



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:35 pm BST

PDB ID : 1KCG  
Title : NKG2D in complex with ULBP3  
Authors : Radaev, S.; Sun, P.  
Deposited on : 2001-11-08  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

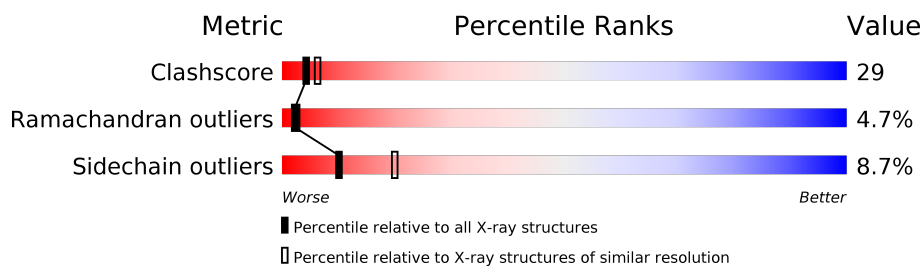
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	124	52% 39% 6% ..
1	B	124	59% 34% 6% ..
2	C	178	42% 43% 10% ..

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3546 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.

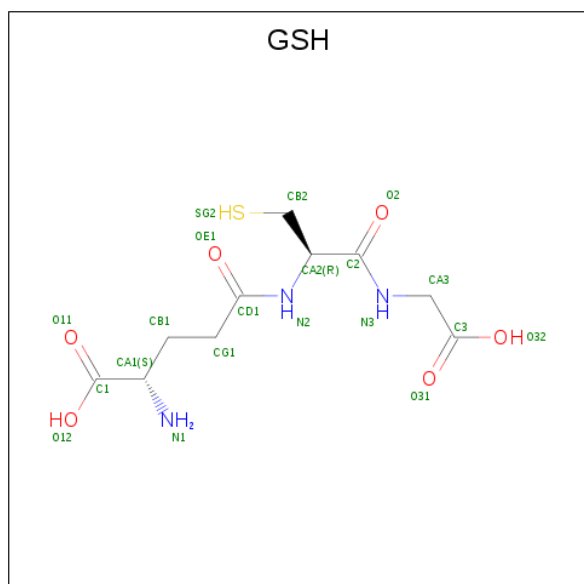
- Molecule 1 is a protein called NKG2-D type II integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	122	Total 987	C 628	N 159	O 188	S 12	2	0	0
1	B	123	Total 996	C 633	N 160	O 191	S 12	0	0	0

- Molecule 2 is a protein called ULBP3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	170	Total 1421	C 897	N 257	O 255	S 12	7	0	0

- Molecule 3 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



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

- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	29	Total 29	O 29	0	0
4	B	41	Total 41	O 41	0	0
4	C	52	Total 52	O 52	0	0

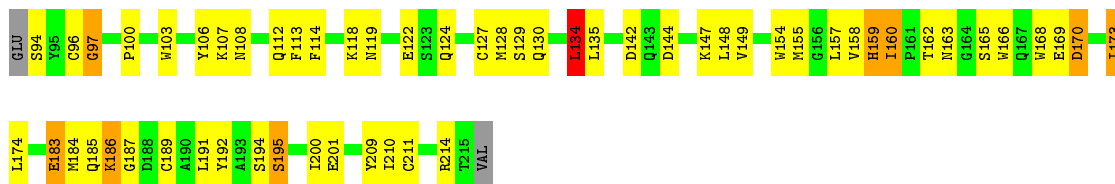
### 3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

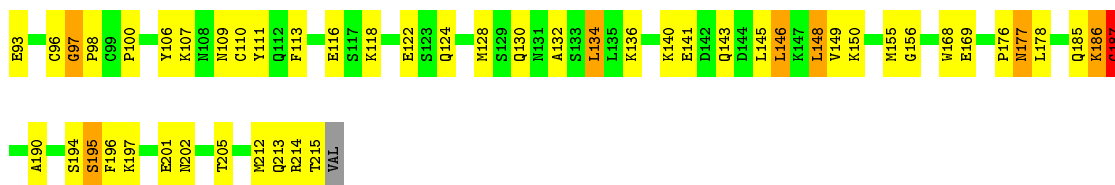
- Molecule 1: NKG2-D type II integral membrane protein

Chain A: 



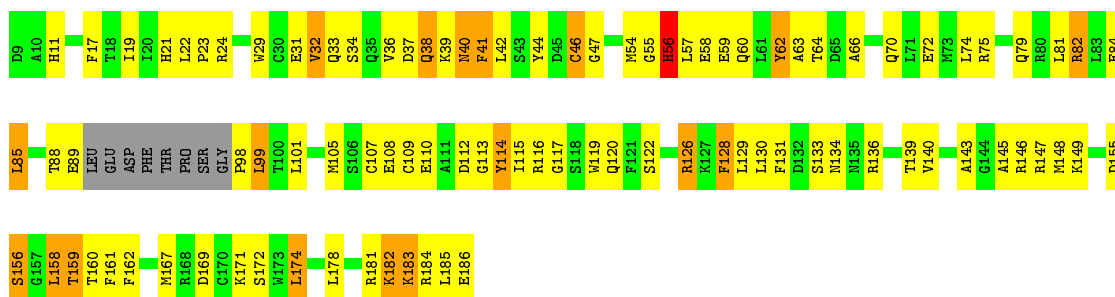
- Molecule 1: NKG2-D type II integral membrane protein

Chain B: 



- Molecule 2: ULBP3 protein

Chain C: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.05Å 62.05Å 237.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (41.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 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	0.42	0/1015	0.78	1/1376 (0.1%)
1	B	0.40	0/1024	0.67	1/1388 (0.1%)
2	C	0.43	0/1454	0.69	1/1949 (0.1%)
All	All	0.42	0/3493	0.71	3/4713 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	183	GLU	N-CA-C	7.05	130.03	111.00
1	B	187	GLY	N-CA-C	5.81	127.63	113.10
2	C	62	TYR	N-CA-C	-5.41	96.39	111.00

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	987	0	927	53	0
1	B	996	0	933	48	0
2	C	1421	0	1375	101	0
3	C	20	0	13	1	0
4	A	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	41	0	0	3	0
4	C	52	0	0	5	0
All	All	3546	0	3248	195	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 29.

All (195) 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:108:ASN:HB2	1:A:214:ARG:HH21	1.06	1.18
1:B:149:VAL:O	1:B:194:SER:HB2	1.57	1.04
1:A:108:ASN:HB2	1:A:214:ARG:NH2	1.79	0.95
1:B:177:ASN:OD1	1:B:178:LEU:HG	1.77	0.85
1:A:159:HIS:HB3	1:A:166:TRP:CE3	2.12	0.84
2:C:64:THR:HG22	2:C:66:ALA:H	1.43	0.82
2:C:55:GLY:O	2:C:56:HIS:HB2	1.80	0.79
1:A:191:LEU:HD11	1:A:201:GLU:OE2	1.83	0.78
2:C:120:GLN:HG2	2:C:130:LEU:CD2	2.14	0.78
2:C:155:ASP:O	2:C:159:THR:HG22	1.83	0.78
2:C:129:LEU:HD13	2:C:145:ALA:HB1	1.67	0.77
1:A:159:HIS:HB3	1:A:166:TRP:CD2	2.20	0.76
2:C:147:ARG:HD2	4:C:1005:HOH:O	1.86	0.76
1:A:160:ILE:HD12	1:A:160:ILE:H	1.51	0.75
2:C:29:TRP:CZ3	2:C:82:ARG:HG3	2.21	0.75
2:C:62:TYR:O	2:C:63:ALA:HB3	1.87	0.74
1:B:116:GLU:HB2	4:B:254:HOH:O	1.88	0.73
1:A:155:MET:HE1	1:A:168:TRP:CH2	2.25	0.72
1:B:202:ASN:HB3	1:B:205:THR:HG23	1.71	0.72
2:C:82:ARG:HD3	4:C:1009:HOH:O	1.91	0.70
2:C:11:HIS:HA	2:C:37:ASP:OD1	1.92	0.70
2:C:126:ARG:H	2:C:126:ARG:HD2	1.57	0.69
2:C:140:VAL:HG23	2:C:149:LYS:HD2	1.76	0.67
1:A:155:MET:HG2	1:A:192:TYR:HB2	1.76	0.66
1:B:136:LYS:HE3	1:B:168:TRP:CD1	2.30	0.66
1:A:159:HIS:HB2	1:A:165:SER:O	1.95	0.66
1:A:155:MET:HE1	1:A:168:TRP:HH2	1.60	0.66
1:A:113:PHE:CG	1:B:148:LEU:HD21	2.31	0.66
1:B:109:ASN:OD1	1:B:214:ARG:HD2	1.95	0.66
1:B:124:GLN:HG3	1:B:169:GLU:OE1	1.96	0.65
2:C:136:ARG:HH21	2:C:160:THR:CG2	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:O	1:A:186:LYS:HB2	1.95	0.65
2:C:11:HIS:ND1	2:C:37:ASP:OD2	2.28	0.65
2:C:29:TRP:CE3	2:C:82:ARG:HG3	2.32	0.65
2:C:182:LYS:HB2	2:C:182:LYS:HZ2	1.61	0.64
2:C:38:GLN:HG2	2:C:39:LYS:HE3	1.79	0.64
2:C:32:VAL:HG22	2:C:46:CYS:SG	2.38	0.64
1:A:160:ILE:HD12	1:A:160:ILE:N	2.12	0.64
1:A:194:SER:HB3	1:B:150:LYS:NZ	2.13	0.63
2:C:105:MET:HG3	2:C:119:TRP:CZ2	2.34	0.63
2:C:54:MET:O	2:C:54:MET:HG3	1.99	0.63
2:C:128:PHE:CD2	2:C:145:ALA:HB2	2.34	0.62
1:B:132:ALA:HB1	1:B:212:MET:O	2.00	0.62
2:C:182:LYS:HG3	2:C:183:LYS:N	2.14	0.61
2:C:136:ARG:HH21	2:C:160:THR:HG23	1.65	0.61
1:A:113:PHE:CD2	1:B:148:LEU:HD21	2.36	0.61
1:A:144:ASP:O	1:A:147:LYS:HG2	2.00	0.61
1:B:185:GLN:NE2	4:B:218:HOH:O	2.33	0.60
1:A:160:ILE:HD13	1:A:165:SER:OG	2.02	0.60
1:B:134:LEU:HB3	1:B:156:GLY:N	2.17	0.60
2:C:55:GLY:O	2:C:56:HIS:CB	2.50	0.58
2:C:89:GLU:HG2	2:C:148:MET:SD	2.43	0.58
1:B:96:CYS:O	1:B:97:GLY:O	2.20	0.58
1:B:118:LYS:HB3	1:B:122:GLU:HB2	1.84	0.58
1:A:134:LEU:O	1:A:211:CYS:HA	2.04	0.57
2:C:182:LYS:HB2	2:C:182:LYS:NZ	2.18	0.57
2:C:126:ARG:O	2:C:126:ARG:HG2	2.04	0.57
1:A:107:LYS:O	1:A:214:ARG:NH2	2.38	0.57
1:A:118:LYS:HD3	1:A:209:TYR:CE2	2.39	0.57
2:C:72:GLU:HG2	4:C:1003:HOH:O	2.04	0.57
2:C:156:SER:HA	2:C:159:THR:CG2	2.35	0.57
2:C:182:LYS:HG3	2:C:183:LYS:H	1.70	0.57
1:A:100:PRO:HA	1:B:93:GLU:HA	1.87	0.57
2:C:136:ARG:NH2	2:C:160:THR:HG23	2.20	0.56
2:C:32:VAL:HG23	2:C:44:TYR:O	2.04	0.56
2:C:108:GLU:O	2:C:115:ILE:HD12	2.04	0.56
2:C:41:PHE:HA	2:C:55:GLY:O	2.06	0.56
1:B:140:LYS:HE3	1:B:178:LEU:HA	1.87	0.56
2:C:19:ILE:HD13	2:C:81:LEU:HB2	1.88	0.56
1:B:140:LYS:HE3	1:B:177:ASN:O	2.06	0.55
1:A:194:SER:HB3	1:B:150:LYS:HZ1	1.69	0.55
1:B:185:GLN:HG3	1:B:186:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:MET:CG	1:A:192:TYR:HB2	2.37	0.55
2:C:21:HIS:HB2	2:C:85:LEU:HD13	1.89	0.54
2:C:64:THR:HG22	2:C:66:ALA:N	2.17	0.54
1:A:96:CYS:O	1:A:97:GLY:O	2.25	0.54
2:C:129:LEU:CD1	2:C:145:ALA:HB1	2.36	0.54
2:C:171:LYS:HE3	4:C:1007:HOH:O	2.07	0.54
2:C:11:HIS:HD1	2:C:37:ASP:CG	2.11	0.53
2:C:38:GLN:HG3	2:C:38:GLN:O	2.09	0.53
1:A:112:GLN:OE1	1:A:113:PHE:N	2.42	0.53
2:C:109:CYS:SG	2:C:174:LEU:HD13	2.49	0.53
2:C:75:ARG:O	2:C:79:GLN:HG3	2.08	0.53
1:A:185:GLN:C	1:A:187:GLY:H	2.12	0.52
2:C:31:GLU:HG2	2:C:33:GLN:HE22	1.75	0.52
1:B:134:LEU:HB2	1:B:169:GLU:OE2	2.09	0.52
1:A:149:VAL:O	1:A:194:SER:HB2	2.09	0.52
2:C:116:ARG:HA	2:C:134:ASN:HD21	1.74	0.52
1:B:106:TYR:CE2	1:B:107:LYS:HD3	2.46	0.51
2:C:109:CYS:SG	2:C:115:ILE:HD13	2.50	0.51
2:C:24:ARG:HH11	2:C:24:ARG:HG2	1.75	0.51
2:C:57:LEU:N	2:C:57:LEU:HD12	2.25	0.51
2:C:31:GLU:CG	2:C:33:GLN:HE22	2.24	0.50
2:C:108:GLU:C	2:C:115:ILE:HD12	2.32	0.50
1:A:158:VAL:HG23	1:A:158:VAL:O	2.11	0.50
1:B:143:GLN:HB3	1:B:146:LEU:HD22	1.94	0.50
1:B:187:GLY:HA3	1:B:202:ASN:HA	1.94	0.49
1:B:145:LEU:O	1:B:148:LEU:HB2	2.13	0.49
2:C:113:GLY:O	2:C:115:ILE:N	2.46	0.49
2:C:38:GLN:O	2:C:38:GLN:CG	2.60	0.49
2:C:32:VAL:CG2	2:C:46:CYS:SG	3.01	0.49
1:B:186:LYS:HA	4:B:225:HOH:O	2.11	0.49
1:B:110:CYS:O	1:B:212:MET:HA	2.13	0.49
2:C:109:CYS:SG	2:C:115:ILE:CD1	3.01	0.49
2:C:174:LEU:HD13	3:C:999:GSH:SG2	2.53	0.49
1:A:163:ASN:C	1:A:165:SER:H	2.17	0.48
1:A:113:PHE:CD1	1:B:148:LEU:HD21	2.47	0.48
1:B:176:PRO:O	1:B:177:ASN:CB	2.62	0.48
2:C:62:TYR:O	2:C:63:ALA:CB	2.52	0.48
1:A:154:TRP:CZ3	1:A:189:CYS:HB3	2.48	0.48
2:C:88:THR:HG22	2:C:148:MET:CE	2.44	0.48
2:C:22:LEU:N	2:C:23:PRO:HD3	2.29	0.48
1:B:202:ASN:HB3	1:B:205:THR:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:LEU:HA	2:C:54:MET:HA	1.95	0.47
2:C:70:GLN:O	2:C:74:LEU:HG	2.15	0.47
2:C:21:HIS:O	2:C:98:PRO:HB3	2.13	0.47
2:C:158:LEU:HD22	2:C:162:PHE:CE2	2.50	0.47
1:A:134:LEU:HB2	1:A:169:GLU:OE1	2.14	0.47
1:B:136:LYS:HG3	1:B:168:TRP:CD2	2.49	0.47
2:C:117:GLY:O	2:C:133:SER:HB2	2.14	0.47
2:C:17:PHE:CD1	2:C:32:VAL:HG13	2.49	0.47
2:C:89:GLU:CG	2:C:148:MET:SD	3.03	0.47
1:A:157:LEU:HD13	1:A:168:TRP:CZ3	2.50	0.46
2:C:84:GLU:HG3	2:C:158:LEU:HD11	1.98	0.46
1:A:103:TRP:HZ2	1:A:130:GLN:HE21	1.63	0.46
2:C:107:CYS:HA	2:C:116:ARG:O	2.16	0.46
2:C:126:ARG:N	2:C:126:ARG:HD2	2.28	0.46
1:A:189:CYS:O	1:A:200:ILE:HA	2.16	0.46
2:C:174:LEU:HD22	2:C:178:LEU:CD1	2.46	0.46
2:C:38:GLN:O	2:C:39:LYS:HE3	2.16	0.46
2:C:38:GLN:O	2:C:39:LYS:CD	2.64	0.46
2:C:158:LEU:O	2:C:161:PHE:HB3	2.16	0.46
2:C:54:MET:HE3	2:C:54:MET:HB2	1.81	0.46
1:A:163:ASN:C	1:A:165:SER:N	2.68	0.45
1:B:201:GLU:HG3	1:B:202:ASN:N	2.31	0.45
1:B:176:PRO:O	1:B:177:ASN:HB3	2.15	0.45
2:C:47:GLY:HA3	4:C:1030:HOH:O	2.16	0.45
1:A:114:PHE:HE1	1:A:211:CYS:SG	2.39	0.45
1:B:143:GLN:O	1:B:146:LEU:HB2	2.17	0.45
2:C:136:ARG:HH21	2:C:160:THR:HG22	1.80	0.45
2:C:88:THR:HG22	2:C:148:MET:HE2	1.98	0.45
2:C:19:ILE:HD13	2:C:81:LEU:CB	2.47	0.45
1:A:94:SER:O	1:B:98:PRO:HA	2.17	0.44
1:B:100:PRO:HD3	1:B:213:GLN:OE1	2.16	0.44
2:C:24:ARG:HG3	2:C:98:PRO:CG	2.48	0.44
1:A:127:CYS:SG	1:A:134:LEU:HA	2.57	0.44
1:B:185:GLN:HG3	1:B:186:LYS:CG	2.47	0.44
2:C:38:GLN:O	2:C:39:LYS:HD3	2.16	0.44
2:C:36:VAL:CG2	2:C:41:PHE:CD1	3.01	0.44
2:C:24:ARG:NH1	2:C:24:ARG:HG2	2.31	0.44
2:C:85:LEU:CD2	2:C:99:LEU:HD13	2.48	0.44
1:B:111:TYR:OH	1:B:143:GLN:HG2	2.17	0.44
2:C:39:LYS:HA	2:C:39:LYS:HD3	1.71	0.44
1:A:155:MET:CE	1:A:168:TRP:HH2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:GLU:O	2:C:115:ILE:HA	2.18	0.44
2:C:36:VAL:O	2:C:37:ASP:C	2.56	0.44
1:A:103:TRP:HZ2	1:A:130:GLN:NE2	2.15	0.43
1:A:186:LYS:HD3	1:A:186:LYS:HA	1.77	0.43
2:C:182:LYS:CG	2:C:183:LYS:N	2.81	0.43
1:A:134:LEU:O	1:A:210:ILE:O	2.36	0.43
1:A:160:ILE:CD1	1:A:160:ILE:N	2.79	0.43
1:A:170:ASP:OD1	1:A:170:ASP:C	2.57	0.43
1:A:185:GLN:HB3	1:A:186:LYS:H	1.11	0.43
2:C:182:LYS:O	2:C:184:ARG:N	2.51	0.43
1:A:106:TYR:CZ	1:A:107:LYS:HE3	2.53	0.43
1:B:124:GLN:HB3	1:B:124:GLN:HE21	1.71	0.43
2:C:143:ALA:O	2:C:146:ARG:HG3	2.19	0.43
1:A:112:GLN:HG3	1:A:114:PHE:CE1	2.54	0.43
2:C:109:CYS:HA	2:C:115:ILE:HD12	2.00	0.43
1:B:155:MET:HG2	1:B:190:ALA:O	2.20	0.42
2:C:110:GLU:OE1	2:C:114:TYR:HD1	2.02	0.42
1:B:140:LYS:HE2	1:B:178:LEU:O	2.20	0.42
1:B:116:GLU:OE2	1:B:118:LYS:NZ	2.46	0.42
1:B:106:TYR:CZ	1:B:107:LYS:HD3	2.54	0.42
1:B:98:PRO:HD2	1:B:215:THR:CG2	2.50	0.42
1:B:186:LYS:O	1:B:187:GLY:O	2.37	0.42
2:C:169:ASP:O	2:C:172:SER:HB3	2.19	0.42
2:C:19:ILE:HG22	2:C:85:LEU:HD12	2.02	0.42
1:A:119:ASN:HD21	1:A:122:GLU:HG3	1.85	0.41
2:C:59:GLU:O	2:C:60:GLN:C	2.58	0.41
2:C:115:ILE:HD12	2:C:115:ILE:HA	1.93	0.41
2:C:119:TRP:HB2	2:C:131:PHE:HB3	2.02	0.41
2:C:36:VAL:HG23	2:C:41:PHE:CD1	2.55	0.41
1:A:148:LEU:N	1:A:148:LEU:HD22	2.35	0.41
1:A:114:PHE:HZ	1:A:130:GLN:HE22	1.68	0.41
1:B:195:SER:O	1:B:197:LYS:HG3	2.21	0.41
1:A:173:ILE:HG23	1:A:174:LEU:N	2.36	0.41
1:B:128:MET:C	1:B:130:GLN:H	2.24	0.41
1:A:134:LEU:HB3	1:A:135:LEU:H	1.72	0.41
1:B:113:PHE:N	1:B:113:PHE:CD1	2.88	0.41
2:C:182:LYS:NZ	2:C:186:GLU:CD	2.74	0.41
2:C:120:GLN:HG2	2:C:130:LEU:HD21	2.00	0.41
2:C:101:LEU:HD12	2:C:122:SER:O	2.21	0.41
2:C:34:SER:O	2:C:40:ASN:HA	2.21	0.40
2:C:54:MET:HE1	2:C:62:TYR:HD2	1.87	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	120/124 (97%)	104 (87%)	10 (8%)	6 (5%)	2	2
1	B	121/124 (98%)	98 (81%)	17 (14%)	6 (5%)	2	2
2	C	166/178 (93%)	143 (86%)	16 (10%)	7 (4%)	3	3
All	All	407/426 (96%)	345 (85%)	43 (11%)	19 (5%)	2	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLY
1	B	97	GLY
1	B	177	ASN
1	B	186	LYS
1	B	187	GLY
2	C	56	HIS
2	C	114	TYR
2	C	185	LEU
1	A	195	SER
1	A	134	LEU
1	B	195	SER
2	C	40	ASN
2	C	41	PHE
2	C	183	LYS
1	A	129	SER
1	A	170	ASP
1	A	186	LYS
2	C	38	GLN
1	B	196	PHE

### 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	112/114 (98%)	101 (90%)	11 (10%)	8	15
1	B	113/114 (99%)	109 (96%)	4 (4%)	36	62
2	C	153/160 (96%)	135 (88%)	18 (12%)	5	9
All	All	378/388 (97%)	345 (91%)	33 (9%)	10	20

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

Mol	Chain	Res	Type
1	A	124	GLN
1	A	128	MET
1	A	134	LEU
1	A	142	ASP
1	A	159	HIS
1	A	160	ILE
1	A	162	THR
1	A	173	ILE
1	A	183	GLU
1	A	184	MET
1	A	195	SER
1	B	134	LEU
1	B	141	GLU
1	B	146	LEU
1	B	148	LEU
2	C	32	VAL
2	C	46	CYS
2	C	56	HIS
2	C	58	GLU
2	C	82	ARG
2	C	85	LEU
2	C	99	LEU
2	C	112	ASP
2	C	126	ARG
2	C	128	PHE
2	C	139	THR

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Mol	Chain	Res	Type
2	C	156	SER
2	C	158	LEU
2	C	159	THR
2	C	167	MET
2	C	174	LEU
2	C	181	ARG
2	C	182	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	185	GLN
1	B	102	ASN
1	B	108	ASN
1	B	124	GLN
1	B	131	ASN
1	B	185	GLN
2	C	21	HIS
2	C	33	GLN
2	C	38	GLN
2	C	120	GLN

### 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](#)

1 ligand is 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	GSH	C	999	2	12,19,19	0.98	0	15,24,24	7.80	15 (100%)

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	GSH	C	999	2	-	8/18/24/24	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	999	GSH	CA3-N3-C2	20.27	151.50	122.34
3	C	999	GSH	CG1-CD1-N2	-9.97	98.55	115.83
3	C	999	GSH	CA2-C2-N3	-9.44	97.51	116.54
3	C	999	GSH	C3-CA3-N3	8.39	126.61	110.43
3	C	999	GSH	CA2-CB2-SG2	-7.00	106.33	114.19
3	C	999	GSH	CA2-N2-CD1	6.00	137.08	121.65
3	C	999	GSH	CB2-CA2-N2	5.93	119.74	111.28
3	C	999	GSH	OE1-CD1-N2	5.15	131.64	122.95
3	C	999	GSH	O2-C2-CA2	4.78	130.51	120.45
3	C	999	GSH	CB2-CA2-C2	4.57	119.19	109.76
3	C	999	GSH	O2-C2-N3	4.17	131.95	122.99
3	C	999	GSH	CG1-CB1-CA1	-4.13	104.21	113.84
3	C	999	GSH	C2-CA2-N2	-3.17	102.53	111.16
3	C	999	GSH	CB1-CG1-CD1	-2.23	108.05	113.04
3	C	999	GSH	OE1-CD1-CG1	2.01	125.69	122.02

There are no chirality outliers.

All (8) torsion outliers are listed below:



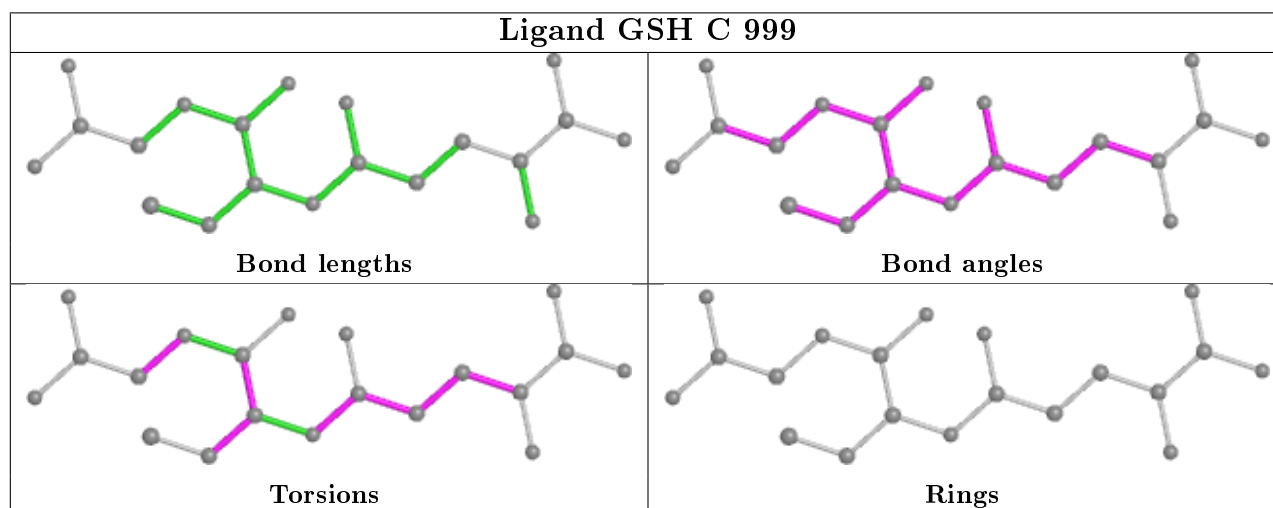
Mol	Chain	Res	Type	Atoms
3	C	999	GSH	C1-CA1-CB1-CG1
3	C	999	GSH	C2-CA2-CB2-SG2
3	C	999	GSH	C3-CA3-N3-C2
3	C	999	GSH	OE1-CD1-CG1-CB1
3	C	999	GSH	CA1-CB1-CG1-CD1
3	C	999	GSH	CG1-CD1-N2-CA2
3	C	999	GSH	O2-C2-CA2-N2
3	C	999	GSH	N2-CD1-CG1-CB1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	999	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 [i](#)

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.