Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:35 PM EDT

PDB ID	:	1ETZ
Title	:	THE THREE-DIMENSIONAL STRUCTURE OF AN ANTI-SWEETENER FAB, NC10.14, SHOWS THE EXTENT OF STRUCTURAL DIVERSITY IN ANTIGEN RECOGNITION BY IMMUNOGLOBULINS
Authors	:	Guddat, L.W.; Shan, L.; Broomell, C.; Ramsland, P.A.; Fan, Z.; Anchin, J.M.; Linthicum, D.S.; Edmundson, A.B.
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 (i) 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 (1)) were used in the production of this report:

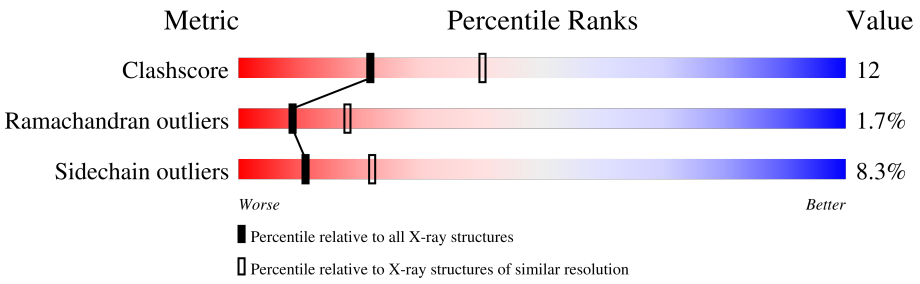
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	215	74% 20% 6%
1	L	215	72% 25% •
2	B	228	71% 26% •
2	H	228	71% 25% •

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.

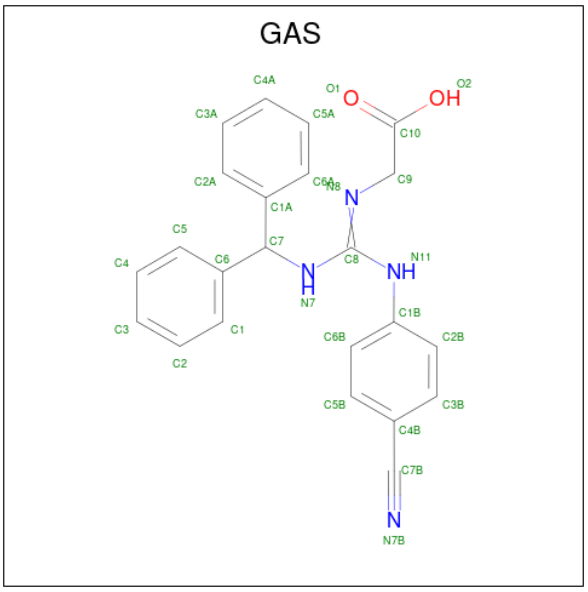
- Molecule 1 is a protein called FAB NC10.14 - LIGHT CHAIN.

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

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

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

- Molecule 3 is N-(P-CYANOPHENYL)-N'-DIPHENYLMETHYL-GUANIDINE-ACETIC ACID (three-letter code: GAS) (formula: $C_{23}H_{20}N_4O_2$).



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

- Molecule 4 is water.

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

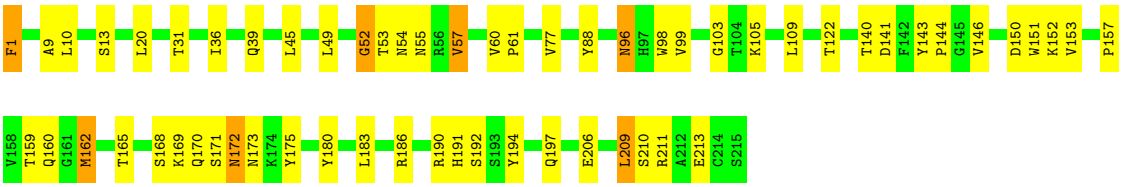
3 Residue-property plots (i)

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.

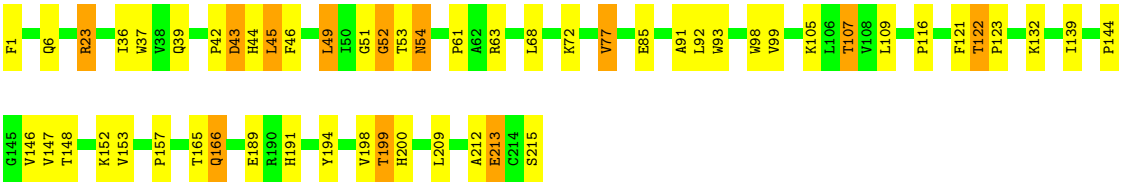
• Molecule 1: FAB NC10.14 - LIGHT CHAIN

Chain L:



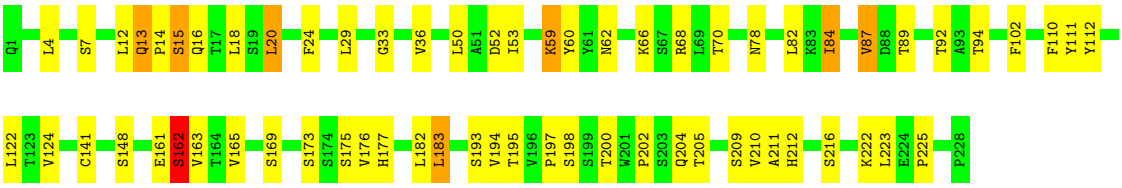
• Molecule 1: FAB NC10.14 - LIGHT CHAIN

Chain A:



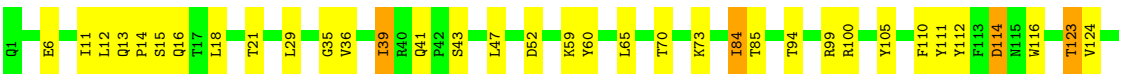
• Molecule 2: FAB NC10.14 - HEAVY CHAIN

Chain H:



• Molecule 2: FAB NC10.14 - HEAVY CHAIN

Chain B:



T129
P136
L137
C141
T144
S148
L151
G152
C153
E161
S162
V163
T164
W167
N168
S169
G170
S171
L172
S173
S174
S175
V176
L182
S193
V194
P197
S198
S199
T200
Q204
T205
V206
T207
C208
S209
V210
K221
K222
L223
E224
P225
P228

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	0.39	0/1665	0.69	1/2275 (0.0%)
1	L	0.40	0/1665	0.71	1/2275 (0.0%)
2	B	0.38	0/1772	0.67	1/2426 (0.0%)
2	H	0.39	0/1772	0.69	0/2426
All	All	0.39	0/6874	0.69	3/9402 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	GLY	N-CA-C	-6.25	97.49	113.10
1	L	52	GLY	N-CA-C	-6.23	97.51	113.10
2	B	171	SER	N-CA-C	-5.14	97.12	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	1627	0	1571	45	0
1	L	1627	0	1571	41	0
2	B	1722	0	1656	45	0
2	H	1722	0	1656	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	158	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 (158) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:136:PRO:HB3	2:B:221:LYS:HZ2	1.77	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
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
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
2:B:164:THR:O	2:B:210:VAL:HA	2.15	0.46
2:H:182:LEU:O	2:H:183:LEU:C	2.54	0.46
1:L:1:PHE:CE1	1:A:189:GLU:HG2	2.51	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:213:GLU:C	1:A:215:SER:H	2.22	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
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
1:L:143:TYR:HA	1:L:144:PRO:C	2.41	0.41
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:A:54:ASN:C	1:A:54:ASN:HD22	2.23	0.41
1:L:172:ASN:ND2	1:L:172:ASN:N	2.69	0.41
1:L:171:SER:C	1:L:173:ASN:H	2.23	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
1:A:166:GLN:H	1:A:166:GLN:CD	2.24	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	11	22
1	L	213/215 (99%)	199 (93%)	12 (6%)	2 (1%)	17	35
2	B	226/228 (99%)	197 (87%)	24 (11%)	5 (2%)	6	12
2	H	226/228 (99%)	199 (88%)	22 (10%)	5 (2%)	6	12
All	All	878/886 (99%)	790 (90%)	73 (8%)	15 (2%)	9	18

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	168 (92%)	15 (8%)	11 22
1	L	183/183 (100%)	164 (90%)	19 (10%)	7 13
2	B	201/201 (100%)	186 (92%)	15 (8%)	13 27
2	H	201/201 (100%)	186 (92%)	15 (8%)	13 27
All	All	768/768 (100%)	704 (92%)	64 (8%)	11 22

All (64) 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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	141	ASP
1	L	146	VAL
1	L	162	MET
1	L	172	ASN
1	L	206	GLU
1	L	209	LEU
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
2	H	78	ASN
2	H	84	ILE
2	H	87	VAL
2	H	94	THR
2	H	162	SER
1	A	23	ARG
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	132	LYS
1	A	166	GLN
1	A	199	THR
1	A	213	GLU
2	B	36	VAL
2	B	39	ILE
2	B	65	LEU
2	B	70	THR
2	B	84	ILE
2	B	85	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	99	ARG
2	B	105	TYR
2	B	114	ASP
2	B	123	THR
2	B	144	THR
2	B	153	CYS
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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	44	HIS
1	L	54	ASN
1	L	96	ASN
1	L	160	GLN
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	78	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	200	HIS
1	A	203	HIS
2	B	41	GLN
2	B	96	HIS
2	B	168	ASN
2	B	184	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 monosaccharides 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	$\#\|Z\| > 2$
3	GAS	H	229	-	28,31,31	3.17	4 (14%)	35,40,40	1.69	6 (17%)
3	GAS	B	229	-	28,31,31	2.78	4 (14%)	35,40,40	1.37	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	-11.18	1.37	1.52
3	B	229	GAS	C6-C7	-9.65	1.39	1.52
3	H	229	GAS	C6-C7	-9.30	1.40	1.52
3	B	229	GAS	C1A-C7	-8.95	1.40	1.52
3	H	229	GAS	C1B-N11	6.88	1.55	1.41
3	B	229	GAS	C1B-N11	4.88	1.51	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	229	GAS	C4B-C7B	3.21	1.51	1.44
3	B	229	GAS	C4B-C7B	3.11	1.51	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	229	GAS	C6-C7-N7	6.05	122.11	111.30
3	B	229	GAS	C1B-N11-C8	4.59	139.37	126.53
3	H	229	GAS	C1B-N11-C8	4.19	138.24	126.53
3	B	229	GAS	C1A-C7-N7	3.79	118.08	111.30
3	H	229	GAS	C1A-C7-N7	3.59	117.72	111.30
3	H	229	GAS	O2-C10-C9	2.99	119.74	111.57
3	B	229	GAS	C6-C7-N7	2.91	116.51	111.30
3	B	229	GAS	O2-C10-C9	2.40	118.13	111.57
3	H	229	GAS	O1-C10-C9	-2.25	117.19	123.07
3	H	229	GAS	C1A-C7-C6	2.20	117.13	112.33
3	B	229	GAS	O1-C10-C9	-2.05	117.71	123.07

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	O1-C10-C9-N8

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

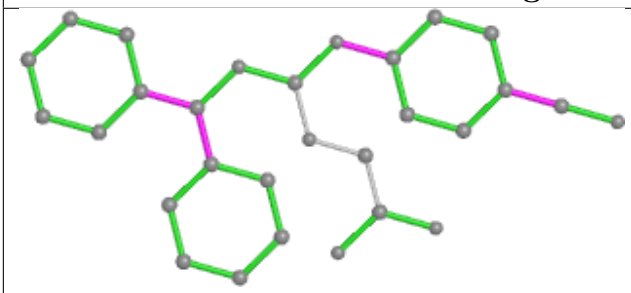
Continued on next page...

Continued from previous page...

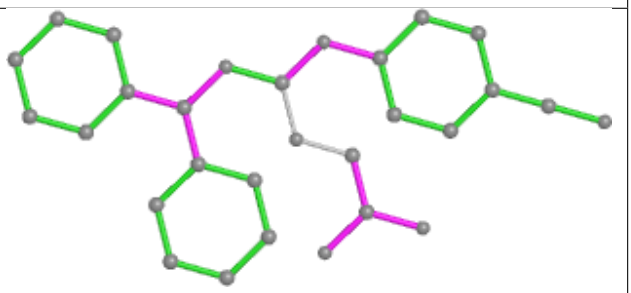
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	229	GAS	5	0

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 then 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.

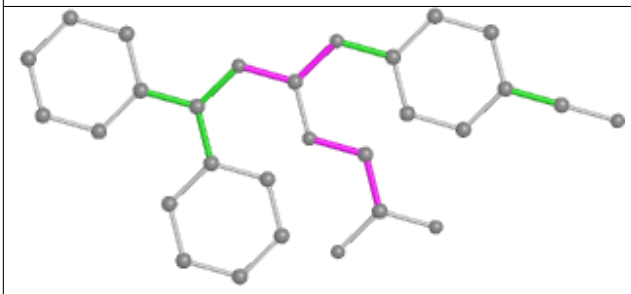
Ligand GAS H 229



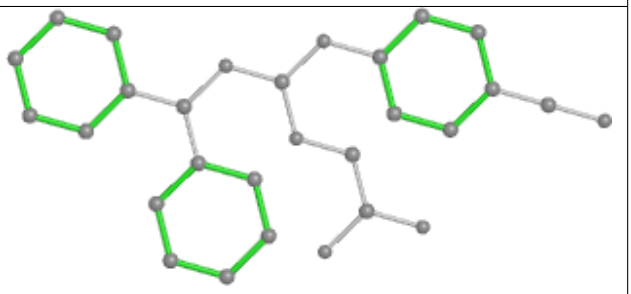
Bond lengths



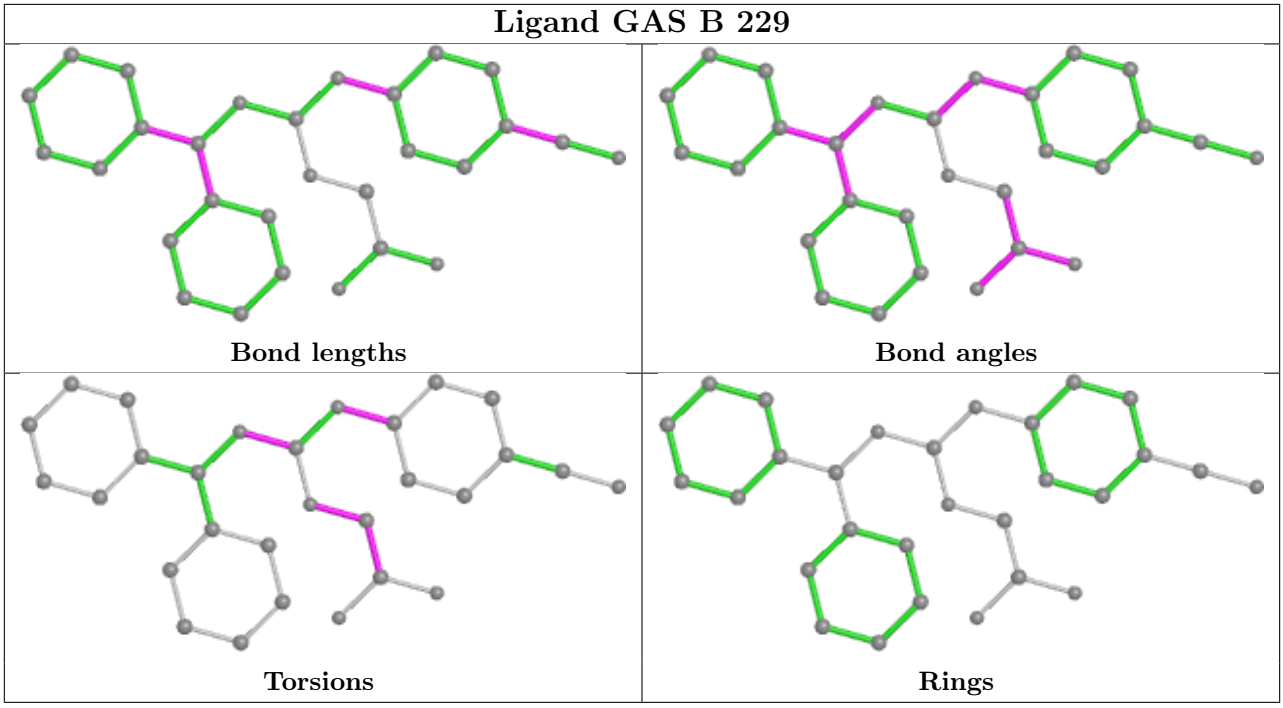
Bond angles



Torsions



Rings



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.