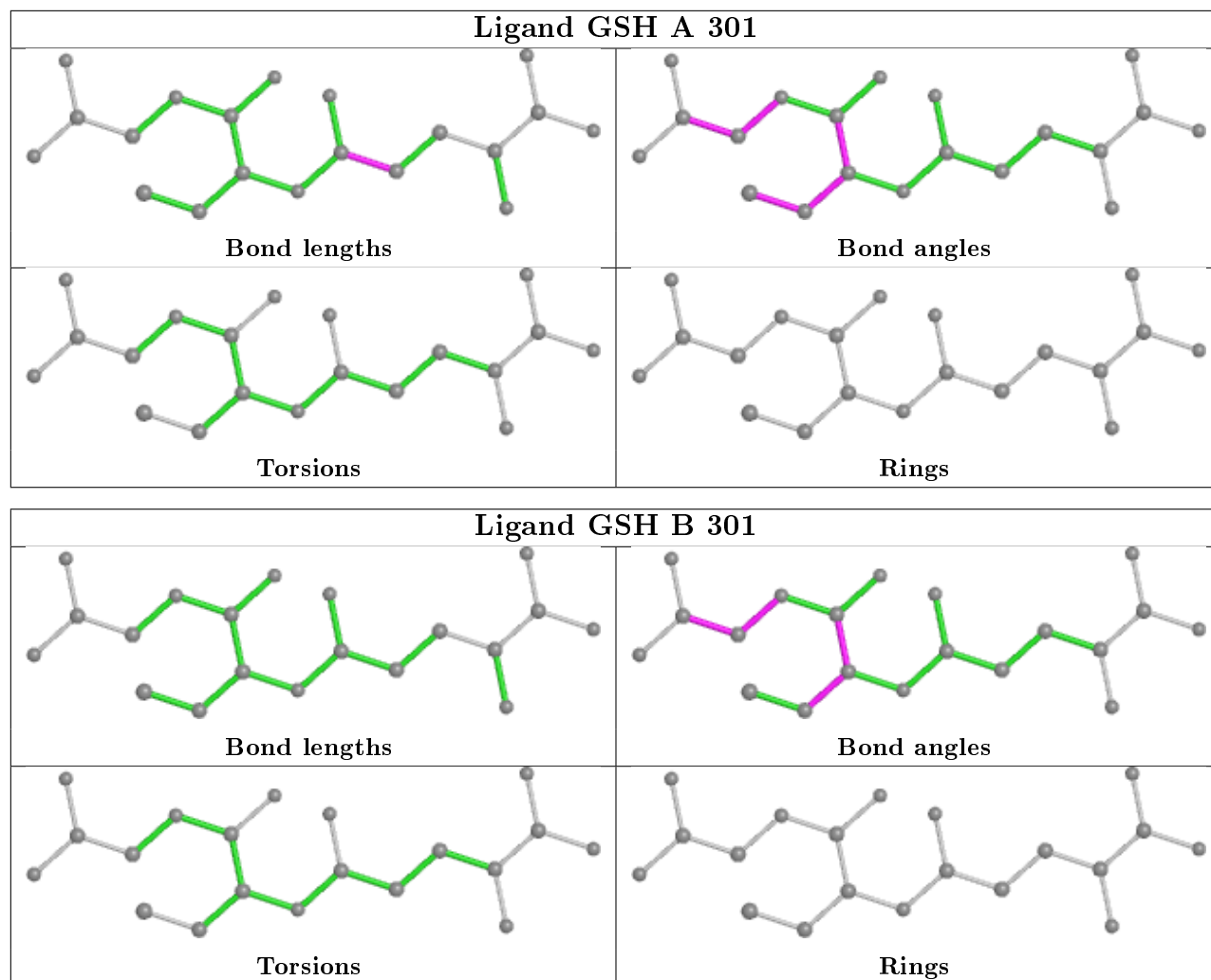
Mol	Chain	Res	Type	Atoms
3	B	302	NNE	OAA-CAJ-CAK-CAM
3	B	302	NNE	CAD-CAJ-CAK-CAM
3	B	302	NNE	CBB-CBI-CBJ-CBM
3	B	302	NNE	OBL-CBI-CBJ-CBM
3	B	302	NNE	CAJ-CAK-CAL-CAN
3	B	302	NNE	CBM-CBJ-CBK-CBN
3	B	302	NNE	NAQ-CAR-CAS-CAY

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/217 (100%)	-0.11	1 (0%) 91 90	9, 18, 29, 44	0
1	B	216/217 (99%)	0.05	2 (0%) 84 84	10, 22, 35, 39	28 (12%)
All	All	433/434 (99%)	-0.03	3 (0%) 87 87	9, 20, 32, 44	28 (6%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	PRO	2.7
1	A	1	PRO	2.4
1	B	37	ALA	2.4

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 carbohydrates 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.

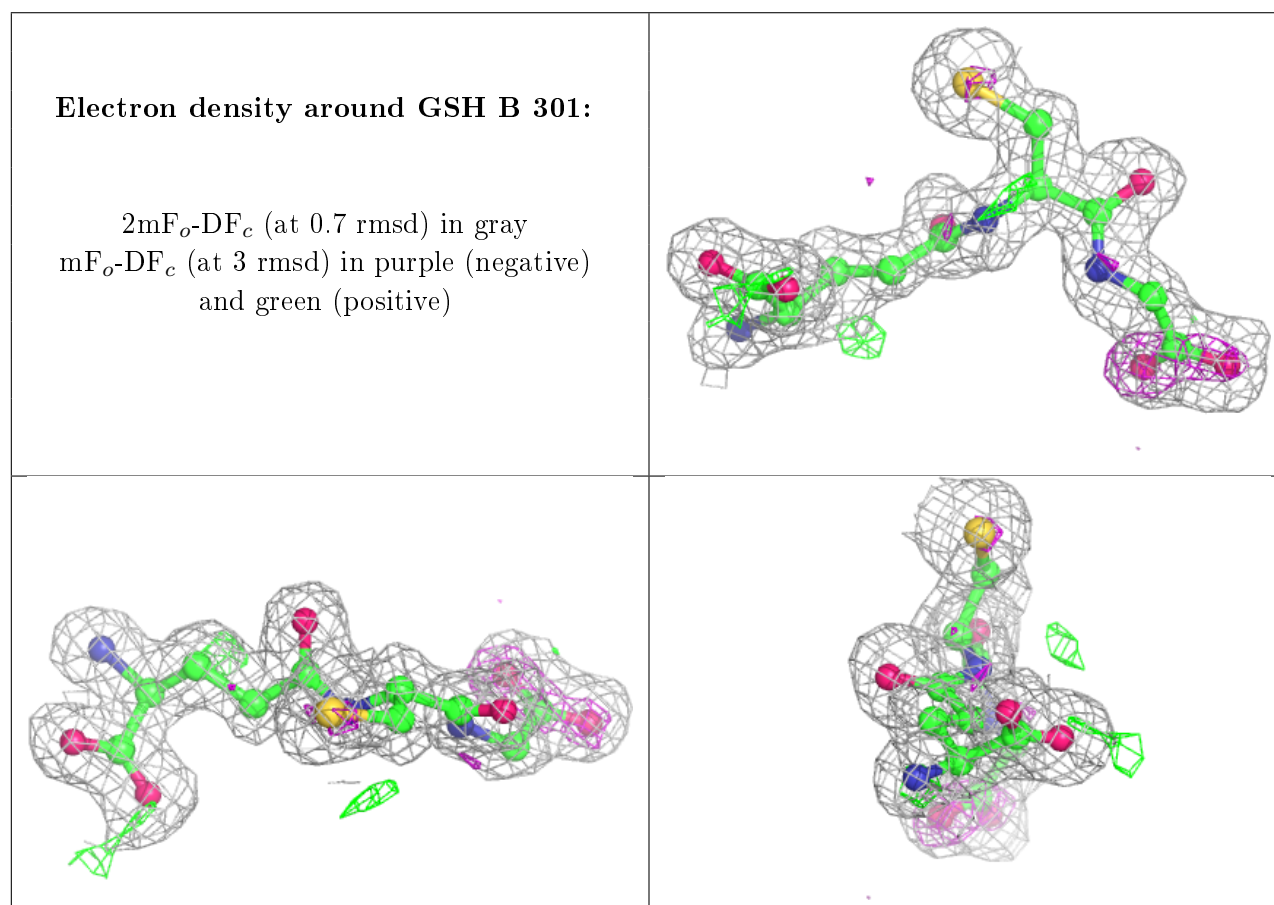
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GSH	B	301	20/20	0.89	0.13	20,20,20,20	0
2	GSH	A	301	20/20	0.90	0.12	20,20,20,20	0

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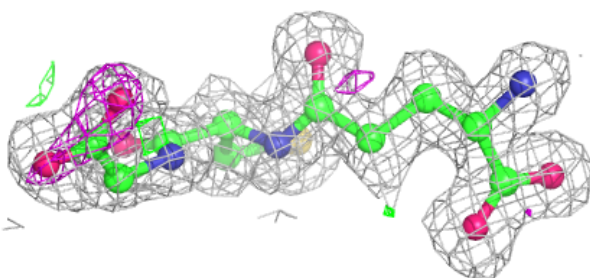
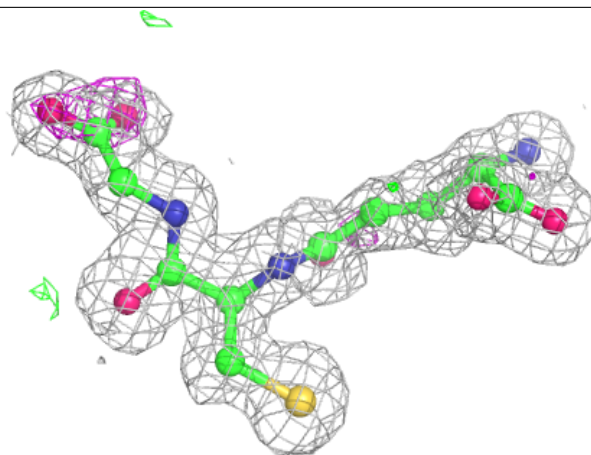
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NNE	B	302	42/42	0.91	0.20	20,20,20,20	0

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.

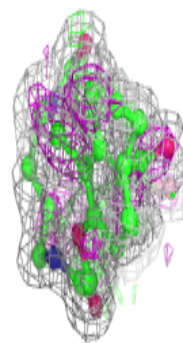
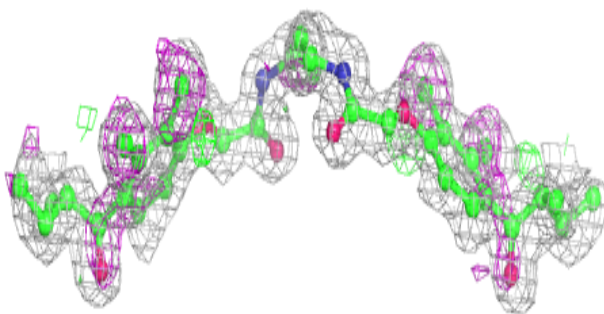
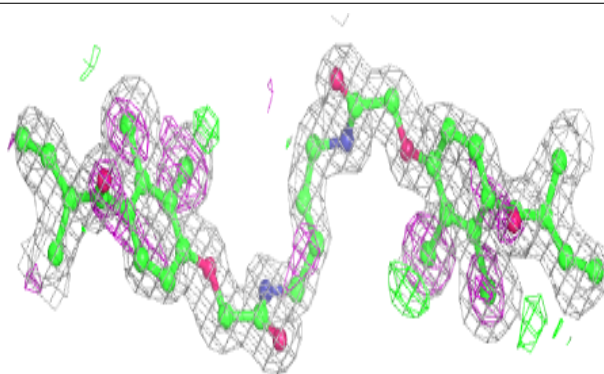


Electron density around GSH A 301:

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

**Electron density around NNE B 302:**

$2mF_o-DF_c$ (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.