



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:51 PM UTC

PDB ID : 1ETZ / pdb_00001etz
Title : THE THREE-DIMENSIONAL STRUCTURE OF AN ANTI-SWEETENER
FAB, NC10.14, SHOWS THE EXTENT OF STRUCTURAL DIVERSITY IN
ANTIGEN RECOGNITION BY IMMUNOGLOBULINS
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Deposited on : 2000-04-13
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

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

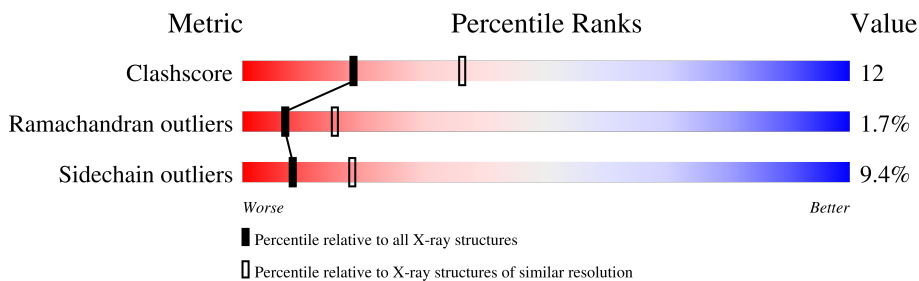
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	215	71% 22% 7%
1	L	215	71% 24% 5%
2	B	228	68% 28% .
2	H	228	69% 27% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6833 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.

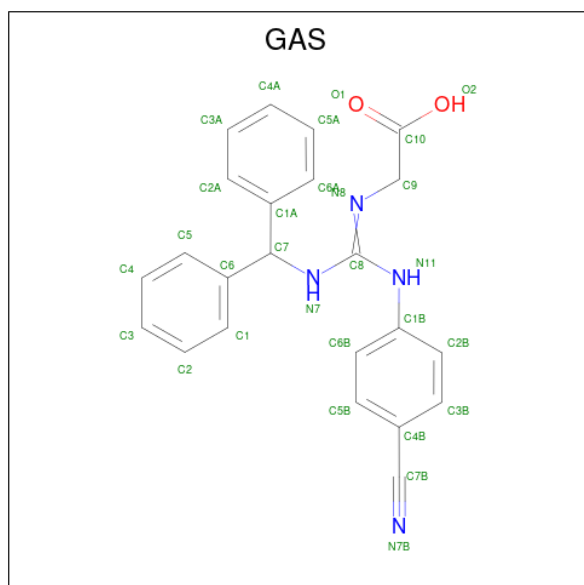
- Molecule 1 is a protein called FAB NC10.14 - LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1627	1019	272	329	7			
1	A	215	Total	C	N	O	S	0	0	0
			1627	1019	272	329	7			

- Molecule 2 is a protein called FAB NC10.14 - HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1722	1091	276	348	7			
2	B	228	Total	C	N	O	S	0	0	0
			1722	1091	276	348	7			

- Molecule 3 is N-(P-CYANOPHENYL)-N'-DIPHENYLMETHYL-GUANIDINE-ACETIC ACID (CCD ID: GAS) (formula: C₂₃H₂₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			29	23	4	2		
3	B	1	Total	C	N	O	0	0
			29	23	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	28	Total	O	0	0
			28	28		
4	H	13	Total	O	0	0
			13	13		
4	A	24	Total	O	0	0
			24	24		
4	B	12	Total	O	0	0
			12	12		

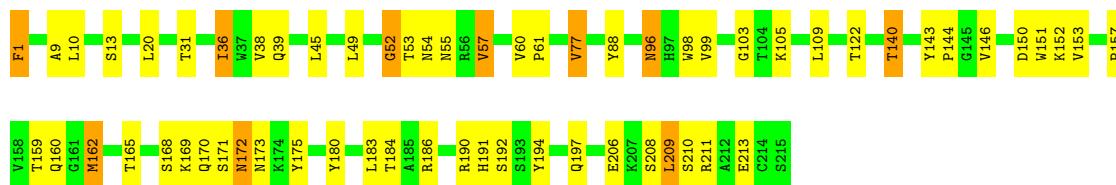
3 Residue-property plots

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. 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.

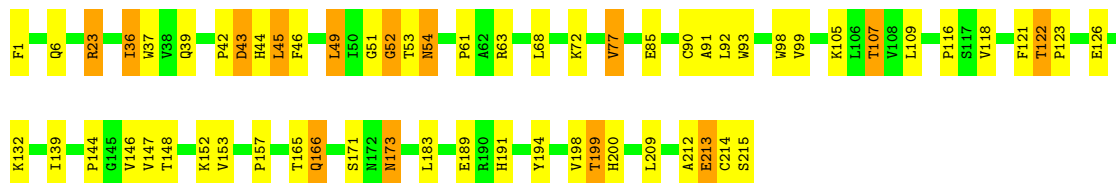
• Molecule 1: FAB NC10.14 - LIGHT CHAIN

Chain L: 



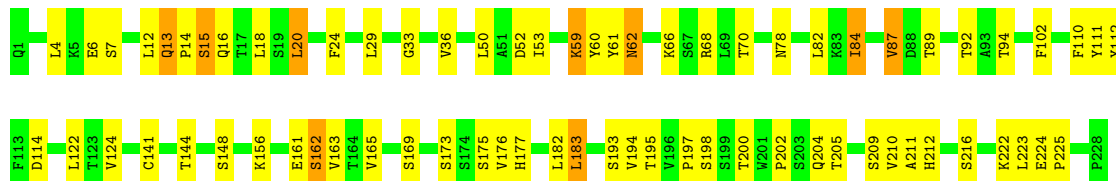
• Molecule 1: FAB NC10.14 - LIGHT CHAIN

Chain A: 



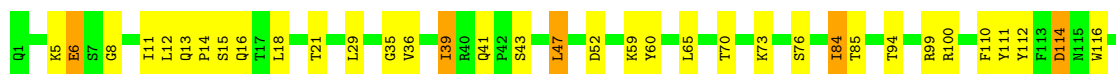
• Molecule 2: FAB NC10.14 - HEAVY CHAIN

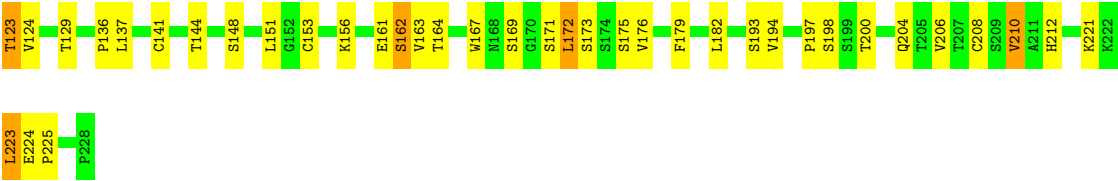
Chain H: 



• Molecule 2: FAB NC10.14 - HEAVY CHAIN

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.90Å 66.30Å 75.20Å 106.70° 107.60° 97.30°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	10.0 (10.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.198 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6833	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GAS

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	0.52	0/1665	0.98	4/2275 (0.2%)
1	L	0.52	0/1665	0.95	5/2275 (0.2%)
2	B	0.48	0/1772	0.98	10/2426 (0.4%)
2	H	0.48	0/1772	1.01	8/2426 (0.3%)
All	All	0.50	0/6874	0.98	27/9402 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	212	HIS	CA-C-N	7.31	127.17	119.05
2	B	212	HIS	C-N-CA	7.31	127.17	119.05
2	B	179	PHE	CA-C-N	7.18	126.94	119.76
2	B	179	PHE	C-N-CA	7.18	126.94	119.76
2	H	224	GLU	CA-C-N	7.13	127.16	119.89
2	H	224	GLU	C-N-CA	7.13	127.16	119.89
1	L	208	SER	N-CA-C	6.89	119.65	108.76
1	A	52	GLY	N-CA-C	-6.88	97.49	110.77
1	L	52	GLY	N-CA-C	-6.61	97.51	113.18
2	B	171	SER	N-CA-C	-6.55	97.12	108.52
2	H	156	LYS	N-CA-C	6.54	120.18	109.72
2	H	61	TYR	N-CA-C	6.27	119.40	109.81
2	H	144	THR	N-CA-C	-6.14	105.95	113.50
2	B	8	GLY	CA-C-N	5.94	125.82	119.28
2	B	8	GLY	C-N-CA	5.94	125.82	119.28
1	L	77	VAL	CB-CA-C	5.64	117.44	110.73
2	B	163	VAL	N-CA-C	-5.54	99.83	108.81
1	A	118	VAL	N-CA-C	5.47	116.66	109.21
1	L	184	THR	N-CA-C	-5.35	102.12	110.42
2	H	62	ASN	CA-C-N	5.18	125.23	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	62	ASN	C-N-CA	5.18	125.23	119.32
1	A	90	CYS	N-CA-C	-5.13	101.57	109.52
2	B	47	LEU	N-CA-C	5.10	116.87	110.24
1	L	140	THR	N-CA-C	5.10	116.73	109.14
2	H	114	ASP	N-CA-C	5.07	119.31	111.56
2	B	156	LYS	N-CA-C	5.07	116.69	109.14
1	A	214	CYS	N-CA-C	-5.05	107.40	113.21

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	1627	0	1571	46	0
1	L	1627	0	1571	41	0
2	B	1722	0	1656	45	0
2	H	1722	0	1656	41	0
3	B	29	0	19	5	0
3	H	29	0	17	1	0
4	A	24	0	0	1	0
4	B	12	0	0	0	0
4	H	13	0	0	0	0
4	L	28	0	0	1	0
All	All	6833	0	6490	160	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 12.

All (160) 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)
2:H:92:THR:HG22	2:H:124:VAL:H	1.38	0.86
1:A:122:THR:HG23	1:A:209:LEU:HD11	1.56	0.86
1:A:122:THR:HG22	1:A:123:PRO:HD2	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:NE2	1:A:166:GLN:H	1.82	0.77
1:L:165:THR:HG22	2:H:182:LEU:HG	1.69	0.73
2:H:222:LYS:HD3	2:H:223:LEU:N	2.05	0.72
1:L:96:ASN:H	1:L:96:ASN:HD22	1.36	0.71
2:B:29:LEU:HD23	2:B:73:LYS:HD2	1.72	0.71
1:L:9:ALA:O	1:L:10:LEU:HD23	1.94	0.67
1:L:140:THR:HG21	2:H:177:HIS:ND1	2.10	0.66
2:H:20:LEU:HD23	2:H:82:LEU:HD23	1.78	0.66
1:L:150:ASP:HB2	1:L:197:GLN:HB3	1.78	0.65
2:B:224:GLU:HG3	2:B:225:PRO:HD2	1.79	0.64
2:H:12:LEU:HD23	2:H:87:VAL:HG11	1.80	0.63
1:L:122:THR:HB	1:L:209:LEU:HD21	1.80	0.63
2:H:68:ARG:NH2	2:H:84:ILE:HD11	2.14	0.62
2:B:100:ARG:NH2	3:B:229:GAS:N7B	2.48	0.62
2:B:175:SER:O	2:B:194:VAL:HA	1.98	0.62
1:L:186:ARG:O	1:L:190:ARG:HG2	1.99	0.62
1:L:170:GLN:HB2	1:L:172:ASN:ND2	2.15	0.62
1:L:36:ILE:HD13	1:L:98:TRP:CH2	2.35	0.62
1:L:96:ASN:HD22	1:L:96:ASN:N	1.94	0.62
2:H:175:SER:HB2	2:H:195:THR:HB	1.82	0.62
1:A:23:ARG:HH11	1:A:23:ARG:HB2	1.65	0.61
1:L:36:ILE:HD11	2:H:111:TYR:O	2.01	0.60
2:H:200:THR:O	2:H:204:GLN:HB2	2.01	0.60
1:A:105:LYS:HE3	1:A:146:VAL:HG22	1.84	0.60
1:A:43:ASP:HB2	1:A:45:LEU:HD22	1.84	0.60
2:B:18:LEU:HB3	2:B:84:ILE:HG23	1.83	0.60
2:B:167:TRP:HB2	2:B:173:SER:HB3	1.83	0.59
1:L:170:GLN:HB2	1:L:172:ASN:HD21	1.68	0.59
2:B:14:PRO:O	2:B:15:SER:HB3	2.01	0.59
2:H:4:LEU:HD13	2:H:24:PHE:HB3	1.84	0.58
1:A:36:ILE:HD13	1:A:98:TRP:CH2	2.39	0.58
1:A:85:GLU:HG3	1:A:107:THR:HA	1.84	0.58
1:A:148:THR:OG1	1:A:199:THR:HG23	2.03	0.58
1:A:23:ARG:HB2	1:A:23:ARG:NH1	2.20	0.57
2:B:169:SER:HB3	2:B:206:VAL:HA	1.87	0.57
1:A:36:ILE:HD11	2:B:111:TYR:O	2.05	0.56
1:A:42:PRO:O	1:A:43:ASP:HB2	2.05	0.56
2:H:163:VAL:HG23	2:H:211:ALA:O	2.06	0.56
2:B:39:ILE:HD11	2:B:47:LEU:HD13	1.86	0.56
2:B:161:GLU:O	2:B:162:SER:HB2	2.05	0.56
1:A:42:PRO:O	1:A:45:LEU:HD22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ILE:HD11	2:B:47:LEU:HB3	1.88	0.55
2:B:100:ARG:NH1	3:B:229:GAS:N7B	2.55	0.55
1:A:152:LYS:HD3	1:A:157:PRO:HA	1.90	0.54
1:L:211:ARG:NH2	1:A:1:PHE:HA	2.23	0.53
1:L:172:ASN:HD22	1:L:172:ASN:N	2.06	0.53
1:A:98:TRP:NE1	3:B:229:GAS:N7B	2.57	0.53
1:A:116:PRO:HB3	1:A:139:ILE:CG2	2.39	0.53
1:A:52:GLY:HA3	2:B:110:PHE:HD2	1.73	0.52
2:B:200:THR:HG23	2:B:204:GLN:HG3	1.91	0.52
1:A:98:TRP:HE1	3:B:229:GAS:C7B	2.21	0.52
2:H:84:ILE:HG13	2:H:84:ILE:O	2.09	0.52
2:H:161:GLU:HG2	2:H:162:SER:N	2.25	0.52
1:A:144:PRO:O	1:A:200:HIS:HE1	1.93	0.52
2:H:14:PRO:O	2:H:15:SER:HB3	2.10	0.51
1:L:192:SER:O	1:L:210:SER:HA	2.11	0.51
2:B:151:LEU:HD23	2:B:223:LEU:HD22	1.92	0.51
1:L:39:GLN:HG3	1:L:88:TYR:CE1	2.45	0.51
1:L:159:THR:O	1:L:160:GLN:HG3	2.10	0.51
2:H:173:SER:HB2	2:H:194:VAL:HG21	1.92	0.51
2:H:182:LEU:O	2:H:183:LEU:C	2.54	0.51
1:L:152:LYS:HD3	1:L:157:PRO:HA	1.92	0.50
2:B:167:TRP:CB	2:B:173:SER:HB3	2.41	0.50
2:B:136:PRO:HB3	2:B:221:LYS:HZ2	1.76	0.50
1:L:96:ASN:N	1:L:96:ASN:ND2	2.57	0.50
1:L:169:LYS:HD3	1:L:173:ASN:HD22	1.77	0.50
1:A:152:LYS:CD	1:A:157:PRO:HA	2.41	0.50
2:H:148:SER:HA	2:H:197:PRO:HA	1.93	0.50
3:B:229:GAS:H7	3:B:229:GAS:H92	1.94	0.50
2:H:165:VAL:HA	2:H:209:SER:O	2.12	0.49
2:H:161:GLU:HG2	2:H:162:SER:H	1.77	0.49
1:A:191:HIS:HB2	1:A:194:TYR:OH	2.13	0.49
2:B:18:LEU:HD23	2:B:84:ILE:CG2	2.43	0.49
2:H:12:LEU:HB2	2:H:122:LEU:HD11	1.94	0.49
2:H:175:SER:O	2:H:194:VAL:HA	2.12	0.49
2:H:205:THR:HG23	2:H:222:LYS:HE2	1.95	0.49
1:L:122:THR:HB	1:L:209:LEU:CD2	2.43	0.48
1:A:213:GLU:C	1:A:215:SER:H	2.22	0.48
2:B:39:ILE:HD13	2:B:116:TRP:CH2	2.49	0.48
2:B:11:ILE:HG13	2:B:123:THR:HG23	1.95	0.48
2:B:173:SER:HB2	2:B:176:VAL:CG2	2.43	0.48
2:H:205:THR:HG23	2:H:222:LYS:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HB3	2:H:84:ILE:HG23	1.96	0.48
2:H:202:PRO:HG3	2:H:225:PRO:HG3	1.95	0.47
1:A:23:ARG:HB3	1:A:72:LYS:HG2	1.95	0.47
1:L:210:SER:HB3	1:L:213:GLU:HG3	1.96	0.47
1:L:162:MET:HA	1:L:180:TYR:O	2.14	0.47
1:L:210:SER:HB2	4:L:243:HOH:O	2.14	0.47
1:L:186:ARG:HG3	1:L:186:ARG:HH11	1.79	0.47
2:H:92:THR:CG2	2:H:124:VAL:H	2.18	0.47
1:A:139:ILE:HD12	1:A:139:ILE:N	2.29	0.47
1:L:170:GLN:HE21	1:L:172:ASN:HD21	1.63	0.47
2:B:18:LEU:HD23	2:B:84:ILE:HG23	1.96	0.47
1:A:93:TRP:HH2	2:B:60:TYR:CD2	2.33	0.46
2:H:52:ASP:HB2	2:H:60:TYR:HB2	1.96	0.46
1:L:183:LEU:HD11	1:L:194:TYR:HE2	1.80	0.46
1:A:51:GLY:HA3	2:B:112:TYR:CE2	2.51	0.46
1:L:143:TYR:HA	1:L:144:PRO:C	2.41	0.46
1:A:54:ASN:C	1:A:54:ASN:HD22	2.23	0.46
2:B:164:THR:O	2:B:210:VAL:HA	2.15	0.46
1:L:1:PHE:CE1	1:A:189:GLU:HG2	2.51	0.46
1:L:171:SER:C	1:L:173:ASN:H	2.23	0.46
2:B:169:SER:CB	2:B:206:VAL:HA	2.45	0.46
1:L:10:LEU:HD12	1:L:20:LEU:HG	1.98	0.45
1:A:139:ILE:HG21	1:A:198:VAL:HG11	1.97	0.45
1:A:166:GLN:H	1:A:166:GLN:CD	2.24	0.45
2:H:176:VAL:HG22	2:H:194:VAL:HG23	1.98	0.45
2:B:29:LEU:HD11	2:B:35:GLY:HA2	1.99	0.45
1:A:39:GLN:O	1:A:46:PHE:HA	2.17	0.45
2:B:148:SER:HA	2:B:198:SER:H	1.82	0.45
1:A:44:HIS:CE1	2:B:94:THR:HG21	2.52	0.45
2:H:169:SER:CB	2:H:173:SER:HB3	2.47	0.44
1:L:170:GLN:NE2	1:L:172:ASN:HD21	2.16	0.44
2:H:165:VAL:HG12	2:H:210:VAL:HG22	1.98	0.44
1:A:37:TRP:O	1:A:49:LEU:HB2	2.18	0.44
2:B:13:GLN:HB2	2:B:16:GLN:OE1	2.17	0.44
2:B:41:GLN:HB2	2:B:47:LEU:HD23	2.00	0.44
2:B:148:SER:HA	2:B:197:PRO:HA	2.00	0.44
2:H:222:LYS:HD3	2:H:222:LYS:C	2.42	0.44
2:B:167:TRP:HB2	2:B:173:SER:CB	2.48	0.44
2:H:53:ILE:HD12	2:H:59:LYS:HG3	2.00	0.43
2:B:12:LEU:O	2:B:124:VAL:HA	2.18	0.43
2:H:33:GLY:HA2	2:H:102:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:CD1	2:B:137:LEU:HB3	2.53	0.43
1:A:122:THR:CG2	1:A:209:LEU:HD11	2.39	0.43
2:B:151:LEU:HD22	2:B:206:VAL:HG11	2.01	0.42
1:A:122:THR:CG2	1:A:123:PRO:HD2	2.40	0.42
1:A:6:GLN:HB2	4:A:234:HOH:O	2.20	0.42
1:A:147:VAL:HG23	1:A:200:HIS:HB2	2.02	0.42
2:B:52:ASP:O	2:B:59:LYS:HA	2.18	0.42
1:L:151:TRP:O	1:L:152:LYS:HD3	2.20	0.42
2:H:59:LYS:N	2:H:59:LYS:HD3	2.34	0.42
1:A:63:ARG:O	1:A:77:VAL:HA	2.19	0.42
1:L:168:SER:O	1:L:175:TYR:HA	2.20	0.42
2:H:176:VAL:HA	2:H:193:SER:O	2.19	0.42
1:A:91:ALA:O	1:A:92:LEU:HD12	2.19	0.42
1:A:165:THR:HG22	2:B:182:LEU:HD21	2.02	0.42
2:B:172:LEU:HD23	2:B:173:SER:N	2.34	0.42
2:H:13:GLN:HB2	2:H:16:GLN:OE1	2.20	0.41
2:H:89:THR:O	2:H:92:THR:HG23	2.21	0.41
1:L:172:ASN:ND2	1:L:172:ASN:N	2.69	0.41
3:H:229:GAS:N11	3:H:229:GAS:C10	2.84	0.41
1:L:52:GLY:HA3	2:H:110:PHE:HD1	1.86	0.41
2:B:11:ILE:HG13	2:B:123:THR:CG2	2.51	0.41
1:L:88:TYR:O	1:L:103:GLY:HA2	2.21	0.41
2:B:6:GLU:HA	2:B:21:THR:O	2.21	0.41
1:L:191:HIS:O	1:L:211:ARG:HD3	2.20	0.40
1:A:147:VAL:CG2	1:A:198:VAL:HG12	2.51	0.40
1:L:57:VAL:HG12	2:H:112:TYR:CD2	2.57	0.40
1:L:57:VAL:HG22	1:L:60:VAL:HG23	2.03	0.40
1:A:171:SER:C	1:A:173:ASN:H	2.28	0.40
2:B:161:GLU:HG3	2:B:162:SER:N	2.36	0.40
2:H:212:HIS:O	2:H:216:SER:N	2.55	0.40
1:A:153:VAL:HG22	1:A:194:TYR:CD2	2.56	0.40
2:B:176:VAL:HA	2:B:193:SER:O	2.21	0.40
1:L:9:ALA:HA	1:L:105:LYS:O	2.21	0.40
1:A:51:GLY:HA3	2:B:112:TYR:CD2	2.56	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	213/215 (99%)	195 (92%)	15 (7%)	3 (1%)	9	19
1	L	213/215 (99%)	199 (93%)	12 (6%)	2 (1%)	14	30
2	B	226/228 (99%)	197 (87%)	24 (11%)	5 (2%)	5	10
2	H	226/228 (99%)	199 (88%)	22 (10%)	5 (2%)	5	10
All	All	878/886 (99%)	790 (90%)	73 (8%)	15 (2%)	7	15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	L	109	LEU
2	H	162	SER
2	H	183	LEU
1	A	212	ALA
2	B	114	ASP
2	H	198	SER
1	A	109	LEU
2	B	43	SER
2	B	141	CYS
2	B	162	SER
2	H	141	CYS
2	H	15	SER
2	B	129	THR
1	L	153	VAL

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	183/183 (100%)	164 (90%)	19 (10%)	7	14
1	L	183/183 (100%)	163 (89%)	20 (11%)	6	13
2	B	201/201 (100%)	183 (91%)	18 (9%)	9	20
2	H	201/201 (100%)	186 (92%)	15 (8%)	12	28
All	All	768/768 (100%)	696 (91%)	72 (9%)	8	18

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	PHE
1	L	13	SER
1	L	31	THR
1	L	36	ILE
1	L	38	VAL
1	L	45	LEU
1	L	49	LEU
1	L	53	THR
1	L	54	ASN
1	L	55	ASN
1	L	57	VAL
1	L	61	PRO
1	L	77	VAL
1	L	96	ASN
1	L	99	VAL
1	L	146	VAL
1	L	162	MET
1	L	172	ASN
1	L	206	GLU
1	L	209	LEU
2	H	6	GLU
2	H	7	SER
2	H	13	GLN
2	H	20	LEU
2	H	29	LEU
2	H	36	VAL
2	H	50	LEU
2	H	59	LYS
2	H	62	ASN
2	H	66	LYS
2	H	70	THR

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Mol	Chain	Res	Type
2	H	78	ASN
2	H	84	ILE
2	H	87	VAL
2	H	94	THR
1	A	23	ARG
1	A	36	ILE
1	A	45	LEU
1	A	49	LEU
1	A	53	THR
1	A	54	ASN
1	A	61	PRO
1	A	68	LEU
1	A	77	VAL
1	A	99	VAL
1	A	107	THR
1	A	122	THR
1	A	126	GLU
1	A	132	LYS
1	A	166	GLN
1	A	173	ASN
1	A	183	LEU
1	A	199	THR
1	A	213	GLU
2	B	5	LYS
2	B	6	GLU
2	B	36	VAL
2	B	39	ILE
2	B	65	LEU
2	B	70	THR
2	B	76	SER
2	B	84	ILE
2	B	85	THR
2	B	99	ARG
2	B	114	ASP
2	B	123	THR
2	B	144	THR
2	B	153	CYS
2	B	172	LEU
2	B	208	CYS
2	B	210	VAL
2	B	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	44	HIS
1	L	54	ASN
1	L	81	GLN
1	L	96	ASN
1	L	166	GLN
1	L	172	ASN
1	L	173	ASN
1	L	200	HIS
1	L	203	HIS
2	H	41	GLN
2	H	62	ASN
2	H	115	ASN
2	H	168	ASN
1	A	44	HIS
1	A	54	ASN
1	A	55	ASN
1	A	111	GLN
1	A	131	ASN
1	A	166	GLN
1	A	173	ASN
1	A	200	HIS
1	A	203	HIS
2	B	41	GLN
2	B	96	HIS
2	B	168	ASN
2	B	177	HIS
2	B	184	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 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
3	GAS	H	229	-	30,31,31	3.15	4 (13%)	35,40,40	1.79	6 (17%)
3	GAS	B	229	-	30,31,31	2.75	4 (13%)	35,40,40	1.38	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAS	H	229	-	-	6/21/23/23	0/3/3/3
3	GAS	B	229	-	-	7/21/23/23	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	GAS	C1A-C7	-11.46	1.37	1.52
3	B	229	GAS	C6-C7	-9.90	1.39	1.52
3	H	229	GAS	C6-C7	-9.54	1.40	1.52
3	B	229	GAS	C1A-C7	-9.18	1.40	1.52
3	H	229	GAS	C1B-N11	6.90	1.55	1.41
3	B	229	GAS	C1B-N11	4.89	1.51	1.41
3	H	229	GAS	C4B-C7B	3.37	1.51	1.44
3	B	229	GAS	C4B-C7B	3.27	1.51	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	229	GAS	C6-C7-N7	6.06	122.11	111.23
3	B	229	GAS	C1B-N11-C8	4.62	139.37	126.70
3	H	229	GAS	N11-C8-N8	-4.27	117.42	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	229	GAS	C1B-N11-C8	4.21	138.24	126.70
3	B	229	GAS	C1A-C7-N7	3.81	118.08	111.23
3	H	229	GAS	C1A-C7-N7	3.61	117.72	111.23
3	B	229	GAS	C6-C7-N7	2.94	116.51	111.23
3	H	229	GAS	O2-C10-C9	2.56	119.74	112.25
3	H	229	GAS	C1A-C7-C6	2.39	117.13	112.33
3	B	229	GAS	N11-C8-N8	-2.02	120.19	122.69
3	B	229	GAS	O2-C10-C9	2.01	118.13	112.25

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	229	GAS	N8-C8-N7-C7
3	H	229	GAS	N11-C8-N7-C7
3	H	229	GAS	C10-C9-N8-C8
3	H	229	GAS	O2-C10-C9-N8
3	B	229	GAS	N8-C8-N7-C7
3	B	229	GAS	N11-C8-N7-C7
3	B	229	GAS	O1-C10-C9-N8
3	B	229	GAS	O2-C10-C9-N8
3	H	229	GAS	N7-C8-N11-C1B
3	B	229	GAS	C2B-C1B-N11-C8
3	B	229	GAS	C10-C9-N8-C8
3	B	229	GAS	C6B-C1B-N11-C8
3	H	229	GAS	C6-C7-N7-C8

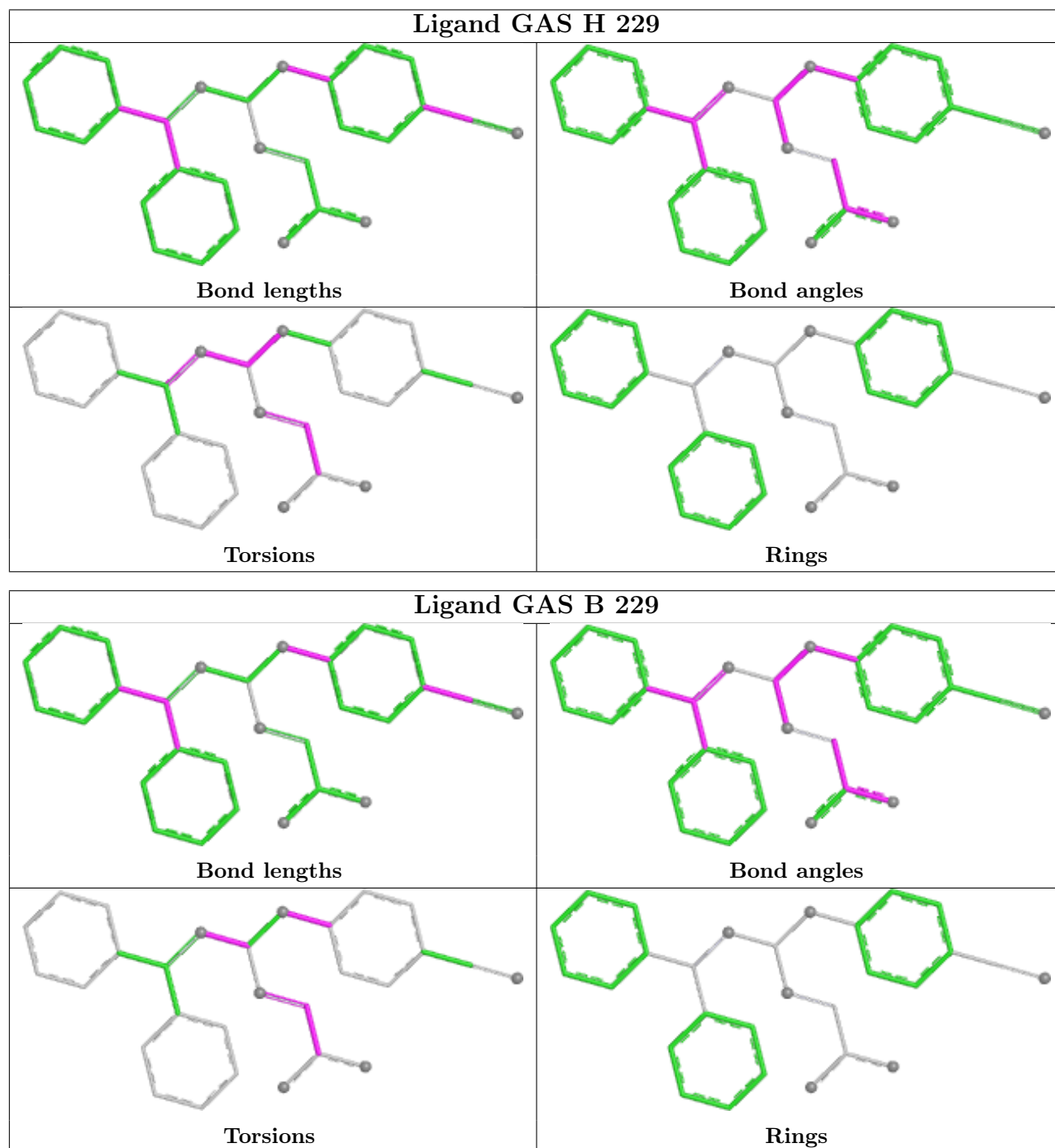
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	229	GAS	1	0
3	B	229	GAS	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.