



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:46 am BST

PDB ID : 1DUG  
Title : STRUCTURE OF THE FIBRINOGEN G CHAIN INTEGRIN BINDING AND FACTOR XIIIa CROSSLINKING SITES OBTAINED THROUGH CARRIER PROTEIN DRIVEN CRYSTALLIZATION  
Authors : Ware, S.; Donahue, J.P.; Hawiger, J.; Anderson, W.F.  
Deposited on : 2000-01-17  
Resolution : 1.80 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

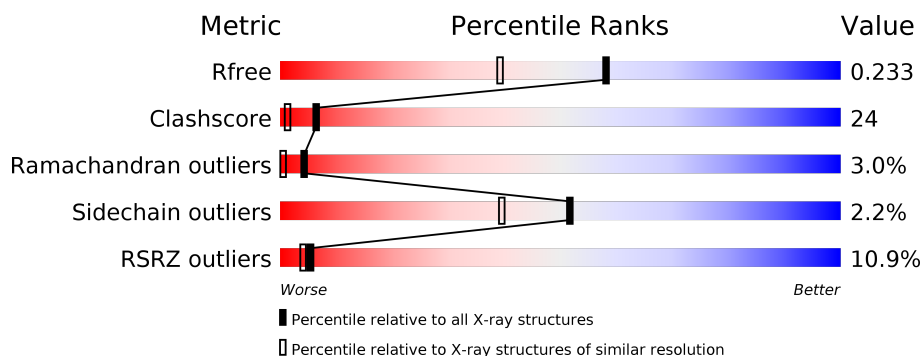
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\leq 5\%$ . 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	234	<div> <div>9%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
1	B	234	<div> <div>13%</div> <div>64%</div> <div>31%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4520 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.

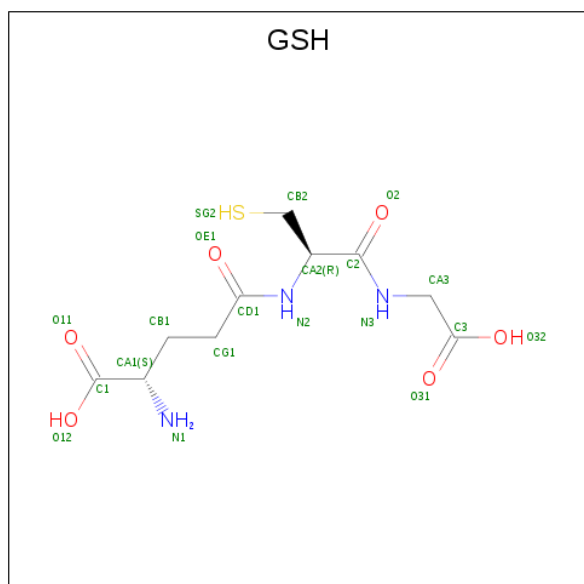
- Molecule 1 is a protein called chimera of GLUTATHIONE S-TRANSFERASE-synthetic LINKER-C-TERMINAL FIBRINOGEN GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1909	1236	315	346	12			
1	B	234	Total	C	N	O	S	0	0	0
			1909	1236	315	346	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	LINKER	UNP P08515
A	219	ASP	-	LINKER	UNP P08515
A	220	PRO	-	LINKER	UNP P08515
B	218	SER	-	LINKER	UNP P08515
B	219	ASP	-	LINKER	UNP P08515
B	220	PRO	-	LINKER	UNP P08515

- Molecule 2 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
2	A	1	Total 20	C 10	N 3	O 6	S 1	0	0
2	B	1	Total 20	C 10	N 3	O 6	S 1	0	0

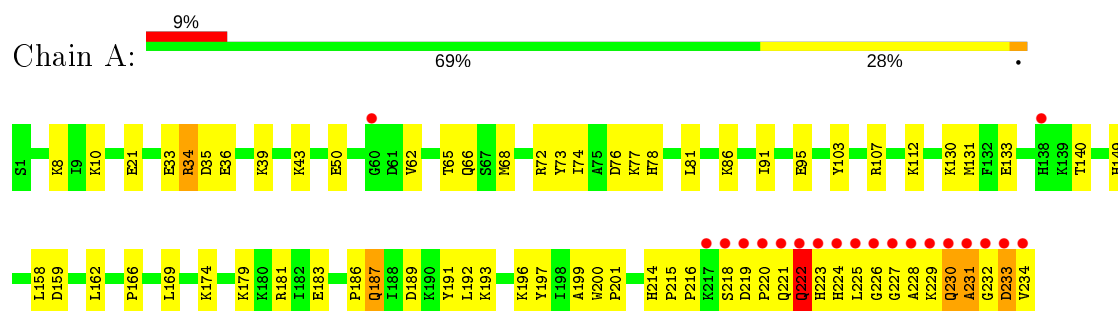
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	364	Total 364	O 364	0	0
3	B	298	Total 298	O 298	0	0

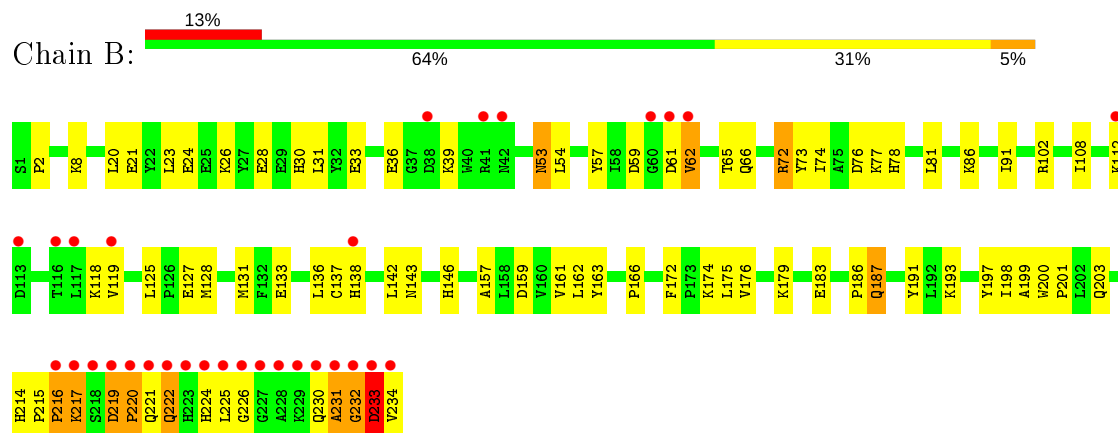
### 3 Residue-property plots [i](#)

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: chimera of GLUTATHIONE S-TRANSFERASE-synthetic LINKER-C-TERMINAL FIBRINOGEN GAMMA CHAIN



- Molecule 1: chimera of GLUTATHIONE S-TRANSFERASE-synthetic LINKER-C-TERMINAL FIBRINOGEN GAMMA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.78 Å   105.78 Å   137.23 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	28.00 – 1.80 27.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.2 (28.00-1.80) 76.2 (27.93-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.70 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.185   ,   0.226 0.209   ,   0.233	Depositor DCC
$R_{free}$ test set	6850 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 66.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.32	0/1961	0.61	0/2646
1	B	0.32	0/1961	0.60	0/2646
All	All	0.32	0/3922	0.60	0/5292

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

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	1909	0	1897	90	1
1	B	1909	0	1897	98	1
2	A	20	0	15	0	0
2	B	20	0	15	2	0
3	A	364	0	0	24	0
3	B	298	0	0	15	0
All	All	4520	0	3824	184	1

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 24.

All (184) 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:68:MET:HE3	3:A:1322:HOH:O	1.52	1.10
1:A:229:LYS:HA	1:A:229:LYS:HE2	1.47	0.96
1:A:131:MET:HG2	3:A:1505:HOH:O	1.69	0.93
1:B:8:LYS:HE2	1:B:231:ALA:HB1	1.50	0.90
3:A:1535:HOH:O	1:B:131:MET:HG3	1.75	0.87
1:B:102:ARG:HH12	1:B:203:GLN:HE22	1.24	0.85
1:A:8:LYS:HE3	1:A:233:ASP:OD2	1.79	0.83
1:A:158:LEU:O	1:A:162:LEU:HG	1.81	0.81
1:A:81:LEU:O	1:A:91:ILE:HD12	1.80	0.80
1:B:53:ASN:HD22	1:B:54:LEU:H	1.27	0.79
1:A:68:MET:HG2	3:A:1529:HOH:O	1.83	0.79
1:B:219:ASP:H	1:B:220:PRO:HD2	1.48	0.79
1:A:222:GLN:HB2	3:A:1576:HOH:O	1.85	0.77
1:B:198:ILE:HA	3:B:1820:HOH:O	1.85	0.77
1:B:72:ARG:HB3	1:B:72:ARG:HH11	1.50	0.76
1:B:108:ILE:HD11	3:B:1650:HOH:O	1.86	0.76
1:B:8:LYS:HE3	1:B:233:ASP:HB2	1.68	0.74
1:B:187:GLN:NE2	1:B:187:GLN:H	1.85	0.74
1:A:225:LEU:HD23	3:A:1511:HOH:O	1.87	0.73
1:A:219:ASP:N	1:A:220:PRO:HD2	2.05	0.72
1:A:222:GLN:HE22	1:A:225:LEU:HD22	1.55	0.71
1:A:112:LYS:HE3	3:A:1477:HOH:O	1.91	0.69
1:A:72:ARG:HD3	3:A:1409:HOH:O	1.92	0.68
1:A:221:GLN:O	1:A:222:GLN:HB2	1.93	0.68
1:A:219:ASP:HB2	3:A:1600:HOH:O	1.93	0.68
1:A:218:SER:C	1:A:220:PRO:HD2	2.14	0.68
1:A:222:GLN:NE2	1:A:225:LEU:HD22	2.08	0.68
1:A:86:LYS:HD2	3:A:1435:HOH:O	1.93	0.67
1:B:23:LEU:HD13	1:B:78:HIS:CD2	2.31	0.65
1:A:179:LYS:NZ	1:A:222:GLN:HG2	2.12	0.65
1:A:74:ILE:O	1:A:78:HIS:HD2	1.79	0.65
1:B:162:LEU:HD12	1:B:179:LYS:HE3	1.78	0.65
1:B:77:LYS:HE2	3:B:1869:HOH:O	1.98	0.64
1:B:31:LEU:CD1	1:B:233:ASP:HB3	2.28	0.64
1:A:166:PRO:HA	1:A:221:GLN:HG2	1.80	0.63
1:B:102:ARG:HH22	1:B:203:GLN:NE2	1.97	0.62
1:B:137:CYS:HB2	3:B:1800:HOH:O	1.99	0.62
1:B:77:LYS:NZ	1:B:77:LYS:HB3	2.14	0.62
1:B:73:TYR:CZ	1:B:77:LYS:HD2	2.35	0.62
1:A:187:GLN:NE2	1:A:187:GLN:H	1.97	0.62
1:B:214:HIS:HE1	1:B:230:GLN:HG3	1.67	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HB2	3:A:1425:HOH:O	2.00	0.60
1:B:28:GLU:HG2	3:B:1794:HOH:O	2.02	0.60
1:B:33:GLU:HB2	1:B:36:GLU:HG3	1.82	0.60
1:B:112:LYS:NZ	1:B:112:LYS:HB2	2.16	0.60
1:B:102:ARG:NH1	1:B:203:GLN:HE22	1.95	0.59
1:A:65:THR:O	1:A:66:GLN:HB2	2.01	0.59
1:B:222:GLN:O	1:B:222:GLN:NE2	2.36	0.59
1:B:61:ASP:O	1:B:62:VAL:HG23	2.03	0.58
1:A:222:GLN:C	1:A:222:GLN:HE21	2.06	0.58
1:A:166:PRO:HB3	1:A:221:GLN:HB2	1.85	0.58
1:B:53:ASN:ND2	1:B:54:LEU:H	2.00	0.58
1:A:133:GLU:OE2	1:A:174:LYS:HD3	2.03	0.58
1:A:179:LYS:O	1:A:183:GLU:HG3	2.04	0.58
1:B:219:ASP:N	1:B:220:PRO:HD2	2.19	0.58
1:B:65:THR:O	1:B:66:GLN:HB2	2.03	0.57
1:A:197:TYR:OH	1:A:225:LEU:HD12	2.04	0.57
1:B:193:LYS:HA	1:B:226:GLY:HA3	1.86	0.57
1:B:215:PRO:HB2	1:B:220:PRO:HB3	1.87	0.57
1:A:73:TYR:CZ	1:A:77:LYS:HD3	2.40	0.56
1:B:8:LYS:CE	1:B:231:ALA:HB1	2.31	0.56
1:B:33:GLU:OE2	1:B:234:VAL:HG21	2.05	0.56
1:A:179:LYS:HZ2	1:A:222:GLN:HG2	1.69	0.56
1:B:221:GLN:HA	1:B:221:GLN:HE21	1.71	0.56
1:B:59:ASP:OD1	1:B:62:VAL:HB	2.06	0.55
1:A:225:LEU:H	1:A:225:LEU:HD23	1.71	0.55
1:A:234:VAL:HG11	3:A:1356:HOH:O	2.06	0.55
1:B:200:TRP:CG	1:B:201:PRO:HA	2.41	0.55
1:B:187:GLN:HE21	1:B:187:GLN:H	1.54	0.55
1:A:192:LEU:O	1:A:226:GLY:N	2.39	0.55
1:A:39:LYS:HE3	3:A:1432:HOH:O	2.06	0.54
1:A:162:LEU:HB3	1:A:221:GLN:O	2.08	0.54
1:B:61:ASP:HA	3:B:1778:HOH:O	2.07	0.54
1:B:137:CYS:O	1:B:138:HIS:HB2	2.07	0.54
1:B:31:LEU:HD12	1:B:234:VAL:HG13	1.89	0.54
1:B:86:LYS:HD2	3:B:1814:HOH:O	2.07	0.54
1:A:200:TRP:CG	1:A:201:PRO:HA	2.43	0.54
1:B:232:GLY:O	1:B:233:ASP:OD1	2.26	0.53
1:B:53:ASN:HD22	1:B:54:LEU:N	2.01	0.53
1:A:50:GLU:O	1:B:131:MET:HE2	2.09	0.53
1:A:149:HIS:CD2	3:A:1322:HOH:O	2.61	0.52
1:A:43:LYS:HG3	3:A:1284:HOH:O	2.07	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HH12	1:B:72:ARG:HE	1.55	0.52
1:B:39:LYS:HG3	3:B:1708:HOH:O	2.08	0.52
1:B:76:ASP:CA	1:B:81:LEU:HD13	2.40	0.52
1:A:34:ARG:HD2	3:A:1350:HOH:O	2.09	0.52
1:A:72:ARG:CD	3:A:1409:HOH:O	2.53	0.52
1:B:20:LEU:HD21	1:B:74:ILE:HD13	1.92	0.51
1:A:162:LEU:HD21	1:A:169:LEU:HG	1.92	0.51
1:B:125:LEU:HA	1:B:128:MET:HE2	1.93	0.51
1:B:222:GLN:HE22	1:B:225:LEU:HD11	1.75	0.51
1:B:166:PRO:HB3	1:B:221:GLN:HG2	1.93	0.51
1:B:214:HIS:CE1	1:B:230:GLN:HA	2.46	0.51
1:A:216:PRO:HD2	3:A:1600:HOH:O	2.11	0.51
1:A:8:LYS:HE2	1:A:231:ALA:CB	2.41	0.51
1:B:57:TYR:HE1	1:B:59:ASP:OD2	1.94	0.51
1:B:127:GLU:HG2	3:B:1796:HOH:O	2.11	0.50
1:A:197:TYR:CE2	1:A:199:ALA:HB2	2.47	0.50
1:B:73:TYR:CE2	1:B:77:LYS:HD2	2.46	0.50
1:A:34:ARG:HG3	1:A:35:ASP:N	2.27	0.50
1:A:33:GLU:HB2	1:A:36:GLU:HG3	1.94	0.49
1:A:220:PRO:HB2	3:A:1594:HOH:O	2.12	0.49
1:B:221:GLN:HA	1:B:221:GLN:NE2	2.27	0.49
1:A:162:LEU:HD21	1:A:169:LEU:CD1	2.43	0.49
1:B:119:VAL:HG12	3:B:1880:HOH:O	2.12	0.49
1:B:230:GLN:O	1:B:230:GLN:HG2	2.13	0.49
1:A:200:TRP:CD1	1:A:201:PRO:HA	2.48	0.48
1:A:219:ASP:N	1:A:220:PRO:CD	2.75	0.48
1:A:34:ARG:HG3	1:A:35:ASP:H	1.78	0.48
1:A:229:LYS:CE	1:A:229:LYS:HA	2.31	0.48
1:B:222:GLN:NE2	1:B:225:LEU:HD11	2.28	0.48
1:B:77:LYS:HD3	3:B:1787:HOH:O	2.13	0.48
1:B:197:TYR:CE2	1:B:199:ALA:HB2	2.49	0.48
1:A:8:LYS:HE2	1:A:231:ALA:HB1	1.95	0.48
1:B:102:ARG:HH12	1:B:203:GLN:NE2	2.04	0.48
1:B:24:GLU:CG	1:B:187:GLN:HG2	2.44	0.48
1:A:186:PRO:HB2	1:A:187:GLN:HE21	1.79	0.48
1:B:217:LYS:O	1:B:217:LYS:HD2	2.13	0.48
1:B:162:LEU:CD1	1:B:179:LYS:HE3	2.44	0.47
1:B:53:ASN:ND2	2:B:1587:GSH:HN3	2.13	0.47
1:B:118:LYS:HA	3:B:1650:HOH:O	2.14	0.47
1:B:76:ASP:HA	1:B:81:LEU:HD13	1.97	0.47
1:A:214:HIS:HE1	1:A:230:GLN:HB2	1.80	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:O	1:B:91:ILE:HD12	2.15	0.46
1:A:223:HIS:O	1:A:224:HIS:HB2	2.16	0.46
1:A:76:ASP:HA	1:A:81:LEU:HG	1.96	0.46
1:A:130:LYS:NZ	3:A:1392:HOH:O	2.47	0.46
1:B:2:PRO:HG3	3:B:1627:HOH:O	2.16	0.46
1:B:77:LYS:HB3	1:B:77:LYS:HZ3	1.79	0.46
1:A:192:LEU:HB3	1:A:225:LEU:HA	1.98	0.46
1:B:215:PRO:HA	1:B:216:PRO:HD2	1.85	0.46
1:A:72:ARG:NH1	1:B:72:ARG:HE	2.14	0.46
1:A:77:LYS:CB	1:A:77:LYS:NZ	2.79	0.46
1:A:228:ALA:HA	3:A:1512:HOH:O	2.16	0.46
1:B:53:ASN:HD21	2:B:1587:GSH:HN3	1.63	0.46
1:B:133:GLU:OE1	1:B:175:LEU:HG	2.15	0.45
1:A:222:GLN:C	1:A:222:GLN:NE2	2.69	0.45
1:B:159:ASP:O	1:B:163:TYR:HD1	2.00	0.45
1:A:196:LYS:HE2	3:A:1394:HOH:O	2.17	0.45
1:A:10:LYS:HE3	1:A:199:ALA:HA	1.98	0.45
1:A:159:ASP:OD1	1:A:222:GLN:HG3	2.17	0.44
1:A:189:ASP:OD2	1:A:193:LYS:HE3	2.17	0.44
1:A:103:TYR:O	1:A:107:ARG:HG3	2.18	0.44
1:B:186:PRO:HB2	1:B:187:GLN:HE21	1.83	0.44
1:B:163:TYR:CE2	1:B:220:PRO:HA	2.53	0.44
1:B:179:LYS:O	1:B:183:GLU:HG3	2.18	0.43
1:A:62:VAL:HG12	1:B:86:LYS:HG3	1.99	0.43
1:B:234:VAL:OXT	1:B:234:VAL:HG23	2.18	0.43
1:A:68:MET:HE1	1:A:95:GLU:CG	2.49	0.43
1:B:219:ASP:H	1:B:220:PRO:CD	2.26	0.43
1:A:36:GLU:HB3	1:A:39:LYS:HD2	2.00	0.43
1:B:26:LYS:HD2	1:B:26:LYS:N	2.34	0.43
1:A:21:GLU:HG3	1:A:191:TYR:CG	2.54	0.43
1:A:68:MET:CE	1:A:95:GLU:CG	2.96	0.43
1:B:230:GLN:O	1:B:231:ALA:HB3	2.18	0.43
1:A:226:GLY:HA3	3:A:1337:HOH:O	2.19	0.43
1:B:112:LYS:HZ2	1:B:112:LYS:HB2	1.84	0.43
1:B:222:GLN:HE22	1:B:225:LEU:CD1	2.31	0.43
1:A:223:HIS:HA	1:A:225:LEU:CD2	2.49	0.43
1:A:229:LYS:HE2	1:A:229:LYS:CA	2.32	0.42
1:A:140:THR:HG23	1:A:181:ARG:HD2	2.01	0.42
1:A:215:PRO:HA	1:A:216:PRO:HD3	1.88	0.42
1:A:162:LEU:HD12	1:A:179:LYS:HE3	2.01	0.42
1:B:24:GLU:HG3	1:B:187:GLN:HG2	2.02	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:CYS:SG	1:B:174:LYS:NZ	2.93	0.42
1:A:74:ILE:O	1:A:78:HIS:CD2	2.67	0.42
1:B:21:GLU:HG3	1:B:191:TYR:CG	2.54	0.42
1:B:61:ASP:O	1:B:62:VAL:CG2	2.66	0.42
1:A:166:PRO:HG3	1:A:219:ASP:O	2.19	0.42
1:A:181:ARG:NH2	3:A:1269:HOH:O	2.52	0.42
1:B:231:ALA:HB2	3:B:1847:HOH:O	2.19	0.42
1:A:76:ASP:HB2	1:A:81:LEU:HD11	2.01	0.41
1:A:162:LEU:HD21	1:A:169:LEU:CG	2.50	0.41
1:B:143:ASN:OD1	1:B:146:HIS:CE1	2.74	0.41
1:B:157:ALA:O	1:B:161:VAL:HG22	2.21	0.41
1:B:30:HIS:HB2	3:B:1788:HOH:O	2.21	0.41
1:B:172:PHE:O	1:B:176:VAL:HG23	2.21	0.41
1:B:142:LEU:O	1:B:143:ASN:CB	2.68	0.41
1:B:222:GLN:HE22	1:B:225:LEU:CG	2.34	0.41
1:B:136:LEU:HD12	1:B:175:LEU:HD23	2.03	0.40
1:A:162:LEU:HD21	1:A:169:LEU:HD12	2.02	0.40
1:A:68:MET:O	1:A:72:ARG:HG3	2.21	0.40
1:A:234:VAL:O	1:A:234:VAL:HG12	2.21	0.40
1:B:61:ASP:OD1	1:B:61:ASP:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PRO:O	1:B:24:GLU:OE1[5_555]	2.18	0.02

## 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	232/234 (99%)	217 (94%)	9 (4%)	6 (3%)	5 1

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	232/234 (99%)	211 (91%)	13 (6%)	8 (3%)	3	0
All	All	464/468 (99%)	428 (92%)	22 (5%)	14 (3%)	4	0

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	PRO
1	A	222	GLN
1	A	227	GLY
1	A	231	ALA
1	A	232	GLY
1	B	232	GLY
1	A	233	ASP
1	B	219	ASP
1	B	233	ASP
1	A	230	GLN
1	B	224	HIS
1	B	231	ALA
1	B	220	PRO
1	B	62	VAL

### 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	205/205 (100%)	202 (98%)	3 (2%)	65	56
1	B	205/205 (100%)	199 (97%)	6 (3%)	42	29
All	All	410/410 (100%)	401 (98%)	9 (2%)	52	39

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

Mol	Chain	Res	Type
1	A	34	ARG
1	A	187	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	222	GLN
1	B	53	ASN
1	B	72	ARG
1	B	187	GLN
1	B	217	LYS
1	B	222	GLN
1	B	233	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	138	HIS
1	A	187	GLN
1	A	214	HIS
1	A	221	GLN
1	A	222	GLN
1	A	230	GLN
1	B	53	ASN
1	B	78	HIS
1	B	187	GLN
1	B	203	GLN
1	B	214	HIS
1	B	221	GLN
1	B	223	HIS
1	B	224	HIS
1	B	230	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	1239	-	12,19,19	0.92	0	15,24,24	1.00	0
2	GSH	B	1587	-	12,19,19	1.10	2 (16%)	15,24,24	0.90	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	A	1239	-	-	0/18/24/24	-
2	GSH	B	1587	-	-	0/18/24/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1587	GSH	CG1-CD1	2.41	1.55	1.51
2	B	1587	GSH	CB2-CA2	2.13	1.55	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	GSH	CB1-CG1-CD1	-2.10	108.35	113.04

There are no chirality outliers.

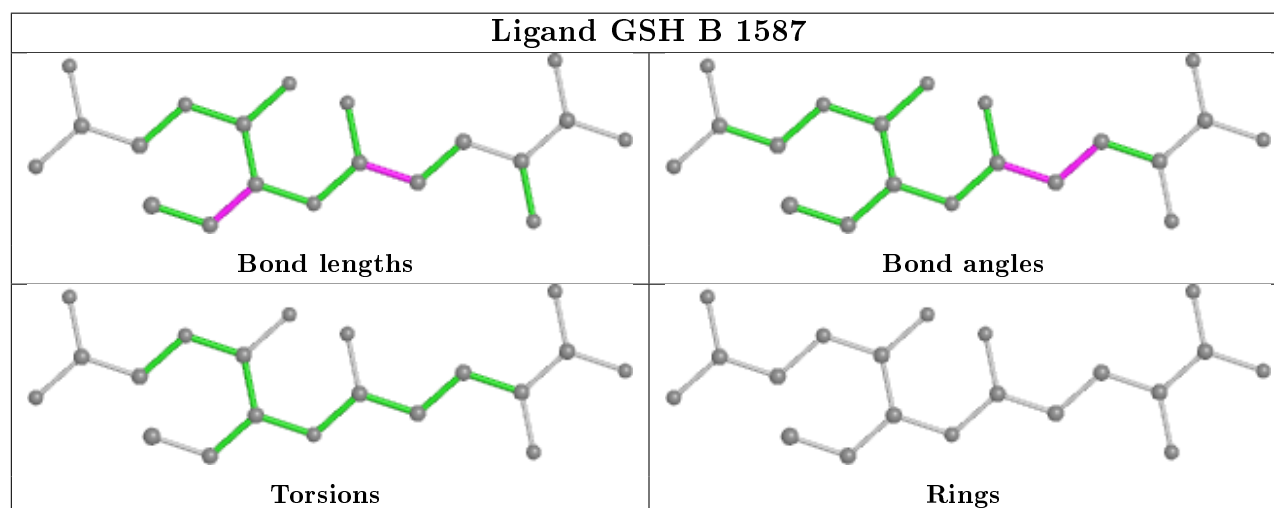
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1587	GSH	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	234/234 (100%)	0.59	20 (8%) 10 8	9, 17, 67, 76	0
1	B	234/234 (100%)	0.89	31 (13%) 3 2	10, 22, 69, 76	0
All	All	468/468 (100%)	0.74	51 (10%) 5 4	9, 19, 69, 76	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	28.6
1	A	234	VAL	18.8
1	A	227	GLY	14.7
1	B	218	SER	14.3
1	B	232	GLY	14.2
1	B	231	ALA	13.6
1	A	220	PRO	13.5
1	B	234	VAL	12.5
1	A	226	GLY	12.3
1	B	228	ALA	11.8
1	A	231	ALA	11.1
1	B	220	PRO	10.7
1	B	217	LYS	10.7
1	B	226	GLY	10.5
1	A	224	HIS	10.4
1	A	232	GLY	10.4
1	B	219	ASP	10.1
1	B	227	GLY	9.5
1	A	219	ASP	9.4
1	B	230	GLN	9.2
1	A	230	GLN	8.4
1	B	233	ASP	8.1
1	B	225	LEU	8.1
1	B	221	GLN	7.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	225	LEU	7.8
1	B	224	HIS	7.7
1	B	223	HIS	7.4
1	A	229	LYS	7.3
1	B	61	ASP	7.1
1	A	223	HIS	6.9
1	A	221	GLN	6.5
1	B	222	GLN	6.3
1	A	233	ASP	5.5
1	B	229	LYS	5.4
1	B	216	PRO	5.0
1	A	218	SER	4.5
1	B	60	GLY	4.2
1	A	222	GLN	4.1
1	B	119	VAL	4.0
1	B	112	LYS	3.6
1	B	138	HIS	3.6
1	A	217	LYS	3.4
1	A	138	HIS	3.3
1	B	62	VAL	3.0
1	B	116	THR	2.8
1	B	113	ASP	2.7
1	B	117	LEU	2.5
1	B	41	ARG	2.5
1	A	60	GLY	2.4
1	B	42	ASN	2.4
1	B	38	ASP	2.3

## 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.

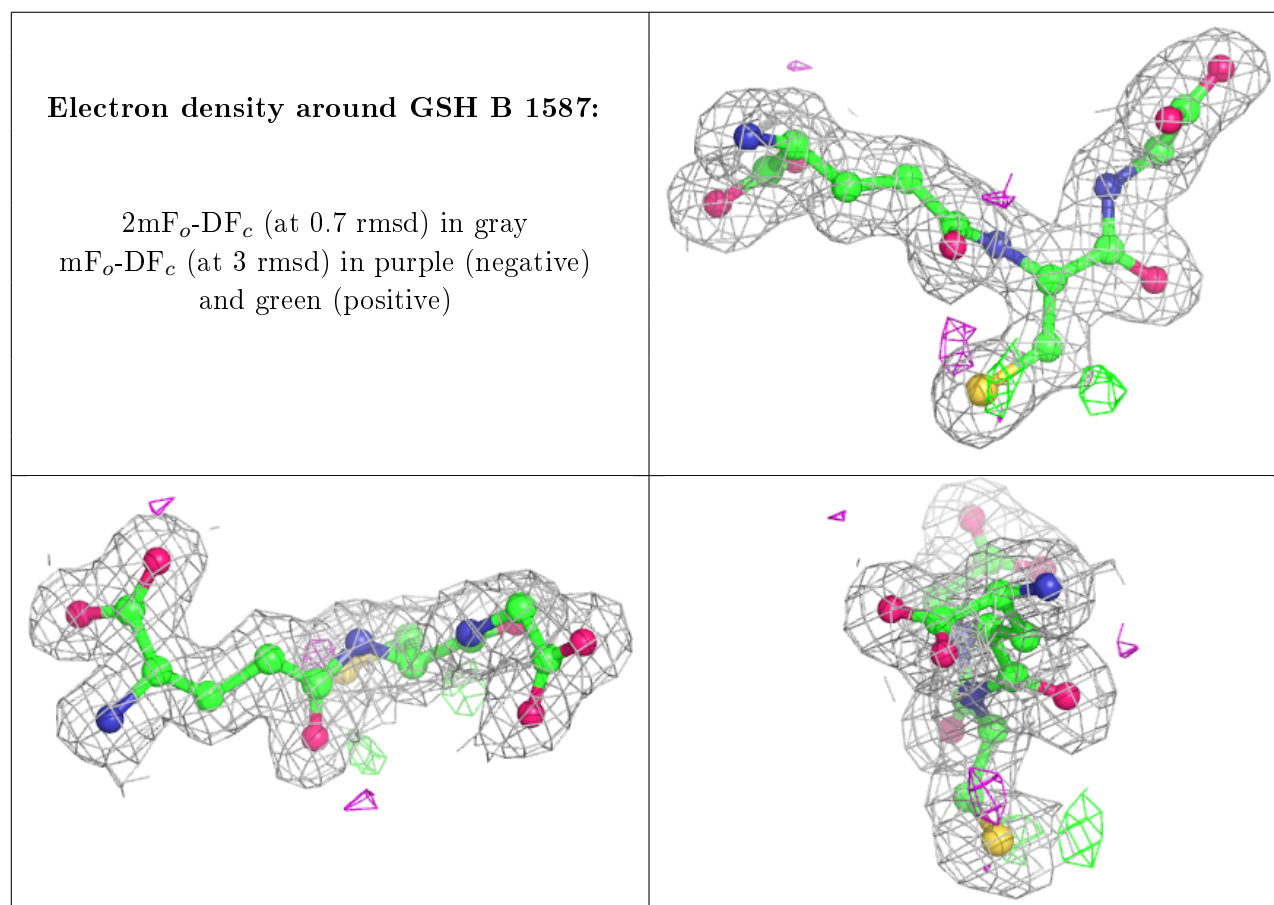
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	1239	20/20	0.96	0.08	10,15,22,26	0
2	GSH	B	1587	20/20	0.96	0.08	8,15,23,29	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.