



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 PM UTC

PDB ID : 5HWL / pdb_00005hwL
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 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

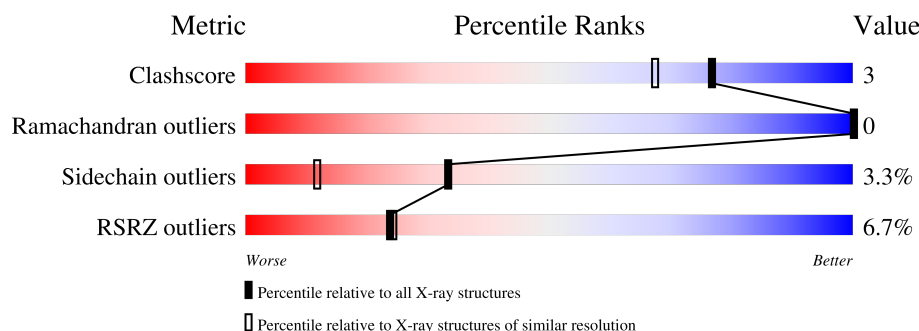
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 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	217	2% 7% 87% 6%
1	B	217	11% 5% 85% 9%

2 Entry composition [i](#)

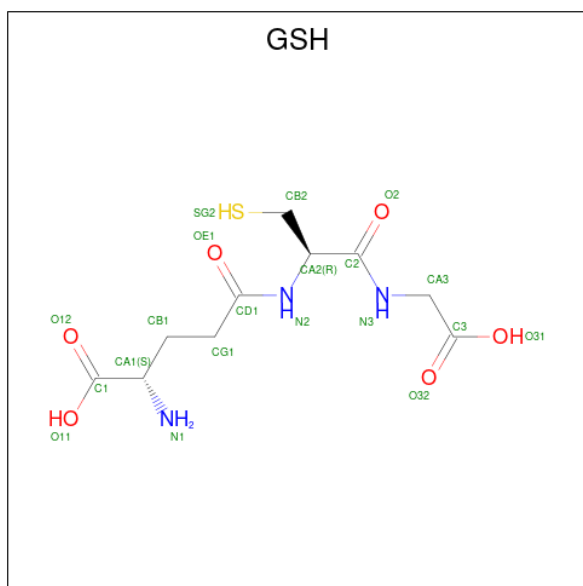
There are 4 unique types of molecules in this entry. The entry contains 3798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

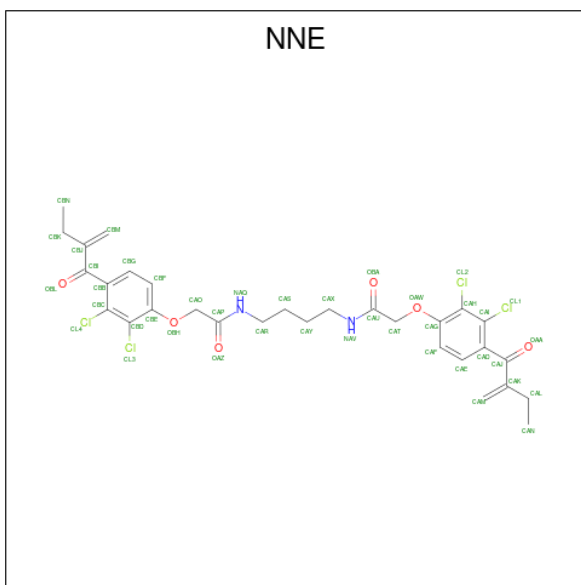
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1729	1128	273	318	10			
1	B	216	Total	C	N	O	S	110	0	0
			1764	1149	287	318	10			

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



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} (CCD ID: NNE) (formula: C₃₀H₃₂Cl₄N₂O₆).



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

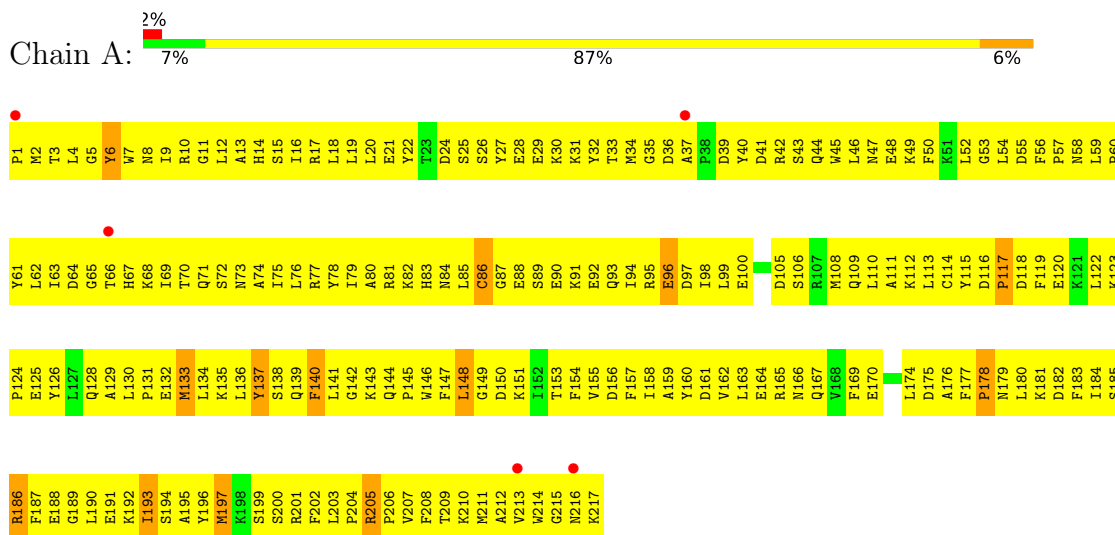
- Molecule 4 is water.

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

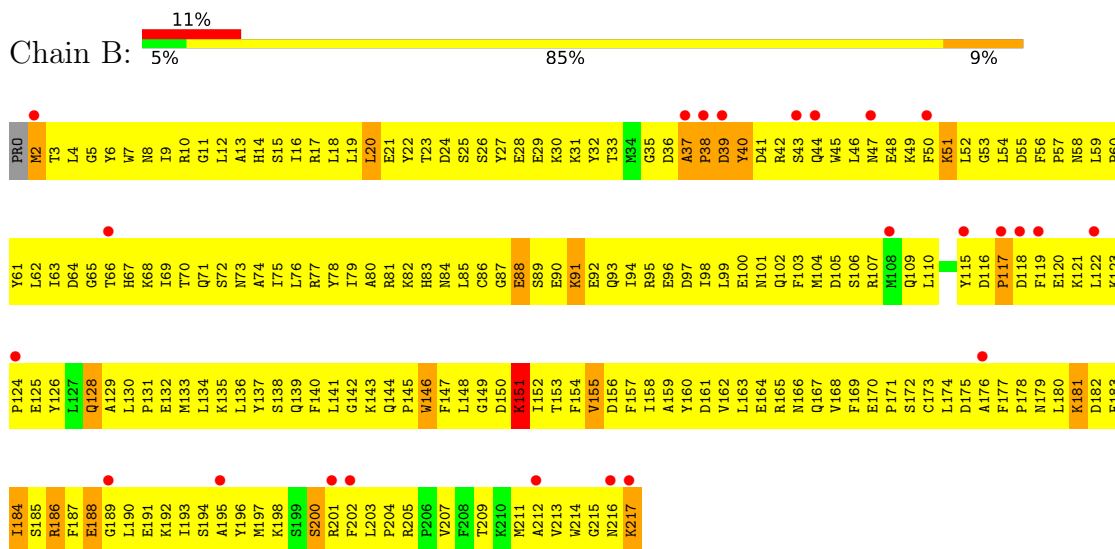
3 Residue-property plots

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 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 , 45.7	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 [i](#)

5.1 Standard geometry [i](#)

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	4.12	299/1777 (16.8%)	1.71	17/2412 (0.7%)
1	B	4.16	300/1811 (16.6%)	1.77	22/2446 (0.9%)
All	All	4.14	599/3588 (16.7%)	1.74	39/4858 (0.8%)

All (599) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	VAL	C-O	-19.65	1.02	1.24
1	A	205	ARG	C-O	-18.58	1.07	1.24
1	B	205	ARG	C-O	-16.83	1.06	1.24
1	A	56	PHE	C-O	-16.57	1.04	1.24
1	A	123	LYS	C-O	-16.40	1.08	1.24
1	B	128	GLN	C-O	-16.32	1.03	1.24
1	A	207	VAL	C-O	-16.08	1.05	1.24
1	B	58	ASN	C-O	-16.03	1.06	1.23
1	A	98	ILE	C-O	-15.97	1.06	1.24
1	B	53	GLY	C-O	-15.61	1.03	1.24
1	B	137	TYR	C-O	-15.51	1.06	1.24
1	A	72	SER	C-O	-15.40	1.05	1.24
1	A	73	ASN	C-O	-15.37	1.05	1.24
1	A	184	ILE	C-O	-15.34	1.06	1.24
1	B	163	LEU	C-O	-15.31	1.06	1.24
1	A	109	GLN	C-O	-15.17	1.06	1.24
1	B	124	PRO	C-O	-15.16	1.05	1.24
1	B	170	GLU	C-O	-15.02	1.07	1.24
1	A	203	LEU	C-O	-14.88	1.06	1.24
1	B	140	PHE	C-O	-14.84	1.07	1.24
1	B	15	SER	C-O	-14.73	1.06	1.24
1	A	177	PHE	C-O	-14.41	1.07	1.24
1	B	74	ALA	C-O	-14.34	1.07	1.24
1	A	14	HIS	C-O	-14.28	1.07	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	PHE	C-O	-14.25	1.07	1.24
1	B	73	ASN	C-O	-14.24	1.07	1.24
1	B	107	ARG	C-O	-14.23	1.07	1.24
1	B	105	ASP	C-O	-13.97	1.07	1.24
1	B	190	LEU	C-O	-13.95	1.07	1.23
1	A	151	LYS	C-O	-13.94	1.07	1.24
1	B	19	LEU	C-O	-13.94	1.07	1.24
1	A	68	LYS	C-O	-13.91	1.08	1.24
1	B	78	TYR	C-O	-13.75	1.08	1.24
1	B	72	SER	C-O	-13.56	1.08	1.24
1	B	102	GLN	C-O	-13.55	1.08	1.24
1	A	134	LEU	C-O	-13.52	1.08	1.24
1	B	157	PHE	C-O	-13.48	1.08	1.24
1	B	95	ARG	C-O	-13.46	1.08	1.24
1	A	161	ASP	C-O	-13.43	1.08	1.24
1	B	184	ILE	C-O	-13.40	1.08	1.24
1	A	63	ILE	C-O	-13.32	1.09	1.24
1	B	158	ILE	C-O	-13.19	1.09	1.24
1	A	193	ILE	C-O	-13.17	1.09	1.24
1	A	19	LEU	C-O	-13.09	1.08	1.24
1	B	187	PHE	C-O	-13.08	1.09	1.24
1	B	88	GLU	C-O	-13.04	1.06	1.24
1	A	149	GLY	C-O	-13.00	1.06	1.23
1	A	111	ALA	C-O	-12.87	1.09	1.24
1	B	135	LYS	C-O	-12.87	1.09	1.24
1	A	25	SER	C-O	-12.79	1.08	1.23
1	B	36	ASP	C-O	-12.78	1.05	1.23
1	A	20	LEU	C-O	-12.71	1.09	1.24
1	B	144	GLN	C-O	-12.70	1.07	1.23
1	B	109	GLN	C-O	-12.69	1.09	1.24
1	A	15	SER	C-O	-12.69	1.09	1.24
1	A	190	LEU	C-O	-12.68	1.08	1.23
1	B	191	GLU	C-O	-12.63	1.08	1.24
1	A	95	ARG	C-O	-12.61	1.09	1.24
1	B	120	GLU	C-O	-12.58	1.09	1.24
1	B	54	LEU	C-O	-12.54	1.08	1.23
1	B	193	ILE	C-O	-12.53	1.10	1.24
1	B	132	GLU	C-O	-12.51	1.09	1.24
1	A	87	GLY	C-O	-12.49	1.06	1.23
1	A	67	HIS	C-O	-12.47	1.08	1.24
1	A	76	LEU	C-O	-12.39	1.09	1.24
1	A	75	ILE	C-O	-12.38	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	LEU	C-O	-12.38	1.09	1.24
1	A	33	THR	C-O	-12.36	1.08	1.24
1	A	170	GLU	C-O	-12.28	1.10	1.24
1	A	59	LEU	C-O	-12.25	1.10	1.24
1	A	78	TYR	C-O	-12.25	1.10	1.24
1	A	91	LYS	C-O	-12.19	1.09	1.24
1	A	142	GLY	C-O	-12.18	1.08	1.24
1	A	137	TYR	C-O	-12.16	1.09	1.24
1	B	35	GLY	C-O	-11.98	1.12	1.23
1	B	87	GLY	C-O	-11.96	1.07	1.23
1	B	149	GLY	C-O	-11.93	1.07	1.23
1	A	180	LEU	C-O	-11.88	1.09	1.24
1	B	14	HIS	C-O	-11.87	1.10	1.24
1	B	96	GLU	C-O	-11.81	1.10	1.24
1	B	52	LEU	C-O	-11.78	1.08	1.24
1	A	120	GLU	C-O	-11.76	1.10	1.24
1	B	180	LEU	C-O	-11.71	1.08	1.24
1	A	138	SER	C-O	-11.69	1.10	1.24
1	B	48	GLU	C-O	-11.67	1.09	1.24
1	A	18	LEU	C-O	-11.63	1.10	1.24
1	B	212	ALA	C-O	-11.62	1.09	1.23
1	A	209	THR	C-O	-11.58	1.07	1.23
1	A	66	THR	C-O	-11.54	1.08	1.24
1	B	67	HIS	C-O	-11.54	1.09	1.24
1	A	96	GLU	C-O	-11.53	1.10	1.24
1	A	128	GLN	C-O	-11.53	1.09	1.24
1	B	25	SER	C-O	-11.52	1.09	1.23
1	A	28	GLU	C-O	-11.47	1.09	1.23
1	B	32	TYR	C-O	-11.47	1.09	1.23
1	B	154	PHE	C-O	-11.44	1.10	1.24
1	A	45	TRP	C-O	-11.42	1.10	1.24
1	A	183	PHE	C-O	-11.34	1.11	1.24
1	B	45	TRP	C-O	-11.34	1.10	1.24
1	A	146	TRP	C-O	-11.30	1.09	1.23
1	A	187	PHE	C-O	-11.27	1.11	1.24
1	A	4	LEU	C-O	-11.26	1.10	1.24
1	B	17	ARG	C-O	-11.24	1.11	1.24
1	B	174	LEU	C-O	-11.23	1.08	1.23
1	A	116	ASP	C-O	-11.22	1.09	1.24
1	B	197	MET	C-O	-11.21	1.09	1.24
1	B	97	ASP	C-O	-11.18	1.10	1.24
1	B	139	GLN	C-O	-11.16	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	ASN	C-O	-11.13	1.09	1.24
1	A	50	PHE	C-O	-11.06	1.09	1.24
1	A	70	THR	C-O	-11.05	1.09	1.23
1	A	160	TYR	C-O	-11.01	1.11	1.24
1	B	86	CYS	C-O	-10.99	1.09	1.23
1	B	145	PRO	C-O	-10.98	1.11	1.24
1	A	164	GLU	C-O	-10.98	1.11	1.24
1	B	59	LEU	C-O	-10.96	1.11	1.24
1	A	132	GLU	C-O	-10.92	1.11	1.24
1	A	163	LEU	C-O	-10.91	1.11	1.24
1	A	58	ASN	C-O	-10.86	1.12	1.23
1	B	93	GLN	C-O	-10.81	1.11	1.24
1	B	151	LYS	C-O	-10.79	1.10	1.24
1	B	209	THR	C-O	-10.76	1.08	1.23
1	A	62	LEU	C-O	-10.67	1.12	1.24
1	A	166	ASN	C-O	-10.66	1.11	1.24
1	A	22	TYR	C-O	-10.65	1.11	1.24
1	B	186	ARG	C-O	-10.62	1.11	1.24
1	A	185	SER	C-O	-10.60	1.11	1.24
1	B	195	ALA	C-O	-10.59	1.11	1.24
1	B	89	SER	C-O	-10.57	1.09	1.23
1	A	12	LEU	C-O	-10.57	1.09	1.24
1	A	69	ILE	C-O	-10.52	1.13	1.24
1	A	83	HIS	C-O	-10.51	1.09	1.24
1	B	214	TRP	C-O	-10.50	1.10	1.24
1	A	32	TYR	C-O	-10.45	1.11	1.23
1	A	200	SER	C-O	-10.45	1.09	1.24
1	B	98	ILE	C-O	-10.45	1.12	1.24
1	B	202	PHE	C-O	-10.39	1.11	1.23
1	B	194	SER	C-O	-10.34	1.12	1.24
1	A	201	ARG	C-O	-10.34	1.10	1.24
1	B	159	ALA	C-O	-10.32	1.12	1.24
1	A	197	MET	C-O	-10.29	1.10	1.24
1	B	4	LEU	C-O	-10.29	1.11	1.24
1	B	155	VAL	C-O	-10.27	1.11	1.24
1	A	53	GLY	C-O	-10.22	1.08	1.23
1	A	135	LYS	C-O	-10.21	1.12	1.24
1	A	158	ILE	C-O	-10.20	1.12	1.24
1	B	46	LEU	C-O	-10.19	1.11	1.24
1	A	167	GLN	C-O	-10.18	1.12	1.24
1	A	202	PHE	C-O	-10.18	1.11	1.23
1	A	3	THR	C-O	-10.14	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	ASP	C-O	-10.08	1.11	1.24
1	A	174	LEU	C-O	-10.08	1.10	1.24
1	A	140	PHE	C-O	-10.05	1.12	1.24
1	B	161	ASP	C-O	-10.03	1.12	1.24
1	B	12	LEU	C-O	-10.02	1.10	1.24
1	B	160	TYR	C-O	-10.02	1.12	1.24
1	B	100	GLU	C-O	-10.02	1.12	1.24
1	A	65	GLY	C-O	-10.01	1.09	1.24
1	A	210	LYS	C-O	-10.01	1.11	1.24
1	B	27	TYR	C-O	-10.00	1.11	1.23
1	A	88	GLU	C-O	-9.98	1.09	1.23
1	B	101	ASN	C-O	-9.92	1.12	1.24
1	B	91	LYS	C-O	-9.85	1.12	1.24
1	B	33	THR	C-O	-9.80	1.12	1.24
1	B	179	ASN	C-O	-9.80	1.11	1.24
1	A	131	PRO	C-O	-9.79	1.12	1.24
1	B	10	ARG	C-O	-9.79	1.11	1.24
1	B	69	ILE	C-O	-9.78	1.14	1.24
1	A	189	GLY	C-O	-9.77	1.10	1.23
1	B	103	PHE	C-O	-9.73	1.11	1.24
1	B	119	PHE	C-O	-9.73	1.11	1.24
1	B	126	TYR	C-O	-9.71	1.12	1.24
1	B	151	LYS	N-CA	-9.71	1.34	1.46
1	A	74	ALA	C-O	-9.69	1.12	1.24
1	B	106	SER	C-O	-9.63	1.12	1.24
1	A	136	LEU	C-O	-9.63	1.12	1.24
1	B	121	LYS	C-O	-9.62	1.11	1.24
1	B	75	ILE	C-O	-9.60	1.13	1.24
1	B	9	ILE	C-O	-9.59	1.12	1.24
1	A	86	CYS	C-O	-9.52	1.11	1.23
1	B	136	LEU	C-O	-9.49	1.12	1.24
1	A	49	LYS	C-O	-9.47	1.13	1.24
1	A	154	PHE	C-O	-9.44	1.13	1.24
1	A	60	PRO	C-O	-9.42	1.04	1.23
1	B	76	LEU	C-O	-9.41	1.13	1.24
1	A	34	MET	C-O	-9.38	1.12	1.23
1	B	99	LEU	C-O	-9.34	1.12	1.24
1	B	196	TYR	C-O	-9.34	1.13	1.24
1	A	94	ILE	C-O	-9.32	1.13	1.24
1	A	192	LYS	C-O	-9.28	1.12	1.24
1	B	40	TYR	C-O	-9.28	1.12	1.23
1	A	17	ARG	C-O	-9.27	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	SER	C-O	-9.24	1.13	1.24
1	A	54	LEU	C-O	-9.23	1.12	1.23
1	B	142	GLY	C-O	-9.23	1.11	1.24
1	B	178	PRO	C-O	-9.22	1.12	1.24
1	B	71	GLN	C-O	-9.22	1.12	1.24
1	B	65	GLY	C-O	-9.20	1.10	1.24
1	B	162	VAL	C-O	-9.19	1.13	1.24
1	A	201	ARG	CZ-NH1	-9.18	1.19	1.32
1	B	147	PHE	C-O	-9.18	1.12	1.24
1	B	146	TRP	C-O	-9.18	1.12	1.23
1	A	150	ASP	C-O	-9.12	1.11	1.24
1	A	216	ASN	CG-ND2	-9.10	1.14	1.33
1	A	5	GLY	C-O	-9.02	1.12	1.23
1	B	104	MET	C-O	-8.99	1.13	1.24
1	A	2	MET	SD-CE	-8.98	1.57	1.79
1	A	48	GLU	C-O	-8.98	1.12	1.24
1	B	203	LEU	C-O	-8.97	1.13	1.24
1	A	175	ASP	C-O	-8.94	1.13	1.24
1	B	148	LEU	C-O	-8.93	1.12	1.24
1	B	62	LEU	C-O	-8.92	1.13	1.24
1	B	181	LYS	C-O	-8.89	1.13	1.24
1	B	18	LEU	C-O	-8.84	1.13	1.24
1	B	63	ILE	C-O	-8.81	1.14	1.24
1	B	61	TYR	C-O	-8.80	1.12	1.23
1	A	124	PRO	C-O	-8.77	1.13	1.24
1	B	94	ILE	C-O	-8.76	1.14	1.24
1	A	84	ASN	C-O	-8.76	1.12	1.23
1	A	126	TYR	C-O	-8.74	1.14	1.24
1	A	204	PRO	C-O	-8.74	1.13	1.24
1	B	66	THR	C-O	-8.73	1.12	1.24
1	A	181	LYS	C-O	-8.73	1.14	1.24
1	B	92	GLU	C-O	-8.71	1.13	1.24
1	A	46	LEU	C-O	-8.71	1.13	1.24
1	A	52	LEU	C-O	-8.71	1.11	1.24
1	A	90	GLU	C-O	-8.70	1.14	1.24
1	B	110	LEU	C-O	-8.68	1.13	1.24
1	A	176	ALA	C-O	-8.66	1.12	1.24
1	B	156	ASP	C-O	-8.66	1.13	1.24
1	A	44	GLN	C-O	-8.65	1.14	1.24
1	A	141	LEU	C-O	-8.65	1.13	1.24
1	B	176	ALA	C-O	-8.64	1.12	1.24
1	A	1	PRO	C-O	-8.59	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	SER	C-O	-8.53	1.14	1.24
1	A	211	MET	C-O	-8.54	1.13	1.24
1	A	61	TYR	C-O	-8.52	1.13	1.23
1	A	64	ASP	C-O	-8.49	1.13	1.23
1	B	165	ARG	C-O	-8.45	1.13	1.24
1	B	67	HIS	CA-CB	-8.45	1.41	1.53
1	B	177	PHE	C-O	-8.45	1.14	1.24
1	A	41	ASP	C-O	-8.45	1.13	1.23
1	A	71	GLN	C-O	-8.41	1.13	1.24
1	B	70	THR	C-O	-8.41	1.13	1.23
1	B	5	GLY	C-O	-8.40	1.12	1.23
1	A	157	PHE	C-O	-8.37	1.13	1.24
1	B	79	ILE	C-O	-8.36	1.14	1.24
1	A	73	ASN	CG-OD1	-8.33	1.07	1.23
1	B	197	MET	N-CA	-8.33	1.35	1.46
1	A	36	ASP	C-O	-8.32	1.12	1.23
1	B	21	GLU	C-O	-8.30	1.14	1.24
1	B	55	ASP	C-O	-8.29	1.14	1.24
1	B	168	VAL	C-O	-8.26	1.14	1.24
1	B	125	GLU	C-O	-8.26	1.14	1.24
1	A	159	ALA	C-O	-8.25	1.14	1.24
1	A	175	ASP	CA-C	-8.24	1.42	1.52
1	A	105	ASP	C-O	-8.24	1.14	1.24
1	B	182	ASP	C-O	-8.24	1.13	1.24
1	B	215	GLY	C-O	-8.21	1.13	1.24
1	B	28	GLU	N-CA	-8.19	1.35	1.45
1	A	139	GLN	C-O	-8.18	1.14	1.24
1	A	179	ASN	C-O	-8.16	1.14	1.24
1	B	68	LYS	C-O	-8.15	1.14	1.24
1	A	195	ALA	C-O	-8.14	1.14	1.24
1	B	13	ALA	C-O	-8.13	1.13	1.24
1	B	81	ARG	C-O	-8.11	1.14	1.24
1	A	182	ASP	CG-OD1	-8.09	1.09	1.25
1	A	125	GLU	C-O	-8.08	1.14	1.24
1	B	83	HIS	C-O	-8.05	1.13	1.24
1	B	135	LYS	N-CA	-8.05	1.36	1.46
1	B	183	PHE	C-O	-7.99	1.15	1.24
1	A	89	SER	C-O	-7.99	1.13	1.23
1	A	99	LEU	C-O	-7.94	1.14	1.24
1	A	64	ASP	CG-OD2	-7.91	1.10	1.25
1	A	196	TYR	C-O	-7.91	1.14	1.24
1	B	57	PRO	C-O	-7.89	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	LYS	CA-C	-7.88	1.42	1.52
1	B	130	LEU	C-O	-7.88	1.16	1.24
1	A	64	ASP	CA-C	-7.84	1.44	1.53
1	B	28	GLU	C-O	-7.83	1.13	1.23
1	B	172	SER	C-O	-7.82	1.13	1.23
1	A	16	ILE	C-O	-7.82	1.15	1.24
1	A	77	ARG	C-O	-7.82	1.15	1.24
1	B	153	THR	C-O	-7.81	1.13	1.23
1	B	36	ASP	CG-OD2	-7.78	1.10	1.25
1	A	165	ARG	C-O	-7.78	1.14	1.24
1	B	73	ASN	CG-OD1	-7.77	1.08	1.23
1	A	37	ALA	C-O	-7.75	1.14	1.23
1	A	48	GLU	CD-OE1	-7.75	1.10	1.25
1	B	24	ASP	CG-OD2	-7.73	1.10	1.25
1	B	192	LYS	C-O	-7.68	1.15	1.24
1	A	21	GLU	C-O	-7.67	1.15	1.24
1	B	92	GLU	CD-OE2	-7.66	1.10	1.25
1	A	113	LEU	C-O	-7.65	1.15	1.24
1	A	31	LYS	C-O	-7.65	1.14	1.24
1	A	40	TYR	CG-CD1	-7.63	1.23	1.39
1	A	47	ASN	C-O	-7.57	1.14	1.24
1	A	147	PHE	C-O	-7.57	1.14	1.24
1	A	97	ASP	C-O	-7.54	1.15	1.24
1	B	50	PHE	C-O	-7.53	1.14	1.24
1	B	88	GLU	CA-C	-7.53	1.44	1.52
1	A	161	ASP	CG-OD1	-7.51	1.11	1.25
1	A	27	TYR	CA-C	-7.47	1.43	1.52
1	A	166	ASN	CG-OD1	-7.46	1.09	1.23
1	B	204	PRO	C-O	-7.45	1.15	1.24
1	A	82	LYS	C-O	-7.44	1.14	1.24
1	B	2	MET	SD-CE	-7.40	1.61	1.79
1	B	200	SER	C-O	-7.39	1.14	1.24
1	B	23	THR	CA-C	7.38	1.63	1.52
1	A	43	SER	CB-OG	-7.38	1.27	1.42
1	A	45	TRP	CE3-CZ3	-7.38	1.16	1.38
1	B	58	ASN	CG-OD1	-7.36	1.09	1.23
1	B	84	ASN	CA-C	7.34	1.62	1.53
1	A	214	TRP	C-O	-7.32	1.15	1.23
1	A	10	ARG	C-O	-7.30	1.14	1.24
1	B	44	GLN	C-O	-7.30	1.15	1.24
1	A	135	LYS	CA-C	-7.29	1.43	1.52
1	A	144	GLN	CD-NE2	-7.29	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	PHE	N-CA	-7.27	1.38	1.46
1	B	44	GLN	N-CA	-7.23	1.37	1.46
1	A	13	ALA	C-O	-7.21	1.14	1.23
1	B	166	ASN	C-O	-7.20	1.15	1.24
1	B	144	GLN	CD-NE2	-7.19	1.18	1.33
1	A	106	SER	C-O	-7.18	1.15	1.24
1	A	42	ARG	C-O	-7.14	1.14	1.24
1	B	40	TYR	CZ-OH	-7.08	1.23	1.38
1	B	211	MET	C-O	-7.07	1.15	1.24
1	A	11	GLY	C-O	-7.02	1.14	1.23
1	B	97	ASP	CG-OD1	-6.99	1.12	1.25
1	A	41	ASP	CG-OD2	-6.99	1.12	1.25
1	A	26	SER	C-O	-6.97	1.15	1.24
1	A	145	PRO	C-O	-6.97	1.15	1.24
1	A	144	GLN	C-O	-6.95	1.15	1.23
1	B	51	LYS	C-O	-6.95	1.14	1.24
1	B	57	PRO	N-CD	6.93	1.57	1.47
1	A	33	THR	CB-OG1	-6.92	1.32	1.43
1	B	21	GLU	CD-OE1	-6.92	1.12	1.25
1	A	119	PHE	C-O	-6.91	1.16	1.24
1	A	199	SER	C-O	-6.89	1.15	1.23
1	B	36	ASP	CA-CB	-6.88	1.43	1.53
1	B	123	LYS	C-O	-6.87	1.17	1.24
1	B	213	VAL	C-O	-6.87	1.15	1.23
1	A	186	ARG	CZ-NH2	-6.87	1.24	1.33
1	B	116	ASP	C-O	-6.86	1.15	1.24
1	A	90	GLU	N-CA	-6.85	1.38	1.46
1	A	118	ASP	CG-OD2	-6.85	1.12	1.25
1	B	77	ARG	C-O	-6.85	1.16	1.24
1	A	169	PHE	C-O	-6.84	1.16	1.24
1	B	217	LYS	C-O	-6.83	1.09	1.23
1	A	85	LEU	C-O	-6.83	1.14	1.23
1	B	88	GLU	CA-CB	-6.83	1.42	1.54
1	A	175	ASP	CG-OD2	-6.82	1.12	1.25
1	A	155	VAL	C-O	-6.82	1.15	1.24
1	A	100	GLU	CD-OE2	-6.81	1.12	1.25
1	B	11	GLY	C-O	-6.80	1.14	1.23
1	B	21	GLU	CD-OE2	-6.79	1.12	1.25
1	B	49	LYS	C-O	-6.79	1.16	1.24
1	A	30	LYS	CA-CB	-6.78	1.43	1.53
1	B	140	PHE	N-CA	-6.78	1.38	1.46
1	A	130	LEU	C-O	-6.77	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	LEU	C-N	-6.76	1.25	1.33
1	A	195	ALA	CA-CB	-6.76	1.42	1.53
1	B	68	LYS	N-CA	-6.76	1.38	1.46
1	A	191	GLU	C-O	-6.75	1.16	1.24
1	B	29	GLU	C-O	-6.75	1.15	1.24
1	A	213	VAL	C-O	-6.73	1.15	1.24
1	B	102	GLN	CD-NE2	-6.73	1.19	1.33
1	A	115	TYR	CA-C	6.73	1.62	1.52
1	A	40	TYR	CE2-CZ	-6.72	1.22	1.38
1	A	143	LYS	C-O	-6.72	1.15	1.24
1	B	85	LEU	C-O	-6.72	1.15	1.24
1	B	31	LYS	C-O	-6.71	1.16	1.24
1	B	24	ASP	C-O	-6.69	1.15	1.23
1	A	55	ASP	C-O	-6.69	1.16	1.24
1	B	164	GLU	CD-OE1	-6.68	1.12	1.25
1	A	76	LEU	N-CA	-6.68	1.38	1.46
1	B	48	GLU	CD-OE1	-6.68	1.12	1.25
1	B	64	ASP	C-O	-6.67	1.15	1.23
1	A	91	LYS	CA-CB	-6.66	1.43	1.53
1	A	216	ASN	C-O	-6.64	1.15	1.24
1	A	39	ASP	CG-OD1	-6.59	1.12	1.25
1	A	27	TYR	C-O	-6.57	1.15	1.23
1	A	118	ASP	CA-CB	-6.56	1.44	1.53
1	B	28	GLU	CA-C	6.56	1.60	1.52
1	A	164	GLU	CD-OE1	-6.55	1.12	1.25
1	A	125	GLU	N-CA	-6.55	1.38	1.46
1	B	41	ASP	C-O	-6.53	1.15	1.23
1	B	189	GLY	C-O	-6.53	1.15	1.23
1	B	198	LYS	C-O	-6.53	1.15	1.24
1	A	199	SER	CB-OG	-6.52	1.29	1.42
1	A	96	GLU	CD-OE2	-6.51	1.12	1.25
1	A	78	TYR	CG-CD1	-6.49	1.25	1.39
1	B	164	GLU	C-O	-6.48	1.16	1.24
1	A	6	TYR	C-O	-6.48	1.16	1.23
1	A	57	PRO	C-O	-6.47	1.14	1.23
1	A	37	ALA	CA-C	-6.47	1.45	1.53
1	B	45	TRP	CE2-CZ2	-6.47	1.26	1.39
1	B	143	LYS	C-O	-6.46	1.15	1.24
1	A	71	GLN	CD-OE1	-6.45	1.11	1.23
1	A	58	ASN	CG-OD1	-6.44	1.11	1.23
1	B	138	SER	C-O	-6.43	1.16	1.24
1	A	153	THR	CA-C	6.42	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	ASP	C-O	-6.42	1.14	1.24
1	B	204	PRO	N-CD	6.42	1.56	1.47
1	A	90	GLU	CD-OE2	-6.41	1.13	1.25
1	A	153	THR	C-O	-6.41	1.15	1.23
1	A	129	ALA	C-O	-6.40	1.15	1.24
1	B	22	TYR	C-O	-6.39	1.16	1.24
1	B	132	GLU	N-CA	-6.38	1.38	1.46
1	B	37	ALA	C-O	-6.36	1.15	1.24
1	B	40	TYR	CG-CD1	-6.36	1.25	1.39
1	B	201	ARG	C-O	-6.36	1.15	1.24
1	A	158	ILE	CA-C	6.35	1.60	1.52
1	A	29	GLU	CD-OE2	-6.33	1.13	1.25
1	A	116	ASP	CG-OD2	-6.33	1.13	1.25
1	A	184	ILE	CA-C	6.32	1.60	1.52
1	A	10	ARG	CA-C	6.29	1.61	1.52
1	A	36	ASP	CG-OD1	-6.29	1.13	1.25
1	A	128	GLN	CA-C	-6.27	1.43	1.52
1	B	175	ASP	C-O	-6.27	1.16	1.24
1	B	176	ALA	CA-CB	-6.26	1.42	1.53
1	A	41	ASP	CG-OD1	-6.25	1.13	1.25
1	B	3	THR	C-O	-6.25	1.16	1.24
1	B	44	GLN	CA-C	6.24	1.60	1.52
1	A	41	ASP	N-CA	-6.24	1.38	1.46
1	B	40	TYR	CE2-CZ	-6.22	1.23	1.38
1	B	90	GLU	C-O	-6.22	1.17	1.24
1	B	51	LYS	CA-C	-6.21	1.44	1.52
1	B	194	SER	CB-OG	-6.21	1.29	1.42
1	A	88	GLU	CA-CB	-6.19	1.43	1.54
1	B	169	PHE	C-O	-6.19	1.16	1.24
1	B	16	ILE	C-O	-6.18	1.17	1.24
1	B	7	TRP	C-O	-6.17	1.15	1.23
1	B	134	LEU	C-O	-6.17	1.16	1.24
1	B	93	GLN	CD-OE1	-6.14	1.11	1.23
1	A	155	VAL	CB-CG1	-6.13	1.32	1.52
1	A	24	ASP	CG-OD1	-6.11	1.13	1.25
1	B	26	SER	C-O	-6.10	1.16	1.24
1	B	70	THR	CA-C	6.09	1.60	1.52
1	B	115	TYR	CA-C	6.08	1.60	1.52
1	B	30	LYS	N-CA	-6.08	1.38	1.46
1	B	106	SER	CB-OG	-6.08	1.30	1.42
1	B	170	GLU	CD-OE1	-6.07	1.13	1.25
1	A	215	GLY	C-O	-6.07	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	LEU	C-O	-6.06	1.16	1.24
1	A	137	TYR	CA-C	6.06	1.60	1.52
1	A	79	ILE	C-O	-6.04	1.17	1.24
1	A	65	GLY	C-N	-6.04	1.24	1.33
1	B	131	PRO	CA-CB	-6.04	1.45	1.53
1	B	70	THR	CB-OG1	-6.02	1.34	1.43
1	A	177	PHE	CA-CB	6.01	1.60	1.53
1	B	150	ASP	CA-C	-6.01	1.44	1.52
1	B	42	ARG	C-O	-6.00	1.15	1.23
1	B	161	ASP	CG-OD1	-5.99	1.14	1.25
1	A	105	ASP	CG-OD1	-5.98	1.14	1.25
1	B	115	TYR	N-CA	-5.97	1.38	1.46
1	B	121	LYS	CA-C	-5.97	1.44	1.52
1	B	7	TRP	N-CA	-5.97	1.38	1.45
1	B	201	ARG	CA-CB	-5.96	1.43	1.53
1	B	172	SER	CB-OG	-5.95	1.30	1.42
1	A	214	TRP	N-CA	-5.95	1.38	1.46
1	B	39	ASP	C-O	-5.95	1.16	1.24
1	B	117	PRO	C-O	-5.94	1.16	1.24
1	B	8	ASN	C-O	-5.93	1.16	1.23
1	A	29	GLU	C-O	-5.93	1.16	1.24
1	A	55	ASP	CG-OD1	-5.92	1.14	1.25
1	B	188	GLU	C-O	-5.91	1.16	1.24
1	A	188	GLU	CD-OE2	-5.90	1.14	1.25
1	B	60	PRO	C-O	-5.89	1.11	1.23
1	B	216	ASN	CG-ND2	-5.89	1.20	1.33
1	A	35	GLY	C-O	-5.89	1.14	1.23
1	B	64	ASP	CG-OD2	-5.87	1.14	1.25
1	A	150	ASP	CG-OD1	-5.86	1.14	1.25
1	B	185	SER	CB-OG	-5.86	1.30	1.42
1	B	29	GLU	CD-OE1	-5.85	1.14	1.25
1	B	20	LEU	C-O	-5.85	1.17	1.24
1	A	133	MET	C-O	-5.84	1.17	1.24
1	B	25	SER	CB-OG	-5.84	1.30	1.42
1	A	61	TYR	CG-CD2	-5.84	1.27	1.39
1	B	102	GLN	N-CA	-5.83	1.39	1.46
1	A	71	GLN	CA-C	5.82	1.60	1.52
1	B	6	TYR	C-O	-5.82	1.17	1.23
1	B	32	TYR	N-CA	-5.82	1.38	1.45
1	B	196	TYR	CA-C	-5.82	1.45	1.52
1	A	160	TYR	CG-CD2	-5.80	1.27	1.39
1	A	55	ASP	CG-OD2	-5.80	1.14	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	GLN	CD-NE2	-5.79	1.21	1.33
1	B	205	ARG	CA-C	-5.79	1.46	1.52
1	B	90	GLU	CD-OE2	-5.79	1.14	1.25
1	A	45	TRP	CA-C	5.78	1.60	1.52
1	B	123	LYS	CA-CB	-5.75	1.47	1.53
1	B	82	LYS	C-O	-5.75	1.16	1.24
1	B	192	LYS	N-CA	-5.74	1.39	1.46
1	A	39	ASP	CG-OD2	-5.72	1.14	1.25
1	A	93	GLN	C-N	-5.71	1.26	1.33
1	B	171	PRO	C-O	-5.71	1.16	1.24
1	B	6	TYR	N-CA	-5.70	1.39	1.46
1	A	148	LEU	CA-C	5.69	1.60	1.52
1	A	216	ASN	CG-OD1	-5.68	1.12	1.23
1	A	26	SER	CA-CB	-5.68	1.45	1.53
1	B	188	GLU	CD-OE2	-5.67	1.14	1.25
1	A	120	GLU	CA-C	-5.67	1.45	1.52
1	A	139	GLN	CD-NE2	-5.64	1.21	1.33
1	A	162	VAL	C-O	-5.63	1.17	1.24
1	A	126	TYR	CG-CD2	-5.63	1.27	1.39
1	B	107	ARG	CZ-NH2	-5.62	1.26	1.33
1	A	43	SER	C-O	-5.61	1.17	1.24
1	A	124	PRO	N-CD	5.61	1.55	1.47
1	A	48	GLU	CD-OE2	-5.60	1.14	1.25
1	B	178	PRO	CA-C	-5.59	1.43	1.52
1	B	216	ASN	CG-OD1	-5.58	1.12	1.23
1	B	95	ARG	N-CA	-5.58	1.39	1.46
1	A	112	LYS	C-N	-5.57	1.26	1.33
1	A	140	PHE	C-N	-5.54	1.26	1.33
1	B	90	GLU	CD-OE1	-5.53	1.14	1.25
1	B	116	ASP	C-N	5.53	1.41	1.33
1	A	116	ASP	CG-OD1	-5.50	1.14	1.25
1	A	176	ALA	CA-CB	-5.50	1.43	1.53
1	A	133	MET	SD-CE	-5.49	1.65	1.79
1	A	110	LEU	C-N	-5.48	1.26	1.33
1	B	31	LYS	CA-C	-5.48	1.46	1.52
1	B	126	TYR	CA-C	-5.47	1.45	1.52
1	A	68	LYS	CA-CB	-5.47	1.45	1.53
1	A	118	ASP	C-N	-5.45	1.26	1.33
1	A	25	SER	CA-C	-5.45	1.45	1.52
1	A	183	PHE	CG-CD2	-5.45	1.27	1.38
1	A	8	ASN	CG-ND2	-5.44	1.21	1.33
1	A	72	SER	CB-OG	-5.44	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ALA	N-CA	-5.44	1.38	1.45
1	A	70	THR	CB-OG1	-5.42	1.35	1.43
1	B	175	ASP	CA-C	-5.42	1.45	1.52
1	B	152	ILE	C-O	-5.41	1.17	1.24
1	A	32	TYR	N-CA	-5.41	1.38	1.46
1	B	61	TYR	CE1-CZ	-5.40	1.25	1.38
1	B	158	ILE	CA-C	5.40	1.59	1.52
1	A	130	LEU	CA-CB	-5.39	1.47	1.53
1	A	28	GLU	CA-C	5.39	1.59	1.52
1	B	156	ASP	N-CA	5.38	1.53	1.46
1	A	61	TYR	CE1-CZ	-5.36	1.25	1.38
1	A	213	VAL	N-CA	-5.36	1.39	1.46
1	A	17	ARG	CA-C	5.36	1.59	1.52
1	B	17	ARG	CZ-NH1	-5.35	1.25	1.32
1	A	110	LEU	C-O	-5.35	1.17	1.24
1	A	114	CYS	C-O	-5.33	1.17	1.24
1	B	129	ALA	N-CA	-5.33	1.39	1.46
1	A	92	GLU	CD-OE1	-5.32	1.15	1.25
1	B	123	LYS	CA-C	-5.32	1.46	1.52
1	B	50	PHE	CG-CD2	-5.32	1.27	1.38
1	B	96	GLU	CD-OE1	-5.30	1.15	1.25
1	B	169	PHE	CG-CD1	-5.30	1.27	1.38
1	A	9	ILE	C-O	-5.29	1.16	1.23
1	A	90	GLU	CD-OE1	-5.27	1.15	1.25
1	B	150	ASP	C-O	-5.27	1.17	1.24
1	A	46	LEU	CA-C	5.27	1.59	1.52
1	B	24	ASP	CA-C	-5.26	1.46	1.53
1	B	185	SER	CA-C	-5.25	1.46	1.52
1	B	75	ILE	CA-CB	5.24	1.60	1.54
1	B	195	ALA	CA-CB	-5.24	1.45	1.53
1	A	175	ASP	CG-OD1	-5.23	1.15	1.25
1	B	182	ASP	N-CA	-5.23	1.39	1.46
1	A	97	ASP	CG-OD1	-5.21	1.15	1.25
1	A	117	PRO	CA-CB	-5.21	1.46	1.53
1	B	89	SER	CB-OG	-5.21	1.31	1.42
1	B	80	ALA	C-O	-5.20	1.18	1.24
1	A	212	ALA	C-O	-5.20	1.17	1.23
1	B	102	GLN	CD-OE1	-5.20	1.13	1.23
1	B	133	MET	SD-CE	-5.20	1.66	1.79
1	A	90	GLU	C-N	-5.19	1.27	1.33
1	B	156	ASP	CG-OD1	-5.18	1.15	1.25
1	A	70	THR	CA-C	5.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	PRO	C-N	-5.17	1.27	1.33
1	B	123	LYS	C-N	5.16	1.40	1.33
1	B	182	ASP	CG-OD1	-5.16	1.15	1.25
1	A	80	ALA	C-O	-5.15	1.18	1.24
1	A	57	PRO	N-CD	5.15	1.54	1.47
1	A	1	PRO	C-N	-5.13	1.26	1.33
1	B	132	GLU	CA-CB	-5.13	1.45	1.53
1	A	157	PHE	CA-C	5.13	1.59	1.52
1	B	202	PHE	CG-CD1	-5.12	1.28	1.38
1	B	200	SER	CA-C	-5.12	1.45	1.52
1	A	8	ASN	C-O	-5.11	1.17	1.23
1	B	100	GLU	CA-C	5.09	1.59	1.52
1	A	100	GLU	CD-OE1	-5.08	1.15	1.25
1	A	186	ARG	CD-NE	-5.08	1.39	1.46
1	A	208	PHE	C-O	-5.08	1.16	1.23
1	A	81	ARG	C-O	-5.08	1.17	1.24
1	A	106	SER	CB-OG	-5.07	1.32	1.42
1	B	2	MET	CB-CG	-5.07	1.37	1.52
1	A	112	LYS	C-O	-5.06	1.18	1.24
1	B	120	GLU	CD-OE1	-5.06	1.15	1.25
1	A	187	PHE	CA-C	5.05	1.59	1.52
1	B	55	ASP	CG-OD1	-5.05	1.15	1.25
1	A	137	TYR	N-CA	5.05	1.52	1.46
1	B	168	VAL	N-CA	-5.05	1.40	1.46
1	B	37	ALA	N-CA	-5.04	1.38	1.45
1	A	186	ARG	C-O	-5.04	1.18	1.24
1	A	178	PRO	N-CD	5.04	1.54	1.47
1	A	140	PHE	CD1-CE1	-5.02	1.23	1.38
1	B	105	ASP	CG-OD1	-5.00	1.15	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ASP	N-CA-C	10.15	124.89	113.21
1	A	205	ARG	O-C-N	-8.18	116.48	121.71
1	B	37	ALA	C-N-CD	8.04	138.28	120.60
1	B	43	SER	N-CA-C	7.32	118.91	111.07
1	A	114	CYS	N-CA-C	7.06	121.15	112.54
1	B	151	LYS	N-CA-CB	-7.06	98.55	110.83
1	B	120	GLU	N-CA-C	7.05	118.96	111.28
1	B	35	GLY	CA-C-O	-6.82	115.46	122.28
1	B	147	PHE	N-CA-C	6.79	119.52	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	SER	N-CA-C	6.73	120.37	111.75
1	B	173	CYS	N-CA-C	6.62	119.32	111.71
1	B	52	LEU	N-CA-C	6.51	121.39	113.38
1	A	133	MET	CG-SD-CE	-6.50	86.60	100.90
1	B	56	PHE	O-C-N	6.15	126.90	121.37
1	A	205	ARG	C-N-CD	6.15	134.12	120.60
1	B	117	PRO	CB-CA-C	-6.14	102.00	112.26
1	B	51	LYS	N-CA-C	6.06	120.70	112.88
1	A	186	ARG	CA-CB-CG	5.92	125.94	114.10
1	B	42	ARG	CA-C-N	5.92	128.13	120.44
1	B	42	ARG	C-N-CA	5.92	128.13	120.44
1	B	50	PHE	N-CA-C	5.89	120.09	113.02
1	B	184	ILE	CB-CA-C	-5.82	104.42	112.04
1	B	192	LYS	N-CA-C	5.70	117.49	111.28
1	B	122	LEU	N-CA-C	5.67	120.26	113.23
1	A	186	ARG	CB-CG-CD	5.60	124.19	111.30
1	B	87	GLY	N-CA-C	-5.59	104.92	112.14
1	A	2	MET	CB-CA-C	5.55	119.00	109.51
1	A	2	MET	N-CA-CB	-5.44	101.54	110.41
1	A	133	MET	CB-CG-SD	5.43	128.98	112.70
1	A	177	PHE	N-CA-C	5.42	119.06	108.21
1	A	41	ASP	N-CA-C	5.38	118.37	110.30
1	A	21	GLU	N-CA-CB	5.30	117.70	110.01
1	A	5	GLY	O-C-N	5.25	128.63	123.80
1	B	171	PRO	N-CA-C	5.16	123.09	112.47
1	A	122	LEU	N-CA-C	5.10	119.21	112.89
1	B	124	PRO	CB-CA-C	-5.09	104.27	112.21
1	B	130	LEU	CA-C-O	5.08	123.30	118.63
1	A	147	PHE	N-CA-C	5.07	117.55	111.71
1	A	166	ASN	N-CA-CB	5.02	117.59	110.16

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	11	0
1	B	1764	0	1715	8	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	19	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 3.

All (19) 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: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:A:133:MET:O	1:A:133:MET:HE3	2.13	0.49
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:140:PHE:CD1	1:A:140:PHE:C	2.96	0.44
1:A:96:GLU:HB2	1:A:148:LEU:HD11	1.99	0.44
1:A:133:MET:HE2	1:A:137:TYR:CE2	2.53	0.44
1:A:205:ARG:HA	1:A:206:PRO:C	2.43	0.43
1:A:133:MET:HE2	1:A:137:TYR:CZ	2.53	0.43
1:B:151:LYS:HB3	4:B:466:HOH:O	2.19	0.43
1:A:206:PRO:HB3	1:A:217:LYS:C	2.45	0.42
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:108:MET:HE2	1:A:108:MET:HB2	1.74	0.41
1:B:2:MET:HE1	1:B:20:LEU:CD2	2.51	0.41
1:A:6:TYR:CG	1:A:7:TRP:N	2.89	0.40
1:B:39:ASP:O	1:B:40:TYR:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	53	30
1	B	186/197 (94%)	177 (95%)	9 (5%)	23	6
All	All	361/394 (92%)	349 (97%)	12 (3%)	33	12

All (12) 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	91	LYS
1	B	117	PRO
1	B	128	GLN

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Mol	Chain	Res	Type
1	B	151	LYS
1	B	181	LYS
1	B	200	SER
1	B	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	167	GLN
1	B	93	GLN
1	B	144	GLN
1	B	166	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](#)

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	41,43,43	3.25	13 (31%)	48,58,58	1.75	9 (18%)
2	GSH	B	301	3	18,19,19	1.23	2 (11%)	21,24,24	1.20	1 (4%)
2	GSH	A	301	3	18,19,19	1.50	3 (16%)	21,24,24	1.44	3 (14%)

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	B	301	3	-	0/24/24/24	-
2	GSH	A	301	3	-	0/24/24/24	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	NNE	CAM-CAK	9.35	1.51	1.32
3	B	302	NNE	CAI-CL1	-8.09	1.55	1.72
3	B	302	NNE	CBM-CBJ	7.97	1.48	1.32
3	B	302	NNE	CAH-CL2	-7.28	1.57	1.72
3	B	302	NNE	CAD-CAI	-6.02	1.34	1.39
3	B	302	NNE	CBB-CBI	-5.67	1.38	1.49
3	B	302	NNE	CAD-CAJ	-4.63	1.40	1.49
2	A	301	GSH	O11-C1	-4.15	1.17	1.30
2	B	301	GSH	O11-C1	-3.62	1.19	1.30
3	B	302	NNE	CBC-CL4	-3.36	1.65	1.72
3	B	302	NNE	CAO-CAP	2.88	1.56	1.51
3	B	302	NNE	OAZ-CAP	-2.79	1.17	1.23
3	B	302	NNE	OBA-CAU	-2.54	1.18	1.23
2	A	301	GSH	O31-C3	-2.40	1.22	1.30
3	B	302	NNE	CBD-CL3	-2.32	1.68	1.72
2	A	301	GSH	CG1-CD1	2.29	1.55	1.51
3	B	302	NNE	CAG-CAH	-2.18	1.37	1.40
2	B	301	GSH	O31-C3	-2.14	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	NNE	CBM-CBJ-CBI	-4.70	104.43	120.04
3	B	302	NNE	CAG-CAH-CAI	4.65	122.94	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	NNE	CAD-CAI-CAH	-4.13	118.05	120.86
2	A	301	GSH	CA2-CB2-SG2	-4.08	109.56	114.16
3	B	302	NNE	CBE-CBD-CBC	3.83	122.40	119.86
3	B	302	NNE	CAT-CAU-NAV	-2.98	111.61	116.63
3	B	302	NNE	CAM-CAK-CAJ	-2.91	110.36	120.04
2	B	301	GSH	CB2-CA2-C2	-2.75	103.52	109.50
2	A	301	GSH	CB2-CA2-C2	-2.47	104.14	109.50
2	A	301	GSH	C3-CA3-N3	2.41	120.54	113.06
3	B	302	NNE	OAW-CAG-CAH	2.31	119.49	115.77
3	B	302	NNE	CAS-CAY-CAX	-2.17	103.55	113.56
3	B	302	NNE	CAH-CAI-CL1	2.09	123.86	120.00

There are no chirality outliers.

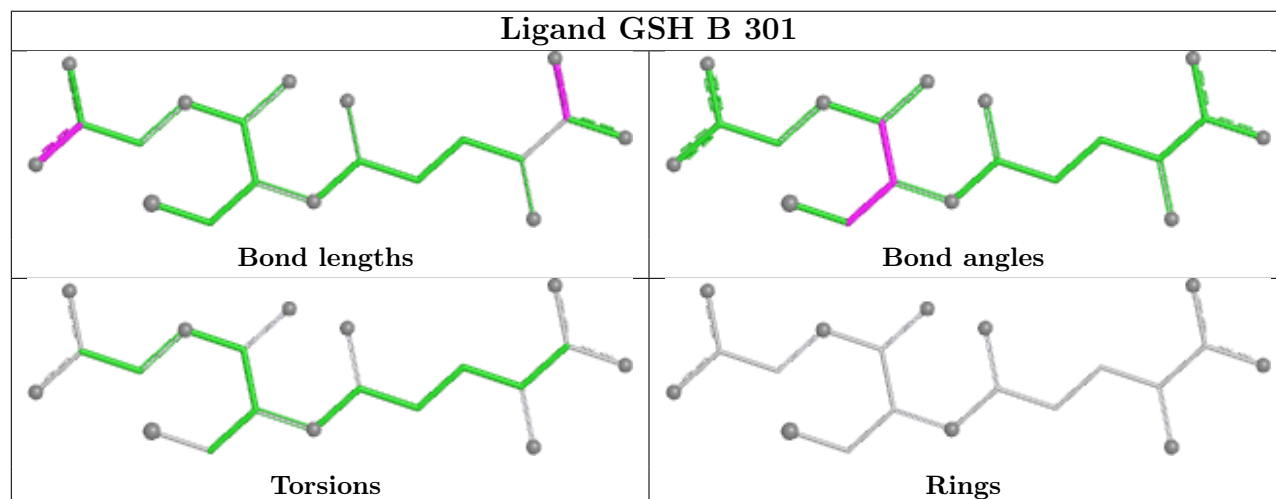
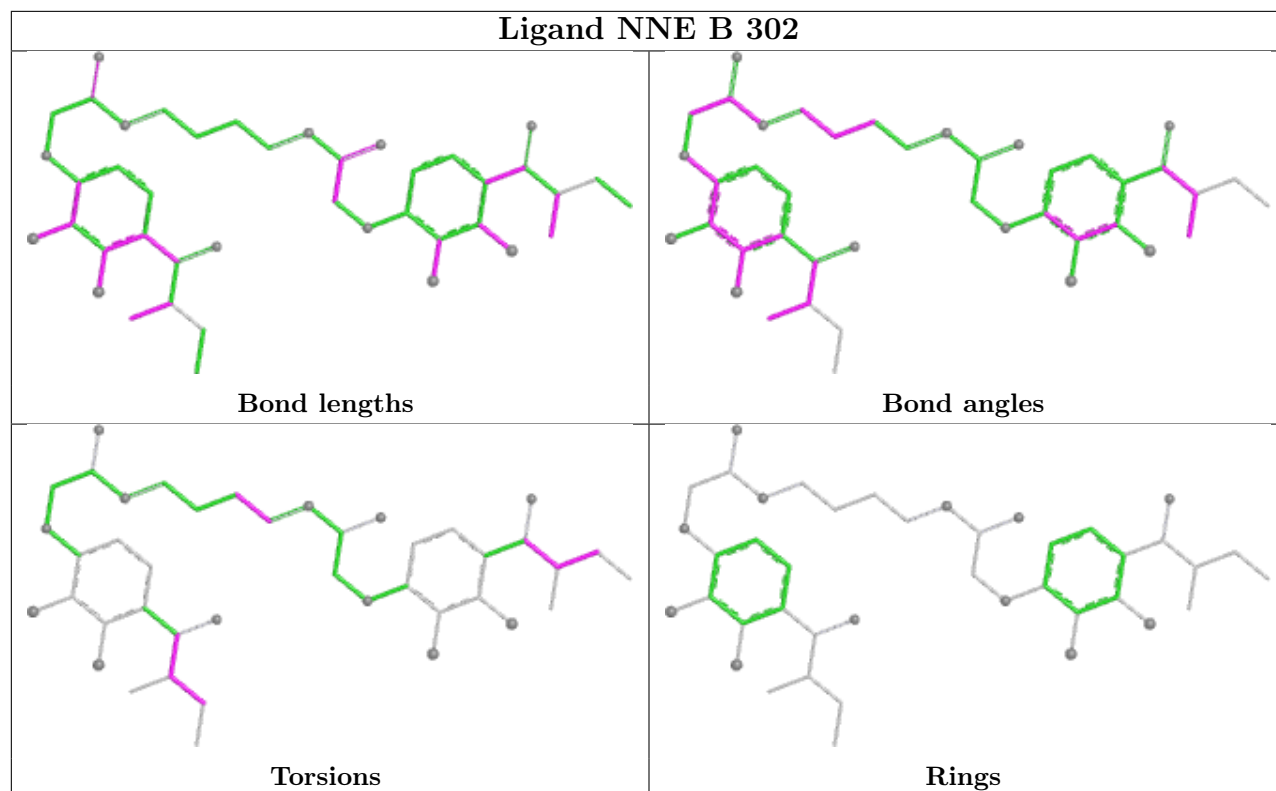
All (7) torsion outliers are listed below:

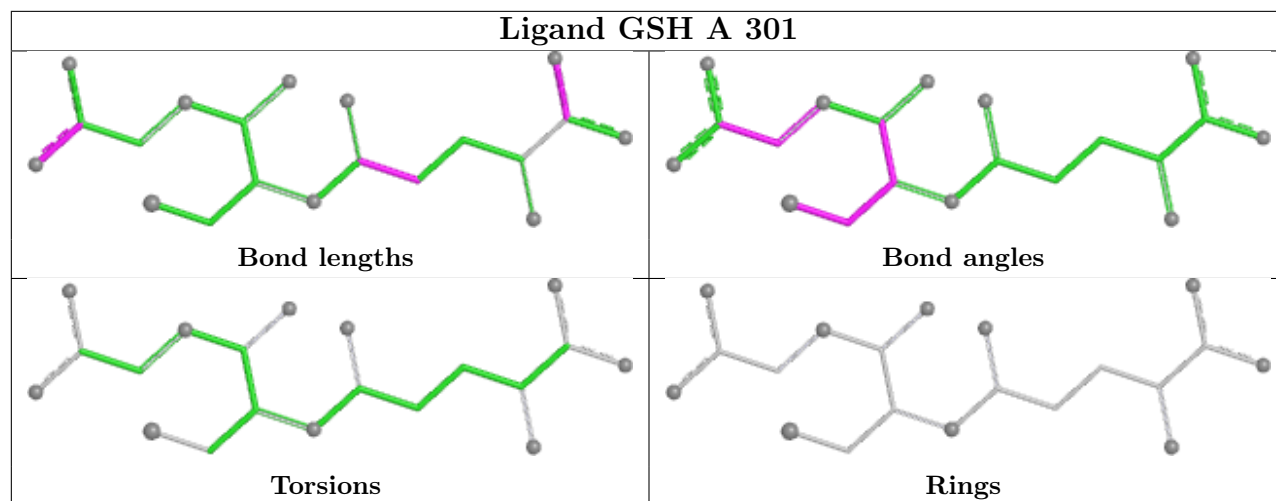
Mol	Chain	Res	Type	Atoms
3	B	302	NNE	OAA-CAJ-CAK-CAM
3	B	302	NNE	CAD-CAJ-CAK-CAM
3	B	302	NNE	CBB-CBI-CBJ-CBM
3	B	302	NNE	OBL-CBI-CBJ-CBM
3	B	302	NNE	CAJ-CAK-CAL-CAN
3	B	302	NNE	CBM-CBJ-CBK-CBN
3	B	302	NNE	NAQ-CAR-CAS-CAY

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

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	217/217 (100%)	0.44	5 (2%) 61 64	9, 18, 29, 44	0
1	B	216/217 (99%)	0.89	24 (11%) 10 10	10, 20, 33, 39	28 (12%)
All	All	433/434 (99%)	0.66	29 (6%) 24 24	9, 19, 31, 44	28 (6%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	PRO	3.8
1	B	38	PRO	3.5
1	B	66	THR	3.5
1	B	119	PHE	3.4
1	B	216	ASN	3.4
1	B	44	GLN	3.2
1	B	122	LEU	3.1
1	B	117	PRO	3.0
1	B	43	SER	2.9
1	A	66	THR	2.9
1	B	37	ALA	2.9
1	B	124	PRO	2.9
1	B	195	ALA	2.8
1	B	39	ASP	2.7
1	B	217	LYS	2.6
1	B	202	PHE	2.4
1	B	2	MET	2.4
1	B	189	GLY	2.4
1	B	50	PHE	2.4
1	B	176	ALA	2.3
1	A	216	ASN	2.3
1	B	108	MET	2.3
1	B	212	ALA	2.2
1	B	118	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	201	ARG	2.2
1	A	37	ALA	2.1
1	B	115	TYR	2.1
1	B	47	ASN	2.0
1	A	213	VAL	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](#)

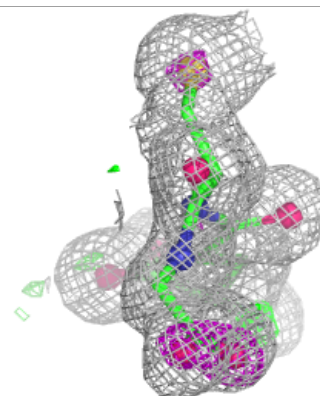
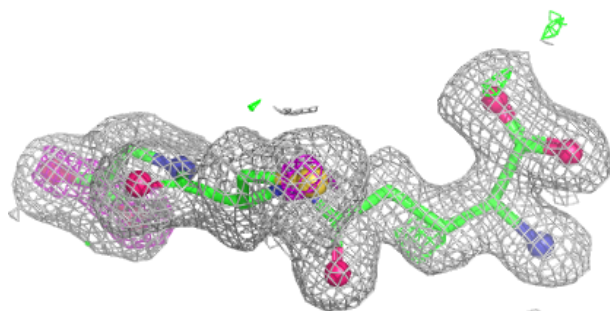
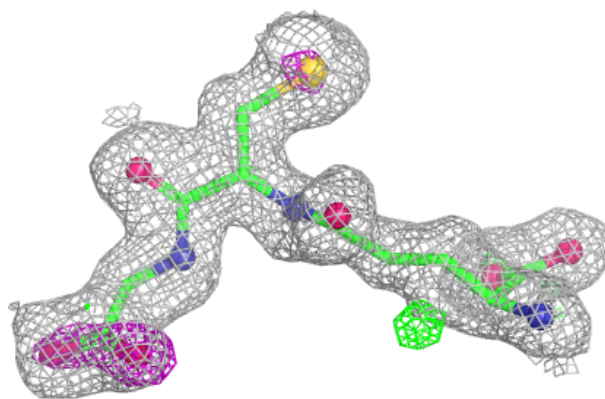
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GSH	B	301	20/20	0.90	0.10	20,20,20,20	0
3	NNE	B	302	42/42	0.91	0.12	20,20,20,20	0
2	GSH	A	301	20/20	0.93	0.10	20,20,20,20	0

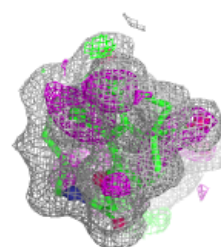
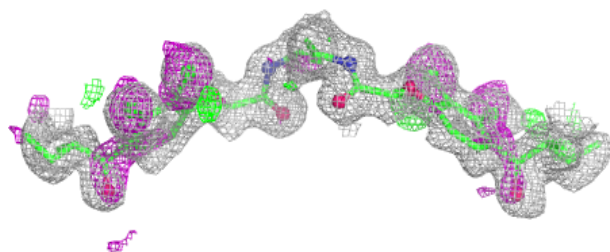
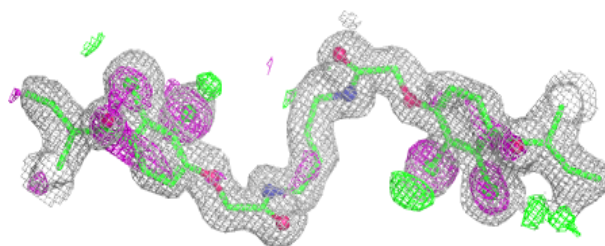
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

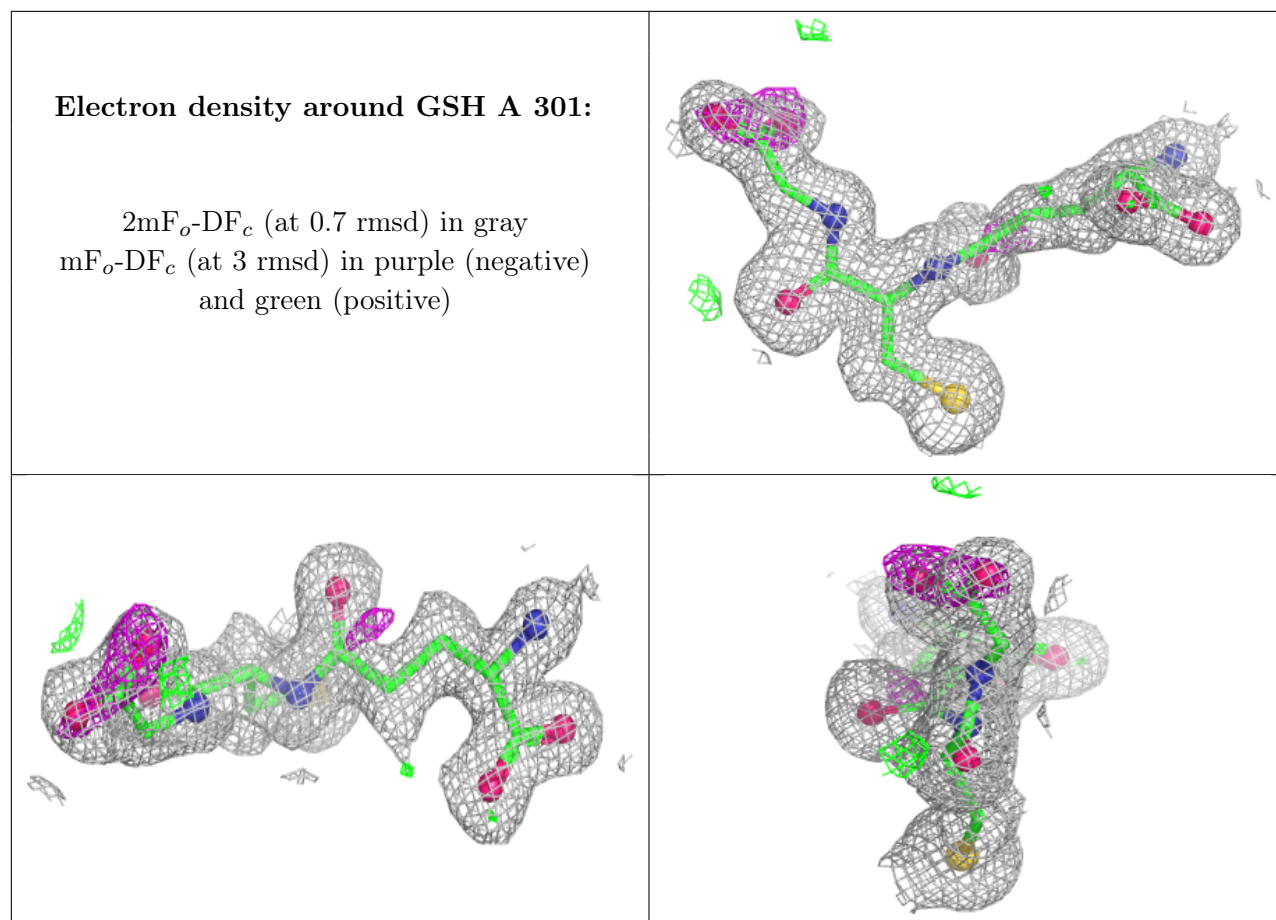
Electron density around GSH B 301:

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

**Electron density around 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 ⓘ

There are no such residues in this entry.