



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 07:46 pm BST

PDB ID : 1K0B
Title : Ure2p in Complex with Glutathione
Authors : Bousset, L.; Belrhali, H.; Melki, R.; Morera, S.
Deposited on : 2001-09-19
Resolution : 2.50 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

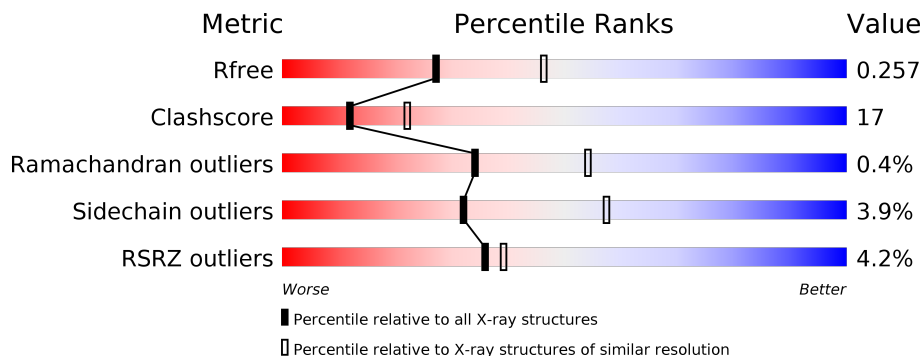
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	260	
1	B	260	
1	C	260	
1	D	260	

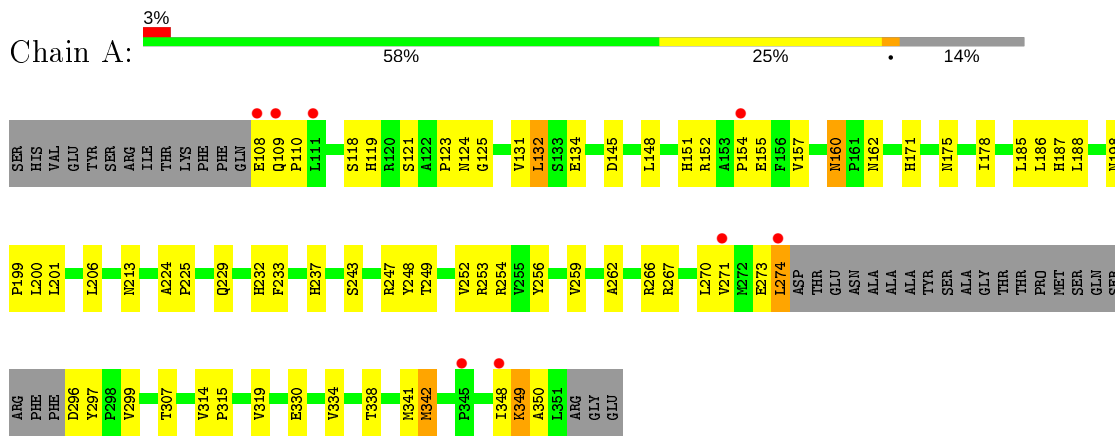
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	57	Total 57	O 57	0	0
3	C	62	Total 62	O 62	0	0
3	D	46	Total 46	O 46	0	0

3 Residue-property plots [i](#)

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.

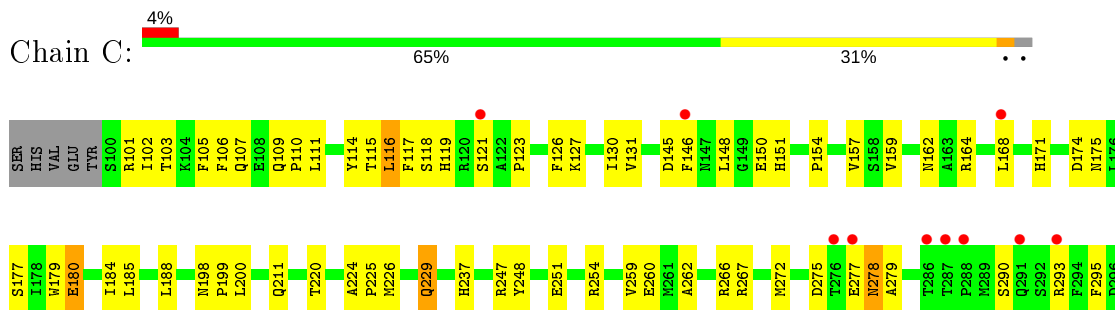
• Molecule 1: URE2 PROTEIN



• Molecule 1: URE2 PROTEIN

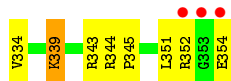


• Molecule 1: URE2 PROTEIN





● 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	54.50Å 124.91Å 160.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.50) 99.9 (19.89-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.50Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.264 0.200 , 0.257	Depositor DCC
R_{free} test set	1943 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtrriage
Anisotropy	0.116	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8205	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% 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

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	0.37	0/1863	0.60	0/2533
1	B	0.37	0/2030	0.58	0/2755
1	C	0.38	0/2123	0.58	0/2884
1	D	0.39	0/2164	0.60	0/2939
All	All	0.38	0/8180	0.59	0/11111

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1812	0	1781	71	0
1	B	1974	0	1936	92	0
1	C	2065	0	2018	69	0
1	D	2104	0	2049	70	0
2	A	20	0	15	0	0
2	C	20	0	15	1	0
3	A	45	0	0	5	0
3	B	57	0	0	2	0
3	C	62	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	46	0	0	2	0
All	All	8205	0	7814	272	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 17.

All (272) 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:247:ARG:HH21	1:B:229:GLN:HE22	1.12	0.97
1:C:352:ARG:HH21	1:C:352:ARG:HB3	1.30	0.95
1:A:131:VAL:HG21	1:A:185:LEU:HD22	1.51	0.92
1:A:162:ASN:ND2	1:B:254:ARG:HH22	1.73	0.87
1:A:229:GLN:HE22	1:B:247:ARG:HH21	1.24	0.82
1:A:145:ASP:OD2	1:A:148:LEU:HG	1.79	0.81
1:B:159:VAL:HG22	1:B:177:SER:CB	2.13	0.78
1:B:131:VAL:HG21	1:B:185:LEU:HD22	1.64	0.77
1:C:247:ARG:HH21	1:D:229:GLN:NE2	1.83	0.77
1:B:173:MET:HE2	1:B:191:LYS:NZ	2.00	0.76
1:B:111:LEU:CD1	1:B:112:GLU:H	1.98	0.76
1:A:254:ARG:HH22	1:B:162:ASN:HD21	1.32	0.76
1:C:226:MET:CE	1:C:251:GLU:HG2	2.18	0.74
1:A:247:ARG:HH21	1:B:229:GLN:NE2	1.85	0.73
1:D:104:LYS:O	1:D:108:GLU:HG2	1.89	0.72
1:C:247:ARG:HH21	1:D:229:GLN:HE22	1.38	0.72
1:B:314:VAL:HG22	1:B:315:PRO:HD3	1.72	0.71
1:A:349:LYS:O	1:A:349:LYS:HD3	1.91	0.70
1:A:162:ASN:HD21	1:B:254:ARG:HH22	1.39	0.70
1:D:159:VAL:HG13	1:D:177:SER:OG	1.92	0.69
1:C:179:TRP:O	1:C:180:GLU:HB2	1.92	0.69
1:D:99:TYR:HB3	1:D:150:GLU:HA	1.74	0.69
1:D:178:ILE:N	1:D:178:ILE:HD12	2.07	0.69
1:B:103:THR:O	1:B:107:GLN:HG2	1.94	0.68
1:B:159:VAL:HG22	1:B:177:SER:HB2	1.75	0.67
1:A:162:ASN:ND2	1:B:254:ARG:NH2	2.43	0.66
1:C:352:ARG:HH21	1:C:352:ARG:CB	2.05	0.66
1:D:323:ILE:HG13	1:D:325:ILE:HD13	1.78	0.66
1:B:326:ASN:O	1:B:330:GLU:HG3	1.96	0.66
1:C:103:THR:O	1:C:107:GLN:HG2	1.96	0.66
1:B:111:LEU:HD13	1:B:112:GLU:H	1.61	0.65
1:C:226:MET:HE2	1:C:251:GLU:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:GLN:HE21	1:C:171:HIS:HE1	1.42	0.65
1:A:314:VAL:HB	1:A:315:PRO:HD3	1.79	0.65
1:C:198:ASN:HD22	1:C:199:PRO:HD2	1.61	0.65
1:B:306:LEU:HD21	1:B:311:LEU:HG	1.78	0.65
1:C:237:HIS:HE1	1:D:243:SER:OG	1.80	0.65
1:A:119:HIS:CD2	1:A:121:SER:H	2.15	0.64
1:B:99:TYR:HB3	1:B:150:GLU:HA	1.78	0.64
1:C:314:VAL:HB	1:C:315:PRO:HD3	1.79	0.64
1:B:267:ARG:NH1	1:B:297:TYR:O	2.28	0.64
1:A:266:ARG:HB3	1:A:299:VAL:HG13	1.80	0.64
1:D:314:VAL:HG13	1:D:315:PRO:HD3	1.80	0.64
1:A:274:LEU:HD22	3:A:392:HOH:O	1.98	0.63
1:A:270:LEU:O	1:A:273:GLU:HB2	1.99	0.63
1:B:326:ASN:C	1:B:326:ASN:HD22	2.02	0.62
1:A:131:VAL:HG21	1:A:185:LEU:CD2	2.26	0.62
1:A:198:ASN:HD22	1:A:199:PRO:HD2	1.63	0.62
1:D:288:PRO:HG2	1:D:291:GLN:HG2	1.80	0.62
1:A:232:HIS:NE2	1:A:237:HIS:HD2	1.97	0.62
1:D:326:ASN:HD22	1:D:329:ILE:H	1.48	0.61
1:B:191:LYS:O	1:B:195:GLU:HG3	2.01	0.61
1:C:226:MET:HE3	1:C:251:GLU:HG2	1.83	0.60
1:B:173:MET:HE3	1:B:187:HIS:NE2	2.15	0.60
1:C:162:ASN:HD21	1:D:254:ARG:HH22	1.47	0.60
1:B:159:VAL:HG22	1:B:177:SER:OG	2.02	0.60
1:C:254:ARG:HH12	1:D:162:ASN:ND2	1.99	0.60
1:B:212:ILE:HG13	1:B:302:VAL:HG21	1.84	0.60
1:C:248:TYR:OH	1:D:229:GLN:HG3	2.02	0.60
1:D:140:ASN:HB2	3:D:381:HOH:O	2.01	0.60
1:C:326:ASN:HD22	1:C:326:ASN:C	2.05	0.59
1:B:173:MET:HE2	1:B:191:LYS:HZ3	1.66	0.59
1:B:314:VAL:CG2	1:B:315:PRO:HD3	2.32	0.59
1:C:159:VAL:HG13	1:C:177:SER:OG	2.02	0.59
1:C:348:ILE:HG22	1:C:352:ARG:HD2	1.84	0.59
1:D:253:ARG:NH1	1:D:325:ILE:HG13	2.18	0.59
1:D:232:HIS:NE2	1:D:237:HIS:HD2	2.00	0.59
1:A:342:MET:HA	1:A:342:MET:CE	2.32	0.59
1:A:247:ARG:NH2	1:B:229:GLN:HE22	1.93	0.58
1:A:187:HIS:HD2	1:B:210:SER:OG	1.85	0.58
1:B:190:ASN:O	1:B:194:LYS:HG2	2.02	0.58
1:B:273:GLU:O	1:B:274:LEU:HB2	2.02	0.58
1:D:271:VAL:HG11	1:D:289:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:HD13	1:B:112:GLU:HG2	1.86	0.58
1:B:178:ILE:HD12	1:B:178:ILE:N	2.18	0.58
1:C:262:ALA:O	1:C:266:ARG:HG2	2.03	0.57
1:A:254:ARG:HH12	1:B:162:ASN:ND2	2.02	0.57
1:D:219:GLN:HE21	1:D:312:ALA:HB1	1.69	0.57
1:A:154:PRO:O	1:A:157:VAL:HG22	2.04	0.57
1:B:224:ALA:HB3	1:B:225:PRO:HD3	1.85	0.57
1:C:119:HIS:HD2	1:C:121:SER:H	1.51	0.57
1:A:178:ILE:HD12	1:A:178:ILE:N	2.20	0.57
1:D:271:VAL:HG11	1:D:289:MET:HE2	1.86	0.57
1:B:127:LYS:HZ3	1:B:219:GLN:HE22	1.54	0.56
1:B:111:LEU:HD12	1:B:112:GLU:H	1.68	0.56
1:A:132:LEU:HD13	1:A:188:LEU:CD1	2.35	0.56
1:A:253:ARG:NH1	1:A:330:GLU:OE1	2.39	0.56
1:C:224:ALA:HB3	1:C:225:PRO:HD3	1.88	0.56
1:A:155:GLU:H	1:A:155:GLU:CD	2.09	0.55
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.71	0.55
1:D:289:MET:HB3	1:D:295:PHE:HE1	1.71	0.55
1:D:289:MET:HB3	1:D:295:PHE:CE1	2.42	0.55
1:C:114:TYR:HB3	1:C:168:LEU:HD11	1.88	0.55
1:D:132:LEU:HD13	1:D:188:LEU:CD1	2.36	0.55
1:A:132:LEU:HD13	1:A:188:LEU:HD11	1.89	0.55
1:C:272:MET:HG3	1:C:279:ALA:HB1	1.89	0.55
1:A:171:HIS:HA	1:A:175:ASN:HD22	1.71	0.54
1:A:237:HIS:HE1	1:B:243:SER:OG	1.89	0.54
1:D:159:VAL:HG13	1:D:177:SER:CB	2.37	0.54
1:D:339:LYS:HA	1:D:339:LYS:NZ	2.22	0.54
1:A:342:MET:HE3	1:A:342:MET:HA	1.90	0.54
1:B:109:GLN:NE2	1:B:169:ILE:HG21	2.23	0.54
1:B:219:GLN:O	1:B:223:HIS:HB3	2.08	0.54
1:A:151:HIS:CE1	1:A:152:ARG:HD3	2.43	0.54
1:A:271:VAL:C	1:A:273:GLU:H	2.11	0.53
1:D:256:TYR:OH	1:D:317:ASN:ND2	2.41	0.53
1:A:160:ASN:HD22	1:A:160:ASN:C	2.11	0.53
1:B:108:GLU:HG3	1:B:108:GLU:O	2.07	0.53
1:B:109:GLN:HE21	1:B:171:HIS:HE1	1.56	0.53
1:C:131:VAL:HG21	1:C:185:LEU:HD22	1.91	0.53
1:C:127:LYS:HD2	1:C:312:ALA:HA	1.90	0.53
1:A:186:LEU:HD21	1:A:213:ASN:HD21	1.74	0.52
1:B:173:MET:HE3	1:B:187:HIS:CE1	2.44	0.52
1:B:310:ASP:HA	1:B:337:TRP:HZ2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:HD23	1:B:307:THR:N	2.23	0.52
1:B:173:MET:HE2	1:B:191:LYS:CE	2.40	0.52
1:C:102:ILE:O	1:C:106:PHE:HD1	1.92	0.52
1:B:101:ARG:NH2	3:B:355:HOH:O	2.42	0.52
1:A:229:GLN:NE2	1:B:247:ARG:HH21	2.01	0.52
1:D:253:ARG:NH1	1:D:330:GLU:OE1	2.43	0.52
1:D:266:ARG:NH2	1:D:304:ASP:H	2.08	0.52
1:A:154:PRO:HA	1:A:157:VAL:HG22	1.92	0.52
1:B:108:GLU:CG	1:B:108:GLU:O	2.58	0.52
1:B:123:PRO:HB2	1:B:316:TRP:CE2	2.44	0.52
1:C:267:ARG:HD2	1:C:333:GLU:OE1	2.10	0.52
1:D:207:ALA:O	1:D:211:GLN:HG2	2.10	0.51
1:C:145:ASP:OD1	1:C:148:LEU:HD13	2.11	0.51
1:C:101:ARG:HD3	1:C:150:GLU:OE2	2.10	0.51
1:C:164:ARG:HG3	3:C:389:HOH:O	2.11	0.51
3:A:367:HOH:O	1:B:210:SER:HA	2.10	0.50
1:A:243:SER:OG	1:B:237:HIS:HE1	1.93	0.50
1:D:128:VAL:HG12	1:D:132:LEU:CD2	2.41	0.50
1:D:339:LYS:O	1:D:343:ARG:HG3	2.11	0.50
1:B:127:LYS:NZ	1:B:219:GLN:HE22	2.09	0.50
1:A:109:GLN:HG3	1:A:110:PRO:HD2	1.94	0.50
1:A:109:GLN:HG2	1:A:175:ASN:ND2	2.27	0.50
1:C:116:LEU:HD23	1:C:117:PHE:N	2.27	0.50
1:C:119:HIS:CD2	1:C:121:SER:H	2.29	0.49
1:D:191:LYS:O	1:D:195:GLU:HG3	2.13	0.49
1:B:111:LEU:HD13	1:B:112:GLU:CG	2.42	0.49
1:C:229:GLN:HE22	1:D:247:ARG:HH21	1.59	0.49
1:B:102:ILE:HG13	1:B:150:GLU:HB3	1.95	0.49
1:B:111:LEU:HD22	1:B:112:GLU:OE1	2.13	0.49
1:C:102:ILE:HD12	1:C:102:ILE:N	2.28	0.49
1:C:123:PRO:HB2	1:C:316:TRP:CE2	2.48	0.48
1:A:349:LYS:C	1:A:349:LYS:HD3	2.33	0.48
1:D:262:ALA:O	1:D:266:ARG:HG2	2.14	0.48
1:A:274:LEU:H	1:A:274:LEU:HD13	1.78	0.48
1:B:97:VAL:HG21	1:B:152:ARG:NH1	2.28	0.48
1:C:116:LEU:HD22	1:C:118:SER:HB2	1.94	0.48
1:D:300:TRP:CZ3	1:D:306:LEU:HD13	2.48	0.48
1:C:116:LEU:CD2	1:C:118:SER:HB2	2.43	0.48
1:D:339:LYS:CE	1:D:339:LYS:HA	2.43	0.48
1:B:212:ILE:CG1	1:B:302:VAL:HG21	2.43	0.48
1:D:354:GLU:H	1:D:354:GLU:CD	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLU:O	1:A:274:LEU:C	2.52	0.47
1:B:201:LEU:HD22	1:B:306:LEU:HD22	1.96	0.47
1:A:119:HIS:HD2	1:A:121:SER:H	1.59	0.47
1:A:160:ASN:ND2	1:A:162:ASN:H	2.13	0.47
1:A:266:ARG:HB3	1:A:299:VAL:CG1	2.44	0.47
1:D:314:VAL:CG1	1:D:315:PRO:HD3	2.43	0.47
1:D:260:GLU:OE1	1:D:331:PHE:HB3	2.14	0.47
1:D:98:GLU:OE2	1:D:98:GLU:HA	2.15	0.47
1:B:184:ILE:O	1:B:188:LEU:HG	2.15	0.47
1:B:97:VAL:N	1:C:293:ARG:NH2	2.63	0.47
1:C:277:GLU:O	1:C:278:ASN:HB2	2.14	0.47
1:B:335:TYR:OH	1:B:339:LYS:NZ	2.45	0.47
1:C:229:GLN:HG3	1:D:248:TYR:OH	2.15	0.47
1:B:306:LEU:HD21	1:B:311:LEU:CG	2.43	0.46
1:A:248:TYR:O	1:A:252:VAL:HG23	2.15	0.46
1:D:132:LEU:HD13	1:D:188:LEU:HD13	1.97	0.46
1:B:148:LEU:HD13	1:C:297:TYR:OH	2.16	0.46
1:B:201:LEU:HA	1:B:307:THR:HA	1.98	0.46
1:C:290:SER:HA	1:C:295:PHE:CD2	2.50	0.46
1:B:111:LEU:HD12	1:B:111:LEU:N	2.31	0.46
1:D:159:VAL:HG13	1:D:177:SER:HG	1.80	0.46
1:D:232:HIS:NE2	1:D:237:HIS:CD2	2.81	0.46
1:D:253:ARG:NH2	3:D:369:HOH:O	2.49	0.46
1:C:220:THR:O	1:D:221:SER:HB2	2.16	0.46
1:B:97:VAL:N	1:C:293:ARG:HH22	2.13	0.46
1:B:111:LEU:HD13	1:B:112:GLU:CD	2.36	0.45
1:A:121:SER:O	1:A:123:PRO:HD3	2.16	0.45
1:A:171:HIS:HA	1:A:175:ASN:ND2	2.31	0.45
1:C:107:GLN:NE2	1:C:107:GLN:HA	2.32	0.45
1:A:134:GLU:HG2	1:A:201:LEU:HD11	1.98	0.45
1:A:206:LEU:HD22	1:B:194:LYS:HD3	1.99	0.45
1:B:322:ARG:HG3	1:B:322:ARG:NH1	2.31	0.45
1:D:118:SER:O	1:D:143:PHE:HA	2.16	0.45
1:A:297:TYR:HD1	3:A:390:HOH:O	2.00	0.45
1:B:262:ALA:O	1:B:266:ARG:HG2	2.17	0.45
1:C:154:PRO:O	1:C:157:VAL:HG12	2.17	0.45
1:A:187:HIS:CD2	1:B:210:SER:OG	2.67	0.45
1:C:110:PRO:HG2	1:C:171:HIS:CD2	2.52	0.45
1:C:339:LYS:O	1:C:343:ARG:HG3	2.17	0.45
1:B:117:PHE:HE1	1:B:169:ILE:HD12	1.81	0.44
1:B:270:LEU:HD12	1:B:299:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:SER:O	1:B:185:LEU:HG	2.17	0.44
1:B:151:HIS:H	1:B:151:HIS:CD2	2.34	0.44
1:D:344:ARG:HA	1:D:345:PRO:HD3	1.88	0.44
1:A:201:LEU:HA	1:A:307:THR:HA	1.98	0.44
1:B:170:ASP:OD2	1:B:187:HIS:HE1	2.00	0.44
1:B:201:LEU:CD2	1:B:306:LEU:HD22	2.47	0.44
1:D:103:THR:O	1:D:107:GLN:HG3	2.17	0.44
1:B:173:MET:CE	1:B:191:LYS:NZ	2.74	0.44
1:C:115:THR:O	1:C:168:LEU:HD12	2.17	0.44
1:C:179:TRP:O	1:C:180:GLU:CB	2.65	0.44
1:C:344:ARG:HA	1:C:345:PRO:HD3	1.87	0.44
1:A:319:VAL:O	1:A:319:VAL:HG22	2.17	0.44
1:B:114:TYR:HB3	1:B:168:LEU:HD11	2.00	0.44
1:A:296:ASP:N	3:A:376:HOH:O	2.50	0.43
1:C:126:PHE:O	1:C:130:ILE:HG13	2.17	0.43
1:C:340:HIS:HA	1:C:343:ARG:NH1	2.33	0.43
1:D:178:ILE:CD1	1:D:178:ILE:N	2.77	0.43
1:A:314:VAL:CG2	1:A:341:MET:SD	3.07	0.43
1:D:260:GLU:OE1	1:D:334:VAL:HG23	2.17	0.43
1:D:247:ARG:HH11	1:D:247:ARG:HG3	1.83	0.43
1:A:271:VAL:C	1:A:273:GLU:N	2.71	0.43
1:A:334:VAL:O	1:A:338:THR:HG22	2.19	0.43
1:C:174:ASP:O	1:C:175:ASN:HB2	2.18	0.43
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.84	0.43
1:C:118:SER:OG	1:C:119:HIS:N	2.51	0.43
1:D:192:TYR:CE2	1:D:200:LEU:HB2	2.54	0.43
1:B:160:ASN:HA	1:B:161:PRO:HD2	1.82	0.43
1:A:124:ASN:HB2	3:A:359:HOH:O	2.19	0.42
1:D:219:GLN:NE2	1:D:312:ALA:HB1	2.33	0.42
1:D:127:LYS:HD2	1:D:312:ALA:HA	2.01	0.42
1:D:253:ARG:NH1	1:D:330:GLU:OE2	2.52	0.42
1:A:249:THR:O	1:A:253:ARG:HG3	2.19	0.42
1:D:128:VAL:HG12	1:D:132:LEU:HD22	2.02	0.42
1:C:275:ASP:OD1	1:C:278:ASN:HB3	2.18	0.42
1:B:319:VAL:HA	1:B:322:ARG:NH1	2.35	0.42
1:C:105:PHE:CZ	1:C:115:THR:HG21	2.55	0.42
1:D:132:LEU:HD13	1:D:188:LEU:HD11	2.00	0.42
1:D:96:HIS:CD2	1:D:97:VAL:HG23	2.55	0.42
1:A:224:ALA:HB3	1:A:225:PRO:HD3	2.01	0.42
1:B:125:GLY:HA2	1:B:166:PRO:HB3	2.02	0.42
1:B:322:ARG:HD3	3:B:367:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASN:O	1:B:164:ARG:HG2	2.20	0.42
1:C:116:LEU:CD2	1:C:116:LEU:C	2.88	0.42
1:C:352:ARG:CG	1:C:352:ARG:HH21	2.32	0.42
1:A:233:PHE:HA	1:A:237:HIS:HB2	2.00	0.42
1:D:282:TYR:HB3	1:D:289:MET:HE1	2.02	0.42
1:C:109:GLN:HE21	1:C:171:HIS:CE1	2.28	0.41
1:C:339:LYS:HA	1:C:339:LYS:HD3	1.76	0.41
1:A:262:ALA:O	1:A:266:ARG:HD3	2.21	0.41
1:A:267:ARG:O	1:A:271:VAL:HG23	2.20	0.41
1:C:260:GLU:OE1	1:C:331:PHE:HB3	2.21	0.41
1:A:132:LEU:HD13	1:A:188:LEU:HD13	2.02	0.41
1:A:348:ILE:O	1:A:350:ALA:N	2.53	0.41
1:B:111:LEU:H	1:B:111:LEU:HD12	1.86	0.41
1:A:254:ARG:NH2	1:B:162:ASN:HD21	2.06	0.41
1:D:266:ARG:HH22	1:D:304:ASP:H	1.68	0.41
1:D:352:ARG:HG2	1:D:352:ARG:HH11	1.85	0.41
1:A:108:GLU:HG2	1:A:108:GLU:O	2.21	0.41
1:A:256:TYR:HA	1:A:259:VAL:HG22	2.03	0.41
1:D:248:TYR:O	1:D:252:VAL:HG23	2.21	0.41
1:C:211:GLN:HE21	1:D:176:LEU:HD11	1.86	0.41
1:D:219:GLN:O	1:D:223:HIS:HB3	2.20	0.41
1:A:118:SER:OG	1:A:125:GLY:HA3	2.20	0.41
1:D:126:PHE:O	1:D:130:ILE:HG13	2.21	0.41
1:D:128:VAL:O	1:D:132:LEU:HD22	2.21	0.41
1:C:184:ILE:O	1:C:188:LEU:HG	2.20	0.41
1:C:314:VAL:CG2	1:C:341:MET:SD	3.09	0.41
1:B:108:GLU:OE1	1:B:108:GLU:O	2.38	0.40
1:D:153:ALA:HA	1:D:154:PRO:HD3	1.95	0.40
1:D:123:PRO:HB2	1:D:316:TRP:CE2	2.56	0.40
1:B:271:VAL:C	1:B:273:GLU:H	2.24	0.40
1:C:146:PHE:CE1	2:C:356:GSH:HA32	2.56	0.40
1:B:248:TYR:O	1:B:252:VAL:HG23	2.22	0.40
1:C:259:VAL:HG23	1:C:334:VAL:HG22	2.03	0.40
1:B:306:LEU:HD23	1:B:306:LEU:C	2.41	0.40
1:C:247:ARG:NH2	1:D:229:GLN:HE22	2.13	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/260 (84%)	211 (96%)	7 (3%)	1 (0%)	29	48
1	B	237/260 (91%)	226 (95%)	10 (4%)	1 (0%)	34	54
1	C	253/260 (97%)	242 (96%)	9 (4%)	2 (1%)	19	35
1	D	257/260 (99%)	247 (96%)	10 (4%)	0	100	100
All	All	966/1040 (93%)	926 (96%)	36 (4%)	4 (0%)	34	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	274	LEU
1	C	278	ASN
1	A	349	LYS
1	C	180	GLU

5.3.2 Protein sidechains [i](#)

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	192/223 (86%)	187 (97%)	5 (3%)	46	72
1	B	209/223 (94%)	198 (95%)	11 (5%)	22	43
1	C	218/223 (98%)	210 (96%)	8 (4%)	34	60
1	D	222/223 (100%)	213 (96%)	9 (4%)	30	55
All	All	841/892 (94%)	808 (96%)	33 (4%)	32	57

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	160	ASN
1	A	200	LEU
1	A	274	LEU
1	A	342	MET
1	B	108	GLU
1	B	111	LEU
1	B	148	LEU
1	B	159	VAL
1	B	194	LYS
1	B	202	TRP
1	B	267	ARG
1	B	273	GLU
1	B	302	VAL
1	B	321	ASP
1	B	326	ASN
1	C	111	LEU
1	C	116	LEU
1	C	151	HIS
1	C	200	LEU
1	C	229	GLN
1	C	299	VAL
1	C	326	ASN
1	C	352	ARG
1	D	96	HIS
1	D	116	LEU
1	D	132	LEU
1	D	162	ASN
1	D	200	LEU
1	D	229	GLN
1	D	289	MET
1	D	339	LYS
1	D	351	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	119	HIS
1	A	147	ASN
1	A	160	ASN

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Mol	Chain	Res	Type
1	A	162	ASN
1	A	175	ASN
1	A	187	HIS
1	A	198	ASN
1	A	209	GLN
1	A	213	ASN
1	A	219	GLN
1	A	229	GLN
1	A	237	HIS
1	A	317	ASN
1	B	109	GLN
1	B	151	HIS
1	B	162	ASN
1	B	209	GLN
1	B	213	ASN
1	B	219	GLN
1	B	229	GLN
1	B	237	HIS
1	B	239	GLN
1	B	318	ASN
1	B	326	ASN
1	C	107	GLN
1	C	109	GLN
1	C	119	HIS
1	C	140	ASN
1	C	162	ASN
1	C	175	ASN
1	C	198	ASN
1	C	209	GLN
1	C	211	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	C	318	ASN
1	C	326	ASN
1	D	96	HIS
1	D	109	GLN
1	D	147	ASN

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Mol	Chain	Res	Type
1	D	162	ASN
1	D	187	HIS
1	D	209	GLN
1	D	213	ASN
1	D	219	GLN
1	D	229	GLN
1	D	237	HIS
1	D	317	ASN
1	D	326	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	C	356	-	12,19,19	1.37	2 (16%)	15,24,24	0.78	0
2	GSH	A	355	-	12,19,19	1.11	1 (8%)	15,24,24	0.93	1 (6%)

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	C	356	-	-	4/18/24/24	-
2	GSH	A	355	-	-	2/18/24/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	356	GSH	CB2-CA2	2.65	1.56	1.53
2	A	355	GSH	CG1-CD1	2.26	1.55	1.51
2	C	356	GSH	CG1-CD1	2.26	1.55	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	355	GSH	CA2-CB2-SG2	-2.46	111.43	114.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	356	GSH	N1-CA1-CB1-CG1
2	C	356	GSH	C1-CA1-CB1-CG1
2	A	355	GSH	N2-CA2-CB2-SG2
2	A	355	GSH	C2-CA2-CB2-SG2
2	C	356	GSH	C2-CA2-CB2-SG2
2	C	356	GSH	C3-CA3-N3-C2

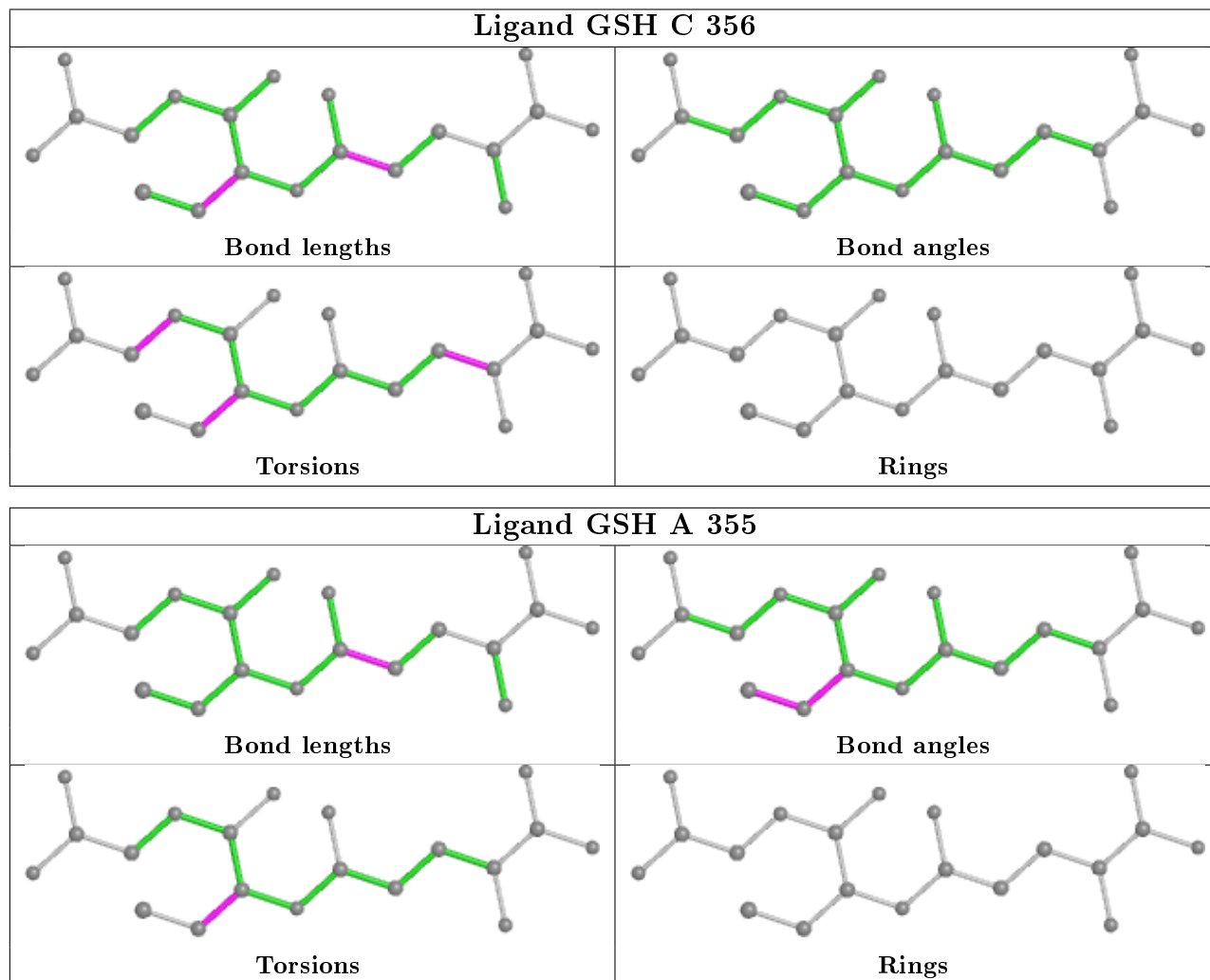
There are no ring outliers.

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	223/260 (85%)	0.00	8 (3%) 42 46	12, 24, 49, 74	0
1	B	241/260 (92%)	0.15	16 (6%) 18 19	13, 28, 61, 80	0
1	C	255/260 (98%)	-0.07	10 (3%) 39 42	11, 22, 54, 67	0
1	D	259/260 (99%)	-0.06	7 (2%) 54 58	9, 23, 44, 73	0
All	All	978/1040 (94%)	0.00	41 (4%) 36 39	9, 25, 54, 80	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	LEU	7.0
1	B	111	LEU	6.6
1	D	353	GLY	5.6
1	D	96	HIS	5.0
1	B	295	PHE	4.6
1	A	108	GLU	4.2
1	A	109	GLN	4.1
1	D	354	GLU	3.7
1	B	107	GLN	3.7
1	A	274	LEU	3.7
1	C	277	GLU	3.6
1	B	293	ARG	3.6
1	A	271	VAL	3.5
1	C	288	PRO	3.5
1	B	275	ASP	3.2
1	B	304	ASP	3.0
1	B	104	LYS	3.0
1	C	293	ARG	3.0
1	B	97	VAL	3.0
1	C	286	THR	3.0
1	B	292	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	352	ARG	2.7
1	C	287	THR	2.6
1	A	348	ILE	2.5
1	C	291	GLN	2.5
1	C	276	THR	2.4
1	C	121	SER	2.4
1	B	138	HIS	2.4
1	A	111	LEU	2.3
1	B	353	GLY	2.3
1	A	345	PRO	2.2
1	B	343	ARG	2.2
1	B	270	LEU	2.2
1	D	97	VAL	2.2
1	D	112	GLU	2.2
1	B	294	PHE	2.1
1	C	168	LEU	2.1
1	A	154	PRO	2.1
1	B	271	VAL	2.1
1	C	146	PHE	2.0
1	D	108	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](#)

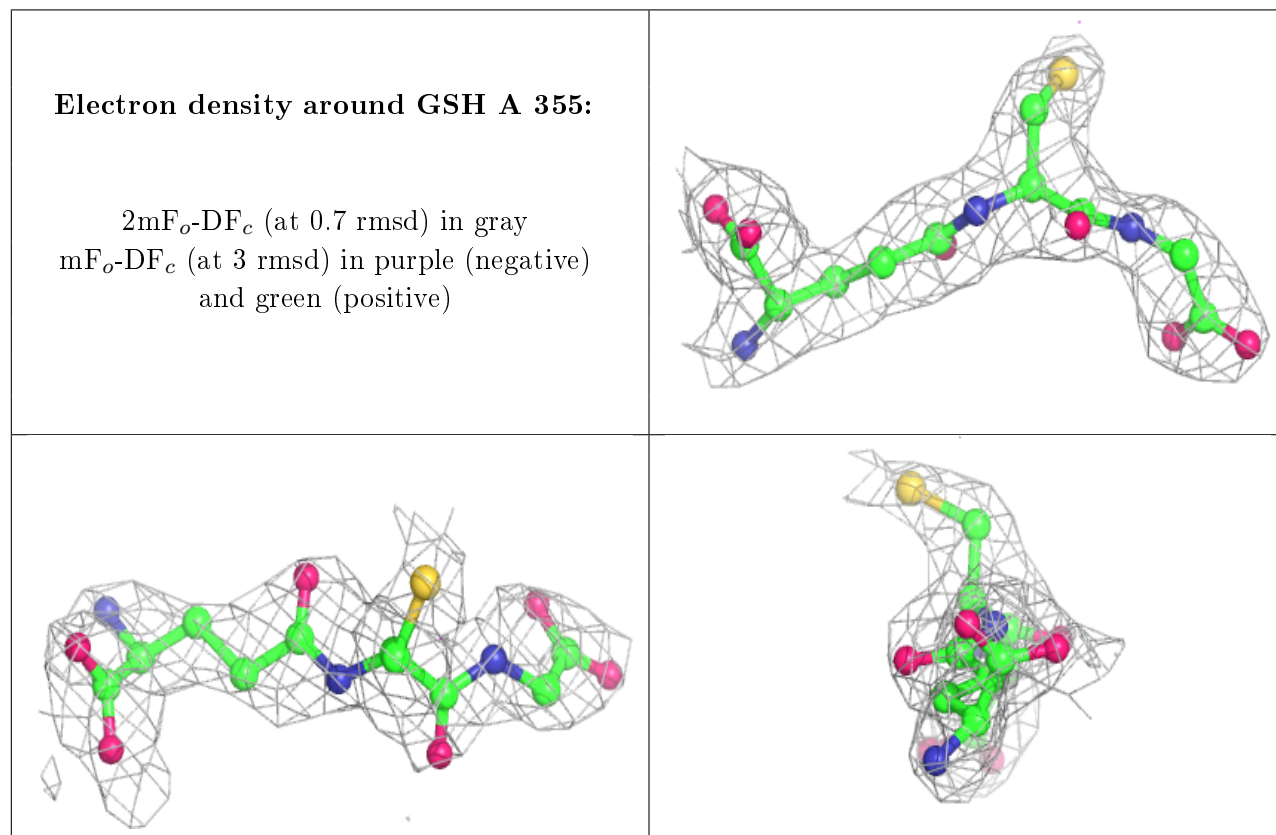
There are no carbohydrates in this entry.

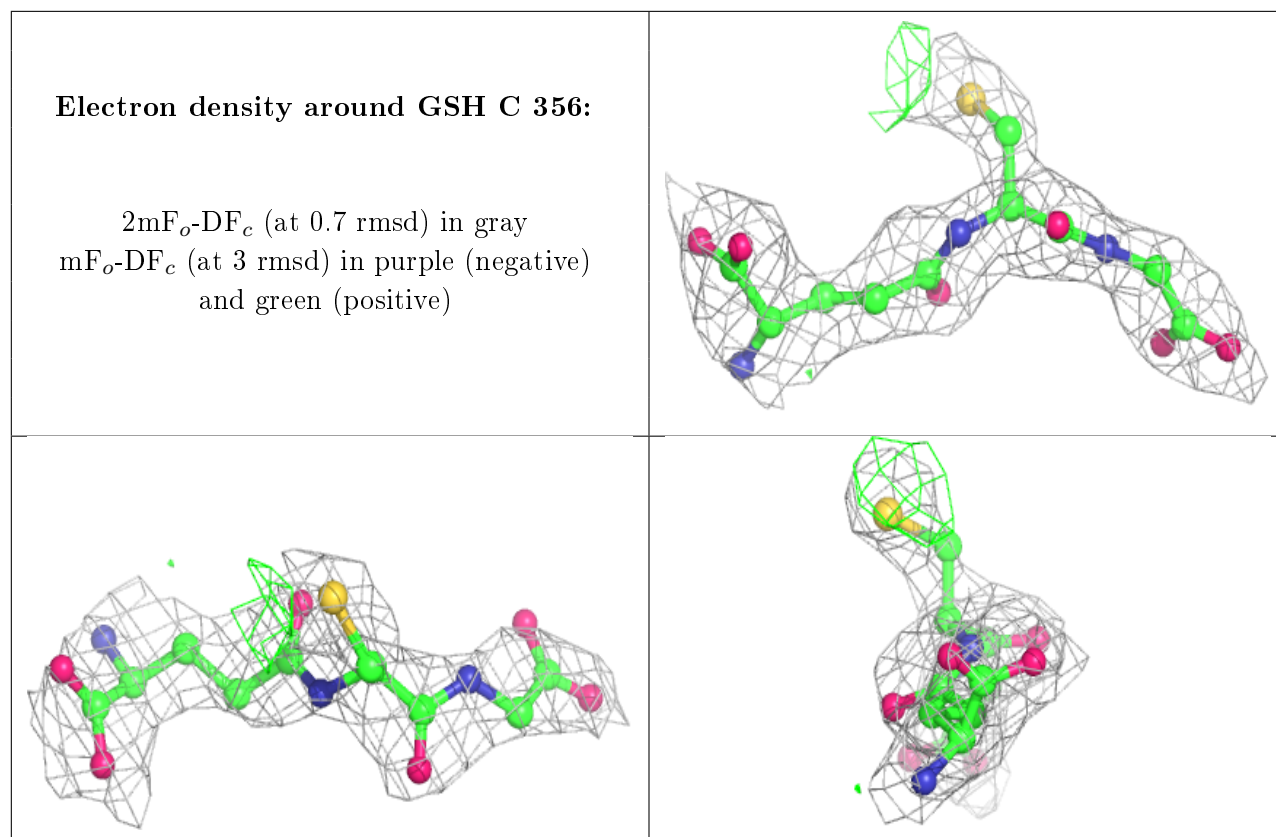
6.4 Ligands [i](#)

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	A	355	20/20	0.84	0.19	41,52,60,64	0
2	GSH	C	356	20/20	0.85	0.23	41,50,59,60	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.