



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:10 PM UTC

PDB ID : 1JZR / pdb_00001jzr
Title : Ure2p in complex with glutathione
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Deposited on : 2001-09-17
Resolution : 2.90 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

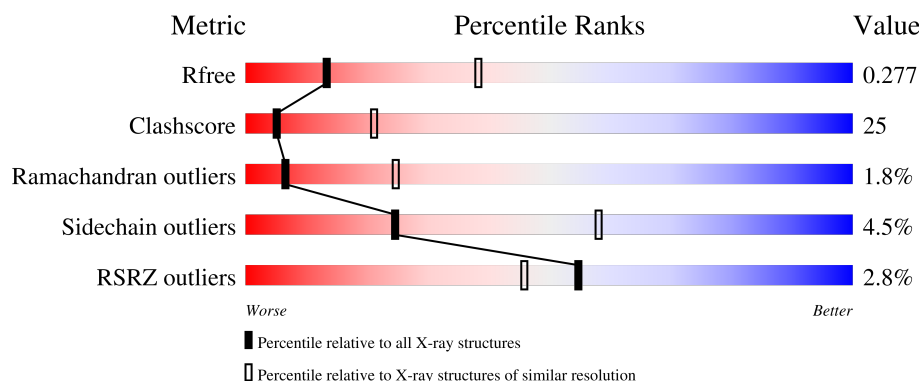
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	260	4% 44% 40% 5% 10%
1	B	260	4% 50% 38% • 7%
1	C	260	% 52% 42% • •
1	D	260	2% 57% 37% 6%

2 Entry composition [i](#)

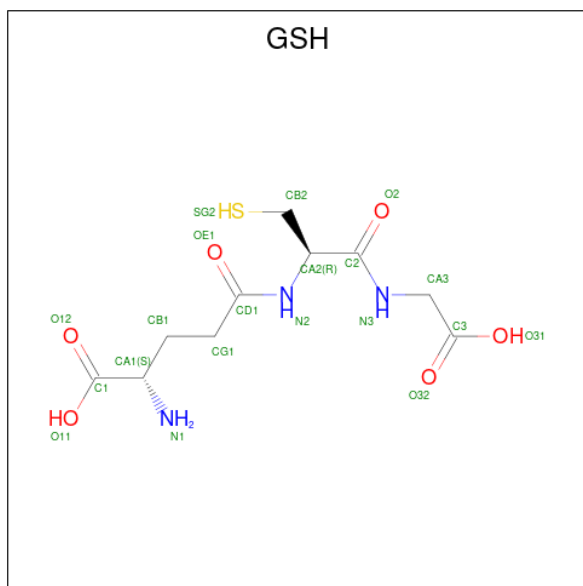
There are 2 unique types of molecules in this entry. The entry contains 8097 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 URE2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1907	1236	329	336	6			
1	B	242	Total	C	N	O	S	0	0	0
			1981	1286	340	349	6			
1	C	255	Total	C	N	O	S	0	0	0
			2065	1333	355	370	7			
1	D	259	Total	C	N	O	S	0	0	0
			2104	1358	361	378	7			

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

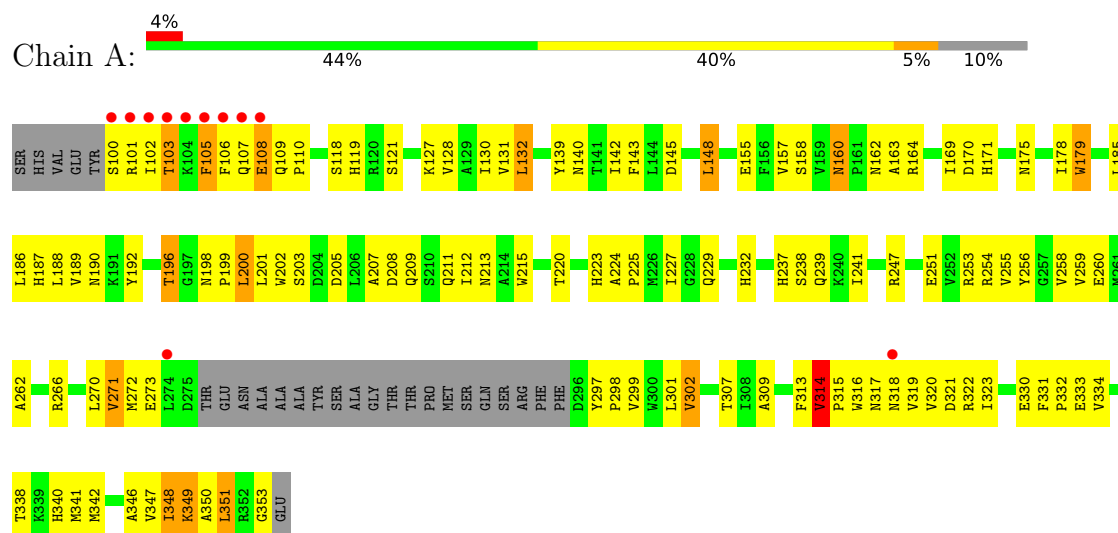


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

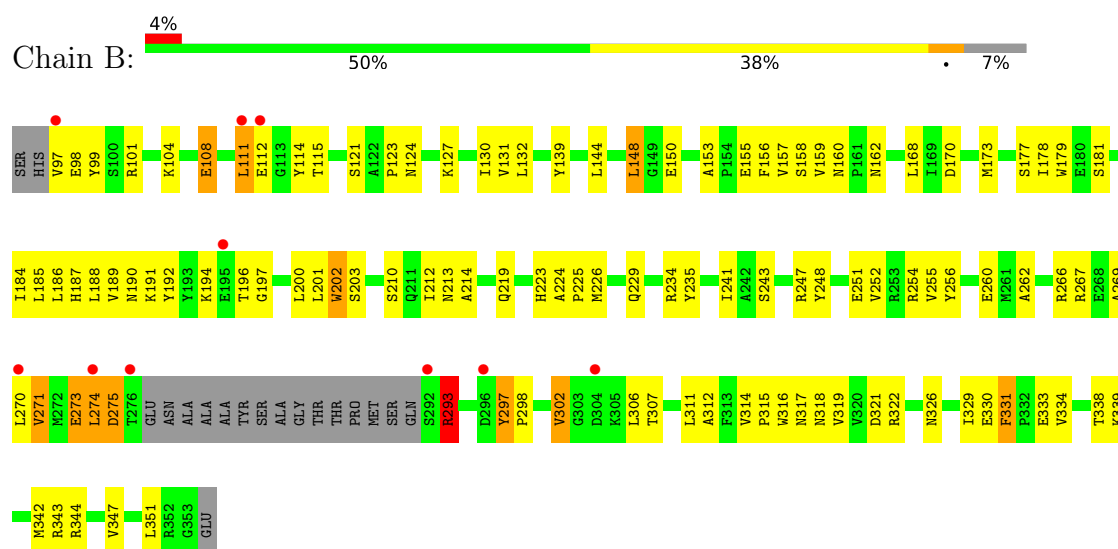
3 Residue-property plots

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: URE2 PROTEIN

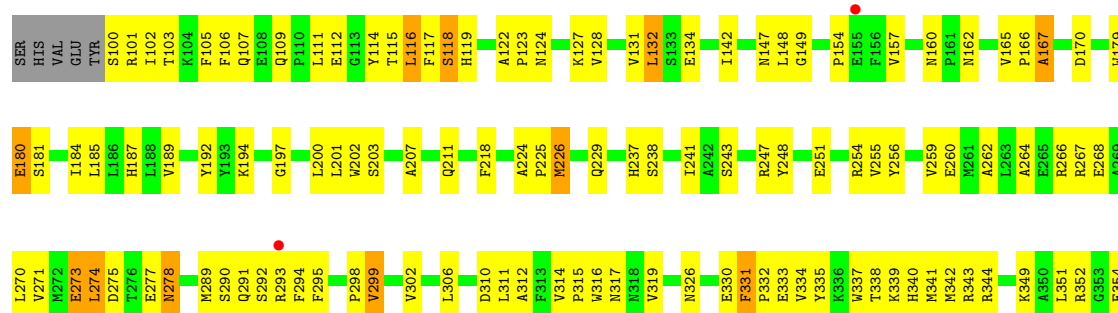


• Molecule 1: URE2 PROTEIN

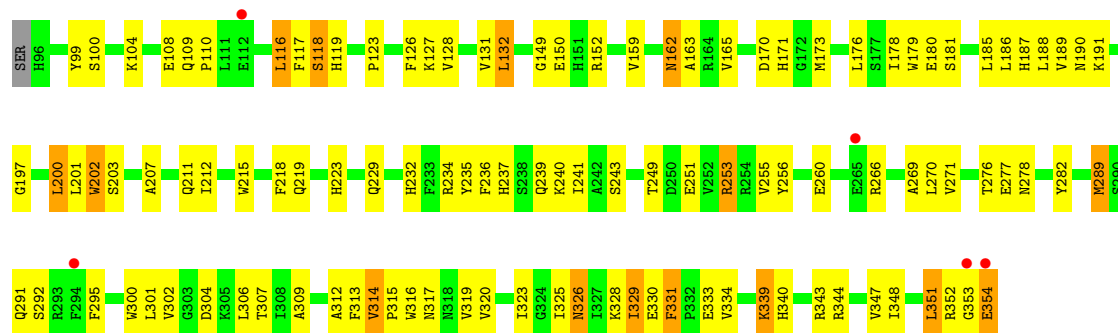


• Molecule 1: URE2 PROTEIN





● Molecule 1: URE2 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.65Å 124.97Å 161.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 99.1 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.97 (at 2.88Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.276 0.210 , 0.277	Depositor DCC
R_{free} test set	1212 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8097	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.98% 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

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	0.49	0/1960	1.01	16/2661 (0.6%)
1	B	0.47	0/2037	0.97	7/2765 (0.3%)
1	C	0.49	1/2123 (0.0%)	0.94	7/2884 (0.2%)
1	D	0.50	0/2164	0.95	13/2939 (0.4%)
All	All	0.49	1/8284 (0.0%)	0.97	43/11249 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	226	MET	SD-CE	-6.36	1.63	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	PHE	N-CA-C	-9.08	102.19	113.18
1	D	302	VAL	N-CA-C	7.40	118.78	108.12
1	A	314	VAL	CB-CA-C	-7.22	106.84	113.70
1	B	331	PHE	CA-C-N	7.09	128.70	119.84
1	B	331	PHE	C-N-CA	7.09	128.70	119.84
1	D	236	PHE	N-CA-C	6.77	121.21	112.41
1	D	179	TRP	N-CA-C	6.74	120.94	111.30
1	A	158	SER	N-CA-C	-6.58	104.72	112.89
1	C	330	GLU	N-CA-C	6.58	119.78	111.69
1	A	348	ILE	N-CA-C	-6.30	105.59	111.45
1	D	197	GLY	N-CA-C	-5.96	107.99	115.08
1	B	197	GLY	N-CA-C	-5.96	106.86	114.37
1	D	313	PHE	N-CA-C	5.93	118.98	111.69
1	A	179	TRP	N-CA-C	5.85	120.80	113.43
1	B	297	TYR	N-CA-C	-5.80	102.77	110.07
1	A	302	VAL	N-CA-C	5.75	116.96	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ALA	N-CA-C	-5.73	99.27	108.55
1	C	331	PHE	CA-C-N	5.73	127.00	119.84
1	C	331	PHE	C-N-CA	5.73	127.00	119.84
1	B	179	TRP	N-CA-C	5.66	121.99	114.12
1	A	331	PHE	CA-C-N	5.65	126.90	119.84
1	A	331	PHE	C-N-CA	5.65	126.90	119.84
1	D	291	GLN	N-CA-C	-5.58	105.98	112.89
1	A	140	ASN	N-CA-C	-5.54	103.38	110.53
1	D	329	ILE	N-CA-C	5.50	117.41	111.58
1	B	158	SER	N-CA-C	-5.46	106.74	113.41
1	A	169	ILE	CB-CA-C	-5.44	104.72	111.08
1	B	235	TYR	N-CA-C	5.41	120.78	114.62
1	C	197	GLY	N-CA-C	-5.38	107.90	115.32
1	A	351	LEU	N-CA-C	-5.38	105.40	113.89
1	D	253	ARG	N-CA-C	-5.37	105.51	111.36
1	D	235	TYR	N-CA-C	5.36	120.18	113.43
1	C	118	SER	N-CA-C	5.34	115.33	108.34
1	D	118	SER	N-CA-C	5.32	115.26	108.24
1	A	313	PHE	N-CA-C	5.27	118.17	111.69
1	D	331	PHE	CA-C-N	5.20	126.34	119.84
1	D	331	PHE	C-N-CA	5.20	126.34	119.84
1	C	302	VAL	N-CA-C	5.19	116.84	108.85
1	D	249	THR	N-CA-C	-5.07	105.83	111.36
1	A	314	VAL	N-CA-C	5.07	119.00	112.67
1	A	148	LEU	N-CA-C	-5.05	107.09	113.20
1	A	139	TYR	N-CA-C	5.04	117.36	108.75
1	A	196	THR	N-CA-C	5.01	119.35	112.68

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	1907	0	1876	109	0
1	B	1981	0	1943	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2065	0	2018	103	0
1	D	2104	0	2049	102	0
2	A	20	0	15	0	0
2	C	20	0	15	1	0
All	All	8097	0	7916	396	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 25.

All (396) 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:D:314:VAL:HG13	1:D:315:PRO:HD3	1.38	1.02
1:A:314:VAL:HG23	1:A:315:PRO:HD3	1.41	1.01
1:B:111:LEU:HD13	1:B:112:GLU:H	1.33	0.93
1:D:266:ARG:NH2	1:D:304:ASP:H	1.66	0.93
1:C:154:PRO:HA	1:C:157:VAL:HG12	1.50	0.92
1:D:266:ARG:HH22	1:D:304:ASP:H	1.09	0.91
1:C:101:ARG:HH11	1:C:101:ARG:HG3	1.40	0.85
1:A:270:LEU:O	1:A:273:GLU:HG2	1.74	0.85
1:A:198:ASN:HD22	1:A:199:PRO:HD2	1.41	0.85
1:D:127:LYS:HD2	1:D:312:ALA:HA	1.59	0.85
1:D:282:TYR:HB3	1:D:289:MET:HE1	1.59	0.85
1:B:111:LEU:CD1	1:B:112:GLU:H	1.90	0.85
1:A:273:GLU:OE2	1:A:273:GLU:HA	1.79	0.82
1:A:254:ARG:HH12	1:B:162:ASN:ND2	1.78	0.82
1:A:196:THR:HG22	1:A:198:ASN:H	1.45	0.81
1:A:162:ASN:ND2	1:B:254:ARG:HH22	1.78	0.80
1:A:131:VAL:HG21	1:A:185:LEU:HD22	1.62	0.80
1:C:154:PRO:HA	1:C:157:VAL:CG1	2.12	0.80
1:B:97:VAL:N	1:C:293:ARG:HH22	1.79	0.80
1:A:171:HIS:HA	1:A:175:ASN:HD22	1.47	0.80
1:C:254:ARG:HH12	1:D:162:ASN:ND2	1.80	0.80
1:A:247:ARG:HH21	1:B:229:GLN:HE22	1.27	0.78
1:D:271:VAL:HG11	1:D:289:MET:HE2	1.64	0.78
1:B:273:GLU:O	1:B:274:LEU:HB2	1.83	0.78
1:D:207:ALA:O	1:D:211:GLN:HG2	1.85	0.76
1:A:109:GLN:HG3	1:A:110:PRO:HD2	1.66	0.76
1:A:334:VAL:O	1:A:338:THR:HG22	1.84	0.76
1:C:179:TRP:O	1:C:180:GLU:HB2	1.86	0.76
1:C:226:MET:HE2	1:C:251:GLU:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:HIS:HD2	1:A:121:SER:H	1.32	0.75
1:C:131:VAL:HG21	1:C:185:LEU:HD22	1.69	0.75
1:A:119:HIS:CD2	1:A:121:SER:H	2.04	0.74
1:B:156:PHE:O	1:B:159:VAL:HG12	1.89	0.73
1:A:314:VAL:HG13	1:A:341:MET:HE3	1.70	0.73
1:C:314:VAL:HB	1:C:315:PRO:HD3	1.70	0.73
1:D:100:SER:O	1:D:104:LYS:HG2	1.89	0.72
1:D:326:ASN:C	1:D:326:ASN:HD22	1.98	0.72
1:A:162:ASN:ND2	1:B:254:ARG:NH2	2.37	0.71
1:B:224:ALA:HB3	1:B:225:PRO:HD3	1.72	0.71
1:A:162:ASN:HD21	1:B:254:ARG:HH22	1.38	0.70
1:D:339:LYS:HA	1:D:339:LYS:HZ3	1.56	0.70
1:C:271:VAL:HG11	1:C:289:MET:HG3	1.74	0.69
1:A:100:SER:HB3	1:A:103:THR:OG1	1.93	0.69
1:B:127:LYS:HZ3	1:B:219:GLN:HE22	1.40	0.69
1:C:119:HIS:HB3	1:C:122:ALA:HB2	1.74	0.69
1:B:267:ARG:NH1	1:B:297:TYR:O	2.27	0.68
1:A:314:VAL:CG2	1:A:315:PRO:HD3	2.22	0.67
1:A:232:HIS:NE2	1:A:237:HIS:HD2	1.92	0.67
1:A:196:THR:HG22	1:A:198:ASN:N	2.09	0.67
1:B:101:ARG:HA	1:B:104:LYS:HD3	1.75	0.67
1:B:159:VAL:HG22	1:B:177:SER:OG	1.95	0.67
1:A:145:ASP:OD2	1:A:148:LEU:HG	1.94	0.67
1:A:247:ARG:HH21	1:B:229:GLN:NE2	1.93	0.67
1:A:347:VAL:O	1:A:351:LEU:HB2	1.94	0.66
1:A:212:ILE:HG23	1:A:309:ALA:HB2	1.78	0.66
1:C:267:ARG:HD2	1:C:333:GLU:OE1	1.96	0.66
1:A:224:ALA:HB3	1:A:225:PRO:HD3	1.78	0.65
1:C:119:HIS:HB3	1:C:122:ALA:CB	2.26	0.65
1:C:127:LYS:HD2	1:C:312:ALA:HA	1.79	0.65
1:B:306:LEU:HD21	1:B:311:LEU:HG	1.77	0.65
1:D:256:TYR:OH	1:D:317:ASN:ND2	2.30	0.64
1:B:225:PRO:O	1:B:229:GLN:HG2	1.98	0.64
1:A:253:ARG:NH1	1:A:330:GLU:OE1	2.30	0.64
1:A:202:TRP:CG	1:A:203:SER:H	2.15	0.63
1:B:127:LYS:NZ	1:B:219:GLN:HE22	1.95	0.63
1:D:253:ARG:NH1	1:D:325:ILE:HG13	2.13	0.63
1:A:102:ILE:HG22	1:A:106:PHE:CZ	2.34	0.63
1:A:171:HIS:HA	1:A:175:ASN:ND2	2.12	0.63
1:D:232:HIS:NE2	1:D:237:HIS:HD2	1.95	0.63
1:D:289:MET:HB3	1:D:295:PHE:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:TYR:HB3	1:D:289:MET:CE	2.28	0.63
1:C:226:MET:CE	1:C:251:GLU:HG2	2.29	0.62
1:D:289:MET:O	1:D:292:SER:HB3	2.00	0.62
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.64	0.62
1:A:254:ARG:HH12	1:B:162:ASN:HD21	1.45	0.62
1:B:131:VAL:HG21	1:B:185:LEU:HD22	1.80	0.62
1:A:229:GLN:HE22	1:B:247:ARG:HH21	1.48	0.62
1:B:173:MET:SD	1:B:191:LYS:NZ	2.72	0.62
1:C:248:TYR:OH	1:D:229:GLN:NE2	2.32	0.61
1:A:348:ILE:C	1:A:350:ALA:H	2.08	0.61
1:B:248:TYR:O	1:B:252:VAL:HG23	2.00	0.61
1:C:147:ASN:C	1:C:149:GLY:H	2.07	0.61
1:D:316:TRP:HA	1:D:319:VAL:HG22	1.81	0.61
1:B:223:HIS:HE1	1:B:316:TRP:HB2	1.66	0.60
1:B:314:VAL:HG22	1:B:315:PRO:HD3	1.82	0.60
1:B:184:ILE:O	1:B:188:LEU:HG	2.01	0.60
1:B:326:ASN:O	1:B:330:GLU:HG3	2.02	0.60
1:D:339:LYS:HA	1:D:339:LYS:NZ	2.16	0.60
1:D:266:ARG:HH22	1:D:304:ASP:N	1.92	0.60
1:A:232:HIS:NE2	1:A:237:HIS:CD2	2.70	0.59
1:A:320:VAL:O	1:A:323:ILE:HG12	2.01	0.59
1:C:103:THR:O	1:C:107:GLN:HG2	2.01	0.59
1:B:97:VAL:HA	1:B:148:LEU:O	2.03	0.59
1:B:344:ARG:HB2	1:B:347:VAL:HG23	1.84	0.59
1:A:298:PRO:HB3	1:A:340:HIS:CE1	2.37	0.59
1:B:226:MET:HG3	1:B:251:GLU:HG2	1.83	0.59
1:B:108:GLU:O	1:B:108:GLU:HG3	2.03	0.59
1:C:181:SER:O	1:C:185:LEU:HG	2.02	0.59
1:A:160:ASN:C	1:A:160:ASN:HD22	2.10	0.58
1:B:314:VAL:CG2	1:B:315:PRO:HD3	2.33	0.58
1:C:326:ASN:C	1:C:326:ASN:HD22	2.11	0.58
1:B:226:MET:HG3	1:B:251:GLU:CG	2.33	0.58
1:C:273:GLU:O	1:C:275:ASP:N	2.36	0.58
1:C:128:VAL:HG12	1:C:132:LEU:HD22	1.86	0.58
1:C:266:ARG:HB2	1:C:299:VAL:CG1	2.34	0.58
1:D:260:GLU:OE1	1:D:331:PHE:HB3	2.03	0.58
1:A:189:VAL:HB	1:A:202:TRP:HB2	1.86	0.58
1:B:319:VAL:HA	1:B:322:ARG:NH1	2.19	0.58
1:B:339:LYS:O	1:B:343:ARG:HG3	2.03	0.58
1:B:124:ASN:ND2	1:B:316:TRP:HZ2	2.02	0.57
1:C:185:LEU:O	1:C:189:VAL:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:O	1:B:108:GLU:CG	2.51	0.57
1:C:349:LYS:HZ3	1:C:354:GLU:C	2.12	0.57
1:B:271:VAL:C	1:B:273:GLU:H	2.13	0.57
1:D:354:GLU:N	1:D:354:GLU:CD	2.63	0.57
1:C:101:ARG:HG3	1:C:101:ARG:NH1	2.13	0.57
1:D:170:ASP:OD2	1:D:187:HIS:HE1	1.87	0.57
1:D:260:GLU:OE1	1:D:334:VAL:HG23	2.05	0.57
1:A:271:VAL:C	1:A:273:GLU:H	2.13	0.56
1:A:128:VAL:O	1:A:132:LEU:HB2	2.05	0.56
1:A:207:ALA:O	1:A:211:GLN:HG2	2.05	0.56
1:A:314:VAL:HG13	1:A:341:MET:CE	2.35	0.56
1:D:223:HIS:NE2	1:D:256:TYR:CE1	2.69	0.56
1:D:189:VAL:HB	1:D:202:TRP:HB2	1.88	0.56
1:A:109:GLN:HG2	1:A:175:ASN:OD1	2.06	0.56
1:C:123:PRO:HB2	1:C:316:TRP:CE2	2.41	0.56
1:C:311:LEU:HA	1:C:314:VAL:HG23	1.88	0.55
1:A:109:GLN:HG3	1:A:110:PRO:CD	2.34	0.55
1:C:107:GLN:HA	1:C:107:GLN:NE2	2.21	0.55
1:D:323:ILE:HG13	1:D:325:ILE:HD13	1.88	0.55
1:A:107:GLN:O	1:A:108:GLU:HB2	2.07	0.55
1:D:271:VAL:HG22	1:D:292:SER:OG	2.07	0.55
1:A:178:ILE:N	1:A:178:ILE:HD12	2.23	0.54
1:A:105:PHE:CZ	1:A:142:ILE:HD11	2.42	0.54
1:A:346:ALA:HA	1:A:349:LYS:HB3	1.89	0.54
1:C:102:ILE:O	1:C:106:PHE:HD1	1.91	0.54
1:A:119:HIS:HD2	1:A:121:SER:N	2.03	0.54
1:D:118:SER:OG	1:D:119:HIS:N	2.39	0.54
1:D:128:VAL:HG12	1:D:132:LEU:HD22	1.90	0.54
1:D:218:PHE:CZ	1:D:255:VAL:HG13	2.43	0.54
1:D:202:TRP:CG	1:D:203:SER:H	2.25	0.54
1:C:277:GLU:O	1:C:278:ASN:HB2	2.07	0.54
1:D:326:ASN:C	1:D:326:ASN:ND2	2.65	0.54
1:C:202:TRP:CG	1:C:203:SER:H	2.26	0.54
1:D:127:LYS:CD	1:D:312:ALA:HA	2.36	0.54
1:B:213:ASN:O	1:B:214:ALA:C	2.51	0.54
1:C:192:TYR:CE2	1:C:200:LEU:HD12	2.43	0.54
1:C:102:ILE:HD12	1:C:102:ILE:N	2.23	0.53
1:B:111:LEU:HD13	1:B:112:GLU:HG2	1.90	0.53
1:C:292:SER:C	1:C:294:PHE:H	2.16	0.53
1:C:254:ARG:HH12	1:D:162:ASN:HD21	1.55	0.53
1:C:243:SER:OG	1:D:237:HIS:HE1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASN:HD22	1:A:199:PRO:CD	2.18	0.53
1:B:234:ARG:HD2	1:B:234:ARG:O	2.08	0.53
1:C:247:ARG:CZ	1:D:232:HIS:CD2	2.92	0.53
1:B:322:ARG:HG3	1:B:322:ARG:NH1	2.24	0.53
1:B:192:TYR:CZ	1:B:196:THR:HG21	2.44	0.53
1:B:297:TYR:CD2	1:B:298:PRO:HD2	2.44	0.53
1:C:247:ARG:HG3	1:C:247:ARG:HH11	1.74	0.52
1:B:186:LEU:O	1:B:190:ASN:ND2	2.42	0.52
1:C:334:VAL:O	1:C:337:TRP:HB3	2.10	0.52
1:A:237:HIS:HE1	1:B:243:SER:OG	1.91	0.52
1:B:130:ILE:HD11	1:B:351:LEU:HD21	1.91	0.52
1:B:157:VAL:HG12	1:B:157:VAL:O	2.09	0.52
1:C:123:PRO:HB2	1:C:316:TRP:CZ2	2.44	0.52
1:C:273:GLU:O	1:C:274:LEU:C	2.52	0.52
1:C:311:LEU:HD23	1:C:341:MET:SD	2.50	0.52
1:D:110:PRO:HD2	1:D:171:HIS:CE1	2.45	0.52
1:A:127:LYS:HG3	1:A:315:PRO:HG2	1.93	0.51
1:B:212:ILE:HG13	1:B:302:VAL:HG21	1.91	0.51
1:D:271:VAL:CG1	1:D:289:MET:HE2	2.38	0.51
1:A:160:ASN:C	1:A:160:ASN:ND2	2.68	0.51
1:D:126:PHE:HB3	1:D:351:LEU:CD1	2.39	0.51
1:D:201:LEU:HA	1:D:307:THR:HA	1.92	0.51
1:D:178:ILE:N	1:D:178:ILE:HD12	2.26	0.51
1:B:338:THR:O	1:B:342:MET:HG2	2.10	0.51
1:D:276:THR:C	1:D:278:ASN:H	2.19	0.51
1:A:160:ASN:HD21	1:A:162:ASN:HB3	1.75	0.51
1:D:116:LEU:HD23	1:D:117:PHE:N	2.26	0.51
1:A:256:TYR:HA	1:A:259:VAL:HG22	1.93	0.51
1:B:186:LEU:HD21	1:B:213:ASN:HD21	1.76	0.51
1:B:273:GLU:O	1:B:273:GLU:CD	2.54	0.51
1:C:259:VAL:HG23	1:C:260:GLU:N	2.25	0.51
1:B:132:LEU:HD23	1:B:139:TYR:CG	2.46	0.50
1:A:253:ARG:NH1	1:A:330:GLU:CD	2.70	0.50
1:A:316:TRP:O	1:A:319:VAL:HG12	2.12	0.50
1:D:239:GLN:HG2	1:D:240:LYS:N	2.26	0.50
1:B:223:HIS:HE1	1:B:316:TRP:CB	2.24	0.50
1:D:126:PHE:CD2	1:D:351:LEU:HA	2.47	0.50
1:B:170:ASP:OD2	1:B:187:HIS:HE1	1.94	0.50
1:B:306:LEU:HD23	1:B:307:THR:N	2.27	0.50
1:C:147:ASN:C	1:C:149:GLY:N	2.66	0.50
1:A:318:ASN:OD1	1:A:342:MET:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:C	1:A:350:ALA:N	2.70	0.49
1:D:126:PHE:HB3	1:D:351:LEU:HD11	1.94	0.49
1:D:314:VAL:CG1	1:D:315:PRO:HD3	2.26	0.49
1:B:97:VAL:N	1:C:293:ARG:NH2	2.54	0.49
1:B:251:GLU:OE2	1:B:251:GLU:HA	2.12	0.49
1:B:316:TRP:C	1:B:318:ASN:H	2.20	0.49
1:D:339:LYS:HA	1:D:339:LYS:CE	2.43	0.49
1:B:326:ASN:C	1:B:326:ASN:HD22	2.21	0.49
1:C:218:PHE:CZ	1:C:255:VAL:HG13	2.48	0.49
1:C:266:ARG:HB2	1:C:299:VAL:HG11	1.94	0.49
1:C:268:GLU:HG3	1:C:289:MET:SD	2.52	0.49
1:D:232:HIS:NE2	1:D:237:HIS:CD2	2.80	0.49
1:A:160:ASN:ND2	1:A:162:ASN:H	2.11	0.48
1:B:114:TYR:HB3	1:B:168:LEU:HD11	1.95	0.48
1:B:219:GLN:O	1:B:223:HIS:HB3	2.13	0.48
1:C:224:ALA:HB3	1:C:225:PRO:HD3	1.95	0.48
1:C:290:SER:HA	1:C:295:PHE:CD2	2.47	0.48
1:C:154:PRO:CA	1:C:157:VAL:HG12	2.33	0.48
1:A:262:ALA:HB1	1:A:266:ARG:NH2	2.28	0.48
1:A:254:ARG:HH22	1:B:162:ASN:HD21	1.60	0.48
1:B:192:TYR:O	1:B:196:THR:HG23	2.13	0.48
1:B:293:ARG:HH11	1:B:293:ARG:CG	2.27	0.48
1:D:185:LEU:O	1:D:189:VAL:HG22	2.13	0.48
1:D:240:LYS:C	1:D:241:ILE:HG13	2.39	0.48
1:D:253:ARG:HG2	1:D:253:ARG:HH11	1.78	0.48
1:A:205:ASP:O	1:A:209:GLN:HG3	2.14	0.48
1:B:108:GLU:O	1:B:108:GLU:OE1	2.30	0.48
1:D:352:ARG:HB2	1:D:354:GLU:OE1	2.14	0.48
1:C:256:TYR:OH	1:C:317:ASN:ND2	2.47	0.48
1:D:186:LEU:O	1:D:190:ASN:HB2	2.13	0.48
1:B:326:ASN:OD1	1:B:329:ILE:HD12	2.13	0.48
1:A:130:ILE:HG12	1:A:347:VAL:HA	1.95	0.47
1:B:155:GLU:CD	1:B:155:GLU:H	2.21	0.47
1:B:192:TYR:CZ	1:B:200:LEU:HD12	2.49	0.47
1:A:162:ASN:HD21	1:B:254:ARG:NH2	2.04	0.47
1:D:237:HIS:C	1:D:239:GLN:H	2.22	0.47
1:C:207:ALA:O	1:C:211:GLN:HG2	2.13	0.47
1:A:215:TRP:CZ3	1:A:259:VAL:HG12	2.50	0.47
1:A:348:ILE:O	1:A:350:ALA:N	2.48	0.47
1:C:117:PHE:HB2	1:C:167:ALA:HB3	1.97	0.47
1:C:266:ARG:CB	1:C:299:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:SER:OG	1:C:119:HIS:N	2.47	0.47
1:D:253:ARG:NH1	1:D:330:GLU:OE1	2.48	0.47
1:A:200:LEU:O	1:A:201:LEU:HB2	2.15	0.47
1:A:266:ARG:HB3	1:A:299:VAL:HG13	1.96	0.47
1:B:144:LEU:HD22	1:B:150:GLU:HB3	1.96	0.47
1:B:251:GLU:O	1:B:255:VAL:HG13	2.14	0.47
1:C:170:ASP:OD2	1:C:187:HIS:HE1	1.98	0.47
1:C:211:GLN:NE2	1:D:176:LEU:HD11	2.30	0.47
1:C:270:LEU:HG	1:C:274:LEU:HD12	1.96	0.47
1:A:110:PRO:HD2	1:A:171:HIS:CE1	2.50	0.47
1:C:124:ASN:HB3	1:C:166:PRO:HD3	1.97	0.47
1:D:251:GLU:OE2	1:D:251:GLU:HA	2.14	0.47
1:B:267:ARG:O	1:B:271:VAL:HG23	2.15	0.47
1:A:127:LYS:HZ1	1:A:220:THR:HG22	1.79	0.47
1:A:349:LYS:HD3	1:A:349:LYS:O	2.15	0.47
1:D:131:VAL:HG21	1:D:185:LEU:HD22	1.96	0.47
1:A:170:ASP:OD2	1:A:187:HIS:HE1	1.97	0.46
1:A:254:ARG:NH1	1:B:162:ASN:HD21	2.10	0.46
1:B:260:GLU:OE2	1:B:334:VAL:HG23	2.15	0.46
1:D:282:TYR:CD2	1:D:289:MET:HE3	2.51	0.46
1:A:251:GLU:OE2	1:A:251:GLU:HA	2.15	0.46
1:A:319:VAL:CG2	1:A:322:ARG:HE	2.29	0.46
1:A:351:LEU:C	1:A:353:GLY:H	2.23	0.46
1:D:348:ILE:O	1:D:352:ARG:HG3	2.16	0.46
1:B:329:ILE:HD11	1:C:112:GLU:CB	2.46	0.46
1:C:264:ALA:O	1:C:267:ARG:HB3	2.15	0.46
1:C:260:GLU:OE1	1:C:331:PHE:HB3	2.16	0.46
1:D:326:ASN:ND2	1:D:329:ILE:H	2.14	0.46
1:D:352:ARG:HH11	1:D:352:ARG:HG2	1.81	0.46
1:A:102:ILE:HB	1:A:155:GLU:HG3	1.98	0.46
1:A:271:VAL:C	1:A:273:GLU:N	2.74	0.46
1:B:178:ILE:N	1:B:178:ILE:HD12	2.31	0.46
1:C:340:HIS:CE1	1:C:343:ARG:HH12	2.33	0.46
1:B:293:ARG:HH11	1:B:293:ARG:HG3	1.81	0.46
1:C:134:GLU:OE2	1:C:344:ARG:NH2	2.49	0.46
1:C:237:HIS:HE1	1:D:243:SER:OG	1.98	0.46
1:A:215:TRP:CE2	1:A:301:LEU:HD22	2.51	0.46
1:A:256:TYR:OH	1:A:317:ASN:ND2	2.49	0.45
1:C:107:GLN:HA	1:C:107:GLN:HE21	1.81	0.45
1:C:194:LYS:O	1:C:194:LYS:HG2	2.16	0.45
1:C:314:VAL:HB	1:C:315:PRO:CD	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LEU:HA	1:C:306:LEU:O	2.16	0.45
1:D:326:ASN:HD21	1:D:328:LYS:HB3	1.82	0.45
1:B:316:TRP:O	1:B:318:ASN:N	2.49	0.45
1:C:298:PRO:HG3	1:C:340:HIS:CE1	2.51	0.45
1:C:116:LEU:C	1:C:116:LEU:CD2	2.89	0.45
1:D:200:LEU:O	1:D:201:LEU:HB2	2.16	0.45
1:A:187:HIS:CD2	1:B:210:SER:OG	2.69	0.45
1:B:316:TRP:C	1:B:318:ASN:N	2.75	0.45
1:C:262:ALA:O	1:C:266:ARG:HG2	2.16	0.45
1:B:159:VAL:CG1	1:B:160:ASN:N	2.79	0.45
1:C:105:PHE:CZ	1:C:115:THR:HG21	2.52	0.45
1:B:234:ARG:NH1	1:C:349:LYS:HG3	2.32	0.45
1:B:269:ALA:O	1:B:273:GLU:HB2	2.17	0.45
1:C:326:ASN:C	1:C:326:ASN:ND2	2.75	0.45
1:A:262:ALA:O	1:A:266:ARG:HD3	2.17	0.45
1:B:200:LEU:C	1:B:202:TRP:H	2.25	0.45
1:C:100:SER:O	1:C:103:THR:N	2.50	0.45
1:A:229:GLN:NE2	1:B:247:ARG:HH21	2.14	0.44
1:B:234:ARG:HH12	1:C:349:LYS:HG3	1.82	0.44
1:B:201:LEU:HA	1:B:307:THR:HA	1.97	0.44
1:C:180:GLU:O	1:C:184:ILE:HG13	2.18	0.44
1:C:101:ARG:HG2	1:C:102:ILE:HD12	1.98	0.44
1:A:186:LEU:HD21	1:A:213:ASN:ND2	2.32	0.44
1:D:132:LEU:HD13	1:D:188:LEU:CD1	2.48	0.44
1:A:163:ALA:O	1:A:164:ARG:NH1	2.46	0.44
1:A:212:ILE:HG13	1:A:302:VAL:HG11	1.99	0.44
1:C:114:TYR:CD1	1:C:114:TYR:N	2.86	0.44
1:A:119:HIS:CD2	1:A:121:SER:N	2.78	0.44
1:C:106:PHE:HA	1:C:109:GLN:HG3	2.00	0.44
1:C:266:ARG:HB2	1:C:299:VAL:HG13	1.98	0.44
1:A:103:THR:C	1:A:105:PHE:H	2.26	0.44
1:C:289:MET:C	1:C:291:GLN:H	2.26	0.44
1:D:123:PRO:HB2	1:D:316:TRP:CE2	2.53	0.44
1:B:271:VAL:C	1:B:273:GLU:N	2.76	0.44
1:C:254:ARG:HH12	1:D:162:ASN:HD22	1.64	0.44
1:B:127:LYS:HE2	1:B:181:SER:HB2	2.00	0.43
1:D:170:ASP:CG	1:D:191:LYS:HZ3	2.26	0.43
1:A:314:VAL:HG23	1:A:315:PRO:CD	2.29	0.43
1:C:134:GLU:CD	1:C:344:ARG:HH21	2.25	0.43
1:D:180:GLU:O	1:D:181:SER:C	2.61	0.43
1:D:260:GLU:OE2	1:D:333:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:C	1:A:202:TRP:H	2.26	0.43
1:A:237:HIS:C	1:A:239:GLN:H	2.25	0.43
1:B:121:SER:O	1:B:123:PRO:HD3	2.17	0.43
1:B:202:TRP:CG	1:B:203:SER:H	2.36	0.43
1:A:202:TRP:CG	1:A:203:SER:N	2.84	0.43
1:A:273:GLU:OE2	1:A:273:GLU:CA	2.56	0.43
1:B:99:TYR:HB3	1:B:150:GLU:HA	1.99	0.43
1:A:192:TYR:O	1:A:196:THR:HB	2.17	0.43
1:A:241:ILE:HG21	1:B:241:ILE:HD13	2.01	0.43
1:C:229:GLN:HB2	1:C:248:TYR:CD2	2.54	0.43
1:D:202:TRP:HE3	1:D:202:TRP:HA	1.84	0.43
1:A:208:ASP:O	1:A:212:ILE:HG13	2.19	0.43
1:D:99:TYR:HB3	1:D:150:GLU:HA	2.00	0.43
1:D:118:SER:HA	1:D:165:VAL:HB	2.00	0.43
1:D:173:MET:HG3	1:D:191:LYS:NZ	2.33	0.43
1:A:132:LEU:HD13	1:A:188:LEU:CD1	2.48	0.43
1:C:105:PHE:CD1	1:C:142:ILE:HD11	2.54	0.43
1:D:269:ALA:O	1:D:270:LEU:C	2.62	0.43
1:D:162:ASN:O	1:D:163:ALA:HB3	2.19	0.43
1:D:202:TRP:HA	1:D:202:TRP:CE3	2.54	0.43
1:B:159:VAL:HG13	1:B:160:ASN:N	2.33	0.42
1:B:262:ALA:O	1:B:266:ARG:HG2	2.19	0.42
1:C:229:GLN:HB2	1:C:248:TYR:CG	2.55	0.42
1:D:212:ILE:HG23	1:D:309:ALA:HB2	2.01	0.42
1:D:253:ARG:NH1	1:D:330:GLU:OE2	2.52	0.42
1:D:352:ARG:HG2	1:D:352:ARG:NH1	2.34	0.42
1:A:314:VAL:HG11	1:A:341:MET:CB	2.49	0.42
1:B:202:TRP:HA	1:B:202:TRP:CE3	2.54	0.42
1:B:252:VAL:O	1:B:256:TYR:HD1	2.03	0.42
1:C:314:VAL:O	1:C:315:PRO:C	2.61	0.42
1:C:192:TYR:CZ	1:C:200:LEU:HD12	2.53	0.42
1:A:223:HIS:O	1:A:227:ILE:HG13	2.20	0.42
1:B:127:LYS:HG3	1:B:312:ALA:HA	2.00	0.42
1:B:160:ASN:C	1:B:160:ASN:OD1	2.62	0.42
1:B:202:TRP:HA	1:B:202:TRP:HE3	1.84	0.42
1:B:189:VAL:HB	1:B:202:TRP:HB2	2.01	0.42
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.90	0.42
1:C:247:ARG:HH21	1:D:229:GLN:HE22	1.66	0.42
1:D:170:ASP:HB3	1:D:176:LEU:HB3	2.01	0.42
1:C:160:ASN:HB2	1:C:179:TRP:HB3	2.01	0.42
1:B:267:ARG:NH2	1:B:333:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ARG:CG	1:B:293:ARG:NH1	2.83	0.41
1:C:256:TYR:HA	1:C:259:VAL:HG22	2.02	0.41
1:D:223:HIS:HD2	1:D:255:VAL:CG1	2.33	0.41
1:D:340:HIS:HA	1:D:343:ARG:NH1	2.35	0.41
1:D:215:TRP:CD2	1:D:301:LEU:HD13	2.55	0.41
1:C:292:SER:C	1:C:294:PHE:N	2.77	0.41
1:A:255:VAL:O	1:A:258:VAL:HB	2.20	0.41
1:C:310:ASP:HA	1:C:337:TRP:HZ2	1.85	0.41
1:D:150:GLU:C	1:D:152:ARG:H	2.29	0.41
1:A:307:THR:C	1:A:309:ALA:N	2.78	0.41
1:C:339:LYS:HD3	1:C:339:LYS:HA	1.59	0.41
1:D:149:GLY:O	1:D:152:ARG:HB2	2.20	0.41
1:D:219:GLN:O	1:D:223:HIS:HB3	2.21	0.41
1:A:270:LEU:HD21	1:A:297:TYR:HB2	2.02	0.41
1:B:115:THR:O	1:B:168:LEU:HD12	2.21	0.41
1:B:339:LYS:HA	1:B:339:LYS:HD3	1.77	0.41
1:D:300:TRP:CZ3	1:D:306:LEU:HD13	2.55	0.41
1:C:241:ILE:CD1	1:D:241:ILE:HG21	2.50	0.41
1:C:165:VAL:HG23	2:C:356:GSH:HB23	2.02	0.41
1:D:344:ARG:HB2	1:D:347:VAL:HG23	2.03	0.41
1:A:101:ARG:O	1:A:101:ARG:HG2	2.21	0.41
1:A:260:GLU:OE2	1:A:333:GLU:HB2	2.20	0.41
1:A:270:LEU:O	1:A:272:MET:N	2.54	0.41
1:B:270:LEU:O	1:B:273:GLU:HB3	2.20	0.41
1:C:162:ASN:ND2	1:D:218:PHE:CE1	2.89	0.41
1:B:98:GLU:O	1:B:98:GLU:HG3	2.21	0.40
1:C:338:THR:O	1:C:342:MET:HG2	2.21	0.40
1:D:354:GLU:CD	1:D:354:GLU:H	2.29	0.40
1:B:260:GLU:OE2	1:B:331:PHE:HB3	2.21	0.40
1:D:109:GLN:HE21	1:D:171:HIS:CE1	2.39	0.40
1:D:173:MET:CG	1:D:191:LYS:HZ2	2.34	0.40
1:C:332:PRO:O	1:C:335:TYR:HB3	2.21	0.40
1:A:118:SER:O	1:A:143:PHE:HA	2.21	0.40
1:A:321:ASP:C	1:A:323:ILE:N	2.80	0.40
1:B:153:ALA:HB1	1:B:155:GLU:OE2	2.22	0.40
1:D:132:LEU:HD13	1:D:188:LEU:HD13	2.03	0.40
1:A:270:LEU:O	1:A:271:VAL:C	2.64	0.40
1:D:234:ARG:NH1	1:D:323:ILE:C	2.79	0.40
1:D:316:TRP:O	1:D:320:VAL:HG13	2.21	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	230/260 (88%)	205 (89%)	19 (8%)	6 (3%)	4	17
1	B	238/260 (92%)	210 (88%)	23 (10%)	5 (2%)	5	21
1	C	253/260 (97%)	224 (88%)	25 (10%)	4 (2%)	7	27
1	D	257/260 (99%)	233 (91%)	21 (8%)	3 (1%)	10	34
All	All	978/1040 (94%)	872 (89%)	88 (9%)	18 (2%)	6	25

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	B	274	LEU
1	B	275	ASP
1	C	274	LEU
1	C	278	ASN
1	A	103	THR
1	A	238	SER
1	A	349	LYS
1	C	273	GLU
1	D	108	GLU
1	B	317	ASN
1	B	293	ARG
1	D	277	GLU
1	C	180	GLU
1	A	271	VAL
1	B	271	VAL
1	A	332	PRO
1	D	353	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/223 (91%)	195 (96%)	7 (4%)	32	66
1	B	210/223 (94%)	200 (95%)	10 (5%)	23	55
1	C	218/223 (98%)	209 (96%)	9 (4%)	27	61
1	D	222/223 (100%)	210 (95%)	12 (5%)	20	51
All	All	852/892 (96%)	814 (96%)	38 (4%)	24	58

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	157	VAL
1	A	160	ASN
1	A	179	TRP
1	A	190	ASN
1	A	200	LEU
1	A	314	VAL
1	B	108	GLU
1	B	111	LEU
1	B	148	LEU
1	B	194	LYS
1	B	202	TRP
1	B	273	GLU
1	B	275	ASP
1	B	293	ARG
1	B	302	VAL
1	B	321	ASP
1	C	111	LEU
1	C	116	LEU
1	C	132	LEU
1	C	148	LEU
1	C	238	SER
1	C	299	VAL
1	C	319	VAL

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Mol	Chain	Res	Type
1	C	351	LEU
1	C	352	ARG
1	D	116	LEU
1	D	132	LEU
1	D	159	VAL
1	D	162	ASN
1	D	200	LEU
1	D	202	TRP
1	D	289	MET
1	D	314	VAL
1	D	326	ASN
1	D	339	LYS
1	D	351	LEU
1	D	354	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	140	ASN
1	A	147	ASN
1	A	160	ASN
1	A	162	ASN
1	A	175	ASN
1	A	187	HIS
1	A	198	ASN
1	A	209	GLN
1	A	211	GLN
1	A	213	ASN
1	A	219	GLN
1	A	229	GLN
1	A	237	HIS
1	A	317	ASN
1	A	340	HIS
1	B	109	GLN
1	B	124	ASN
1	B	151	HIS
1	B	162	ASN
1	B	187	HIS
1	B	209	GLN
1	B	213	ASN
1	B	219	GLN

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Mol	Chain	Res	Type
1	B	229	GLN
1	B	237	HIS
1	B	239	GLN
1	B	318	ASN
1	C	107	GLN
1	C	109	GLN
1	C	119	HIS
1	C	162	ASN
1	C	187	HIS
1	C	198	ASN
1	C	209	GLN
1	C	213	ASN
1	C	219	GLN
1	C	229	GLN
1	C	237	HIS
1	C	239	GLN
1	C	291	GLN
1	C	317	ASN
1	D	96	HIS
1	D	109	GLN
1	D	147	ASN
1	D	162	ASN
1	D	187	HIS
1	D	209	GLN
1	D	219	GLN
1	D	229	GLN
1	D	237	HIS
1	D	317	ASN
1	D	318	ASN
1	D	326	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	GSH	A	355	-	18,19,19	1.33	1 (5%)	21,24,24	0.98	0
2	GSH	C	356	-	18,19,19	1.60	3 (16%)	21,24,24	0.88	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	GSH	A	355	-	-	4/24/24/24	-
2	GSH	C	356	-	-	2/24/24/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	356	GSH	O12-C1	3.32	1.31	1.22
2	A	355	GSH	O12-C1	3.32	1.31	1.22
2	C	356	GSH	CB2-CA2	2.96	1.56	1.53
2	C	356	GSH	CG1-CD1	2.10	1.55	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

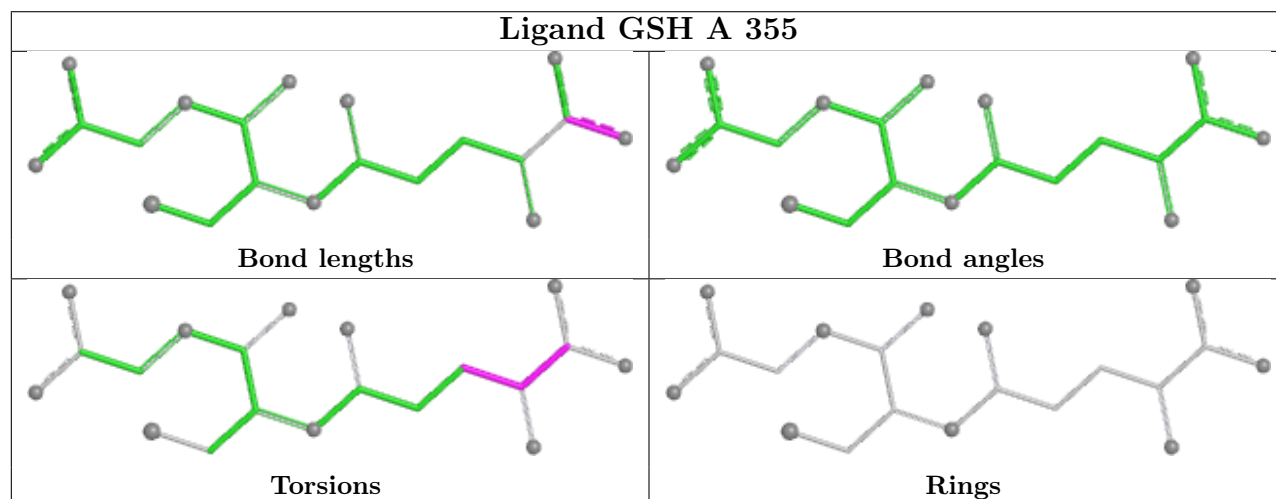
Mol	Chain	Res	Type	Atoms
2	A	355	GSH	N1-CA1-CB1-CG1
2	C	356	GSH	N1-CA1-CB1-CG1
2	A	355	GSH	O11-C1-CA1-N1
2	A	355	GSH	C1-CA1-CB1-CG1
2	A	355	GSH	O12-C1-CA1-N1
2	C	356	GSH	O12-C1-CA1-N1

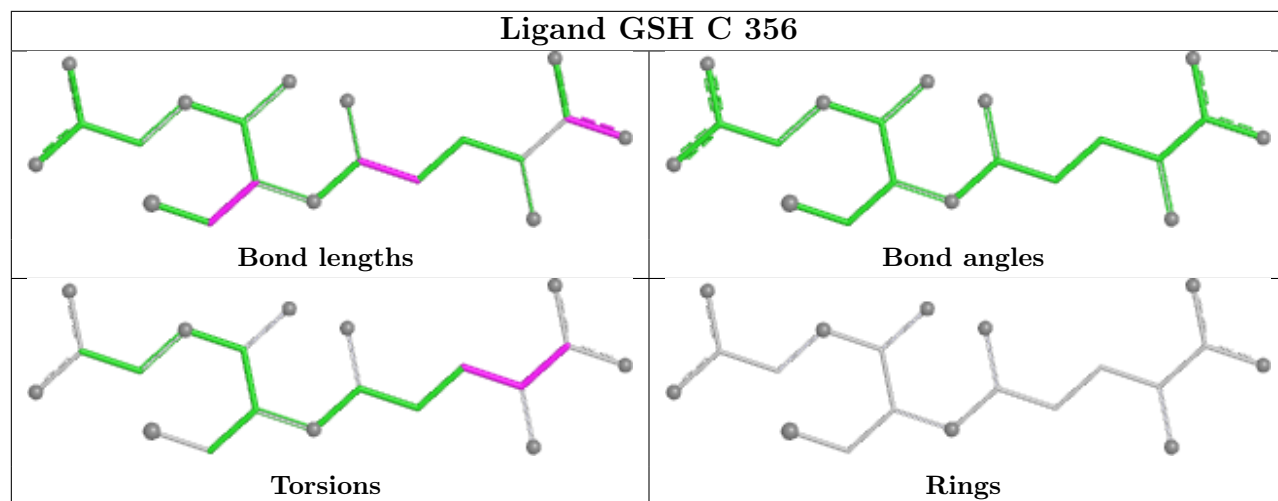
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	356	GSH	1	0

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





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	234/260 (90%)	-0.10	11 (4%) 36 28	2, 12, 43, 64	0
1	B	242/260 (93%)	0.00	10 (4%) 41 33	2, 15, 42, 53	0
1	C	255/260 (98%)	-0.17	2 (0%) 82 77	2, 10, 33, 41	0
1	D	259/260 (99%)	-0.19	5 (1%) 66 58	1, 11, 31, 50	0
All	All	990/1040 (95%)	-0.12	28 (2%) 55 46	1, 12, 36, 64	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	ILE	4.0
1	B	270	LEU	3.9
1	B	111	LEU	3.9
1	A	103	THR	3.8
1	D	353	GLY	3.8
1	A	105	PHE	3.5
1	B	292	SER	3.0
1	A	100	SER	2.9
1	C	293	ARG	2.9
1	B	274	LEU	2.8
1	A	106	PHE	2.7
1	D	112	GLU	2.7
1	B	276	THR	2.6
1	A	108	GLU	2.6
1	A	101	ARG	2.6
1	D	354	GLU	2.6
1	B	97	VAL	2.5
1	A	274	LEU	2.3
1	B	304	ASP	2.3
1	A	107	GLN	2.3
1	A	104	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	318	ASN	2.1
1	B	296	ASP	2.1
1	B	195	GLU	2.1
1	C	155	GLU	2.1
1	B	112	GLU	2.0
1	D	294	PHE	2.0
1	D	265	GLU	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](#)

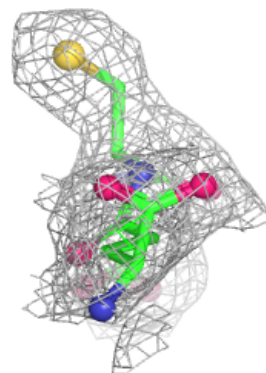
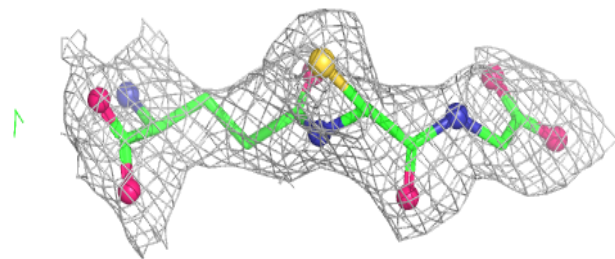
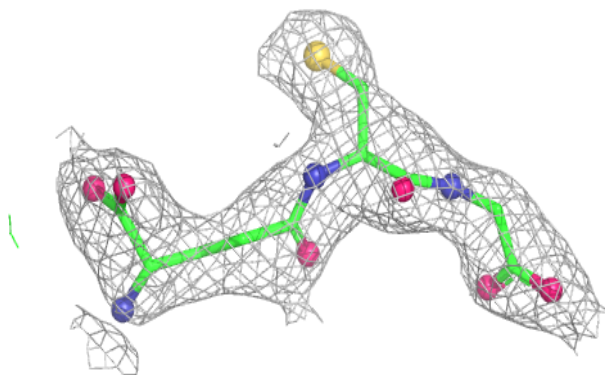
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	355	20/20	0.93	0.09	16,22,26,30	0
2	GSH	C	356	20/20	0.95	0.10	11,15,23,24	0

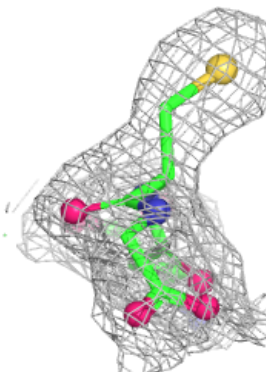
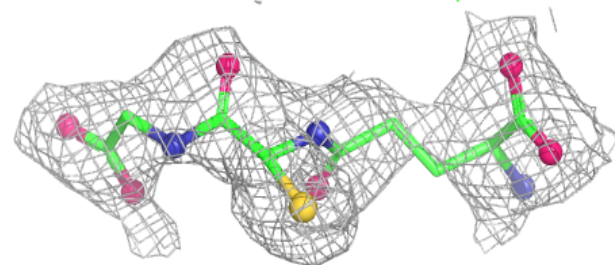
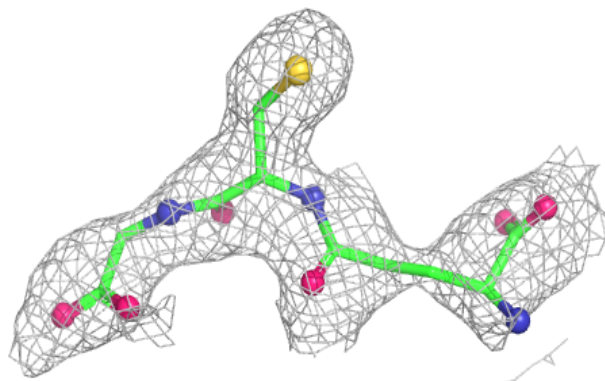
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GSH A 355:

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

**Electron density around GSH C 356:**

$2mF_o-DF_c$ (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.