



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:10 PM BST

PDB ID : 2VDM
Title : Re-refinement of Integrin AlphaIIbBeta3 Headpiece Bound to Antagonist Tirofiban
Authors : Springer, T.A.; Zhu, J.; Xiao, T.
Deposited on : 2007-10-10
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

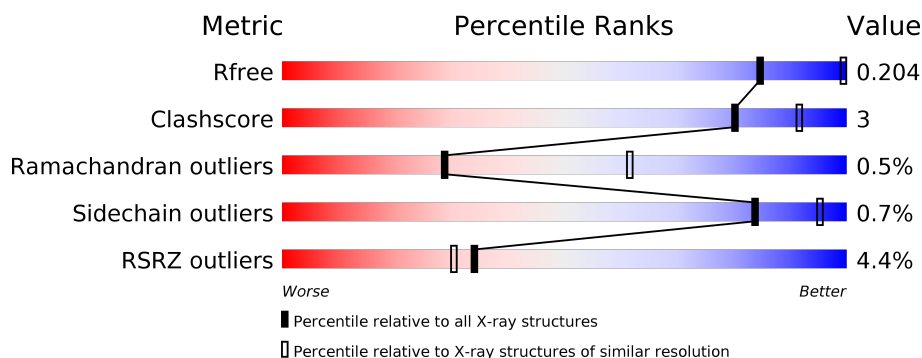
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	452	<div> <div></div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	B	461	<div> <div>11%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
3	H	221	<div> <div></div> <div> <div></div> <div>90%</div> <div>8%</div> </div> </div>
4	L	214	<div> <div></div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
5	C	5	<div> <div></div> <div> <div></div> <div>60%</div> <div>40%</div> </div> </div>
6	D	7	<div> <div></div> <div> <div></div> <div>29%</div> <div>71%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	C	3	X	-	-	-
6	MAN	D	3	X	-	-	-
9	NAG	A	3015	-	-	-	X
9	NAG	A	3249	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10953 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 INTEGRIN ALPHA-IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	4	0
			3504	2224	610	662	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLY	ALA	conflict	UNP P08514

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	456	Total	C	N	O	S	0	2	0
			3545	2209	606	698	32			

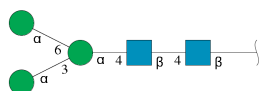
- Molecule 3 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	2	0
			1672	1060	269	337	6			

- Molecule 4 is a protein called MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN.

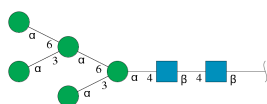
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	1	0
			1642	1022	269	342	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



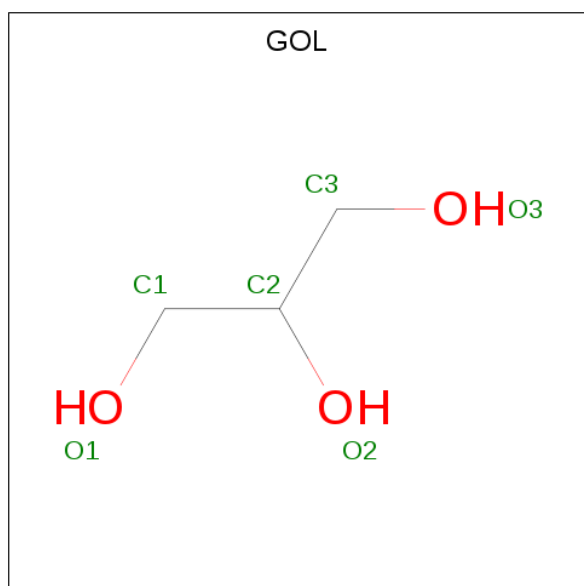
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

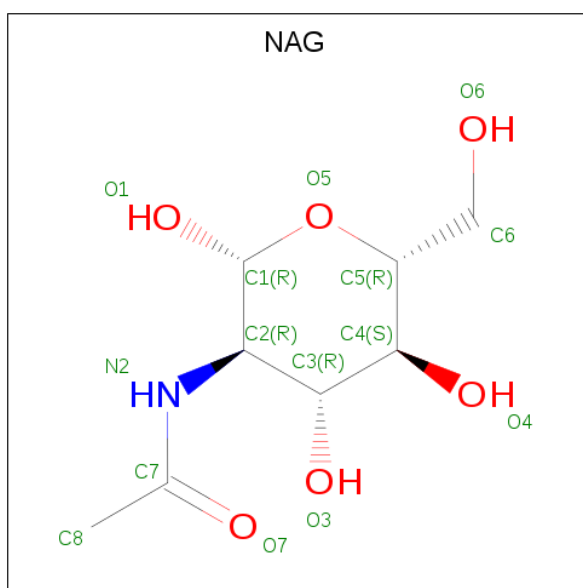


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

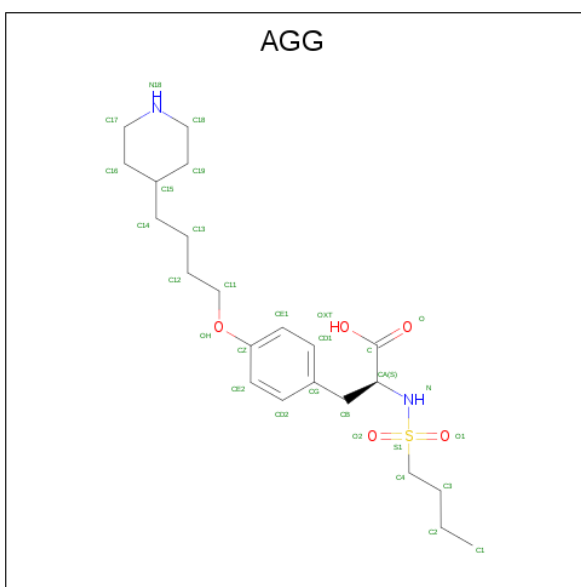
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		
8	A	4	Total	Ca	0	0
			4	4		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is TIROFIBAN (three-letter code: AGG) (formula: C₂₂H₃₆N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			30	22	2	5	1		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Mg	0	0
			1	1		

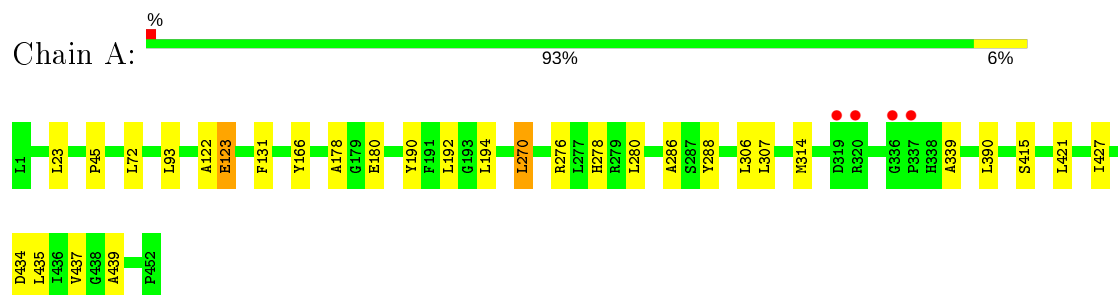
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	139	Total	O	0	0
			139	139		
12	B	75	Total	O	0	0
			75	75		
12	H	73	Total	O	0	0
			73	73		
12	L	68	Total	O	0	0
			68	68		

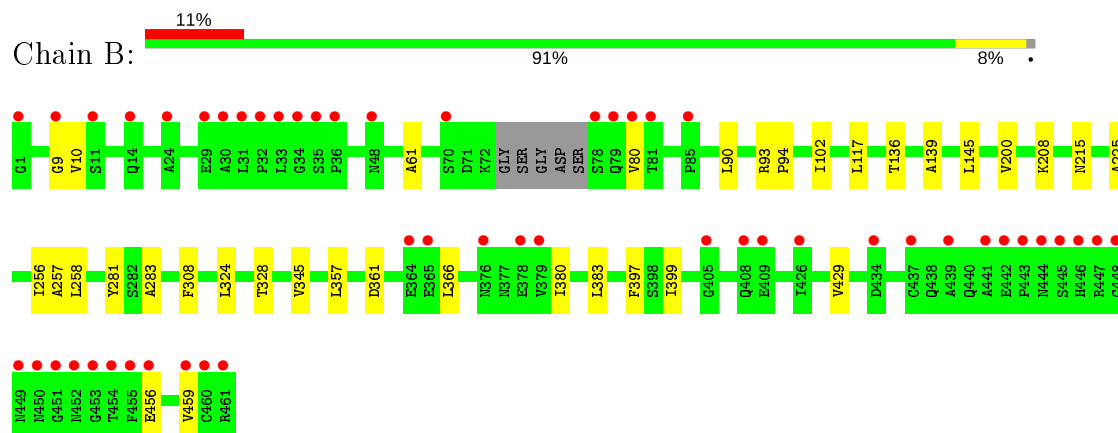
3 Residue-property plots

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 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.

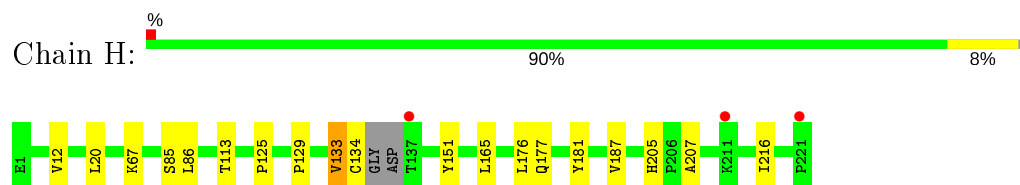
• Molecule 1: INTEGRIN ALPHA-IIB



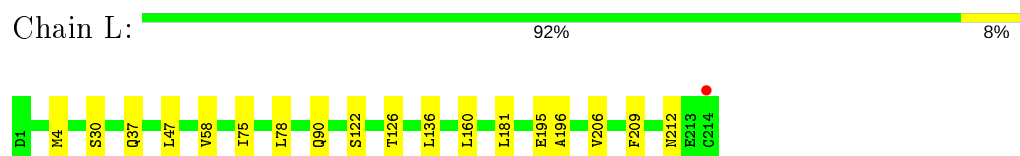
• Molecule 2: INTEGRIN BETA-3



• Molecule 3: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN



• Molecule 4: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN



- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  60% 40%



- Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  29% 71%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.58Å 148.58Å 177.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.23 – 2.90 43.52 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.23-2.90) 91.7 (43.52-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.167 , 0.206 0.174 , 0.204	Depositor DCC
R_{free} test set	2339 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NAG, AGG, CA, MAN

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	0.31	0/3607	0.50	0/4913
2	B	0.30	0/3608	0.47	0/4890
3	H	0.30	0/1721	0.48	0/2357
4	L	0.30	0/1681	0.49	0/2280
All	All	0.30	0/10617	0.49	0/14440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3504	0	3342	18	0
2	B	3545	0	3474	17	0
3	H	1672	0	1629	14	0
4	L	1642	0	1559	12	0
5	C	61	0	52	0	0
6	D	83	0	70	0	0
7	A	6	0	8	0	0
7	B	6	0	7	0	0
8	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	2	0	0	0	0
9	A	28	0	26	0	0
9	B	14	0	13	0	0
10	B	30	0	35	1	0
11	B	1	0	0	0	0
12	A	139	0	0	0	0
12	B	75	0	0	0	0
12	H	73	0	0	0	0
12	L	68	0	0	0	0
All	All	10953	0	10215	57	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 3.

All (57) 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:421:LEU:CD2	1:A:437:VAL:HG22	2.28	0.64
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.84	0.60
2:B:139:ALA:HB1	2:B:200:VAL:HG13	1.82	0.59
2:B:61:ALA:HB2	2:B:90:LEU:HD23	1.85	0.59
1:A:192:LEU:HD13	10:B:1462:AGG:H171	1.85	0.58
1:A:278[A]:HIS:CD2	1:A:339:ALA:HB1	2.42	0.55
2:B:117:LEU:HD22	2:B:225:ALA:HB1	1.89	0.53
3:H:177:GLN:HB3	4:L:160:LEU:HD21	1.91	0.53
3:H:12:VAL:CG2	3:H:86:LEU:HD13	2.40	0.51
4:L:136:LEU:N	4:L:136:LEU:HD12	2.26	0.51
3:H:20:LEU:HD22	3:H:113:THR:HG21	1.92	0.51
2:B:145:LEU:HD22	2:B:345:VAL:HG22	1.93	0.50
1:A:270:LEU:HD23	1:A:276[A]:ARG:HA	1.94	0.50
3:H:205:HIS:CE1	3:H:207:ALA:HB3	2.46	0.49
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.95	0.49
4:L:122:SER:O	4:L:126:THR:HG23	2.12	0.49
3:H:165:LEU:HD21	3:H:187:VAL:HG21	1.93	0.49
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.95	0.49
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.47	0.49
1:A:427:ILE:HG22	1:A:434:ASP:OD1	2.13	0.48
4:L:136:LEU:HD23	4:L:196:ALA:CB	2.44	0.48
3:H:165:LEU:CD2	3:H:187:VAL:HG21	2.43	0.47
1:A:194:LEU:C	1:A:194:LEU:HD12	2.34	0.47
1:A:306:LEU:HD12	1:A:307:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:75:ILE:HG21	4:L:78:LEU:HD23	1.95	0.47
1:A:178:ALA:HB3	1:A:180:GLU:OE1	2.14	0.47
1:A:286:ALA:HA	2:B:256:ILE:HD12	1.97	0.47
1:A:270:LEU:HD23	1:A:276[B]:ARG:HA	1.95	0.47
3:H:176:LEU:HD13	3:H:181:TYR:CE1	2.51	0.46
1:A:421:LEU:HD22	1:A:435:LEU:HD11	1.97	0.46
2:B:456:GLU:O	2:B:459:VAL:HG12	2.16	0.46
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.97	0.46
4:L:181:LEU:N	4:L:181:LEU:HD23	2.31	0.45
4:L:136:LEU:HD23	4:L:196:ALA:HB2	1.98	0.45
2:B:102:ILE:HG21	2:B:399:ILE:HD11	1.99	0.45
1:A:122:ALA:O	1:A:123:GLU:HB2	2.17	0.44
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.52	0.44
1:A:314:MET:HE1	2:B:324:LEU:HB3	2.00	0.44
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.99	0.44
2:B:93:ARG:HB2	2:B:94:PRO:HD2	2.00	0.44
3:H:133:VAL:HG11	4:L:209:PHE:HB2	1.99	0.43
3:H:67:LYS:NZ	3:H:85:SER:O	2.51	0.43
2:B:366:LEU:HD11	2:B:429:VAL:HG21	2.00	0.43
4:L:47:LEU:HA	4:L:58:VAL:HG21	2.01	0.42
3:H:176:LEU:HD13	3:H:181:TYR:CZ	2.54	0.42
1:A:390:LEU:HD12	1:A:390:LEU:N	2.34	0.42
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.02	0.41
1:A:93:LEU:HD13	1:A:131:PHE:CD1	2.55	0.41
2:B:380:ILE:HG21	2:B:383:LEU:HD22	2.03	0.41
2:B:136:THR:HG21	2:B:208:LYS:HE3	2.03	0.40
1:A:415:SER:HB2	1:A:439:ALA:HB1	2.03	0.40
2:B:257:ALA:O	2:B:258:LEU:HB2	2.22	0.40
2:B:357:LEU:HD11	2:B:397:PHE:CD2	2.56	0.40
2:B:102:ILE:CG2	2:B:399:ILE:HD11	2.51	0.40
3:H:133:VAL:HG12	3:H:134:CYS:H	1.87	0.40
3:H:129:PRO:CB	3:H:216:ILE:HD13	2.51	0.40
1:A:45:PRO:HD3	1:A:72:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

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	454/452 (100%)	443 (98%)	10 (2%)	1 (0%)	47	78
2	B	454/461 (98%)	423 (93%)	28 (6%)	3 (1%)	22	54
3	H	217/221 (98%)	209 (96%)	8 (4%)	0	100	100
4	L	213/214 (100%)	204 (96%)	7 (3%)	2 (1%)	17	48
All	All	1338/1348 (99%)	1279 (96%)	53 (4%)	6 (0%)	29	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	9	GLY
4	L	212	ASN
2	B	80	VAL
4	L	30	SER
2	B	10	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	364/360 (101%)	359 (99%)	5 (1%)	67	89
2	B	408/409 (100%)	406 (100%)	2 (0%)	88	96
3	H	191/190 (100%)	190 (100%)	1 (0%)	88	96
4	L	189/188 (100%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1152/1147 (100%)	1144 (99%)	8 (1%)	84	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	215	ASN
2	B	361	ASP
3	H	133	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
2	B	133	ASN
2	B	342	GLN
2	B	428	GLN
3	H	3	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 ⓘ

12 monosaccharides 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	$\# Z > 2$
5	NAG	C	1	2,5	14,14,15	0.65	0	17,19,21	0.86	0
5	NAG	C	2	5	14,14,15	0.58	0	17,19,21	0.68	0
5	MAN	C	3	5	11,11,12	0.57	0	15,15,17	0.98	1 (6%)
5	MAN	C	4	5	11,11,12	0.54	0	15,15,17	0.68	0
5	MAN	C	5	5	11,11,12	0.60	0	15,15,17	0.83	1 (6%)
6	NAG	D	1	2,6	14,14,15	0.56	0	17,19,21	0.78	1 (5%)
6	NAG	D	2	6	14,14,15	0.50	0	17,19,21	0.89	0
6	MAN	D	3	6	11,11,12	0.58	0	15,15,17	0.85	1 (6%)
6	MAN	D	4	6	11,11,12	0.60	0	15,15,17	0.89	1 (6%)
6	MAN	D	5	6	11,11,12	0.58	0	15,15,17	1.17	2 (13%)
6	MAN	D	6	6	11,11,12	0.57	0	15,15,17	1.01	1 (6%)
6	MAN	D	7	6	11,11,12	0.58	0	15,15,17	0.80	0

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
5	NAG	C	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	MAN	C	3	5	1/1/4/5	2/2/19/22	0/1/1/1
5	MAN	C	4	5	-	1/2/19/22	0/1/1/1
5	MAN	C	5	5	-	2/2/19/22	0/1/1/1
6	NAG	D	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	1/6/23/26	0/1/1/1
6	MAN	D	3	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5	6	-	0/2/19/22	0/1/1/1
6	MAN	D	6	6	-	1/2/19/22	0/1/1/1
6	MAN	D	7	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	5	MAN	C1-C2-C3	2.84	113.15	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	4	MAN	C1-O5-C5	2.66	115.80	112.19
6	D	5	MAN	C1-O5-C5	2.59	115.69	112.19
5	C	3	MAN	O5-C5-C6	2.47	111.08	107.20
6	D	1	NAG	O5-C1-C2	-2.37	107.54	111.29
6	D	6	MAN	C1-O5-C5	2.32	115.34	112.19
5	C	5	MAN	C1-C2-C3	2.23	112.40	109.67
6	D	3	MAN	O5-C1-C2	-2.09	107.54	110.77

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	3	MAN	C1
6	D	3	MAN	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	3	MAN	O5-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	C	5	MAN	O5-C5-C6-O6
5	C	3	MAN	C4-C5-C6-O6
5	C	5	MAN	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
5	C	4	MAN	C4-C5-C6-O6
6	D	6	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

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
9	NAG	A	3015	1	14,14,15	0.72	0	17,19,21	1.45	2 (11%)
9	NAG	B	3099	2	14,14,15	0.47	0	17,19,21	0.79	0
10	AGG	B	1462	11	28,31,31	1.36	2 (7%)	33,40,40	1.61	2 (6%)
7	GOL	B	1463	8	5,5,5	0.37	0	5,5,5	0.11	0
7	GOL	A	1453	-	5,5,5	0.40	0	5,5,5	0.12	0
9	NAG	A	3249	1	14,14,15	0.64	0	17,19,21	0.99	0

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
9	NAG	A	3015	1	-	2/6/23/26	0/1/1/1
9	NAG	B	3099	2	-	2/6/23/26	0/1/1/1
10	AGG	B	1462	11	-	9/22/34/34	0/2/2/2
7	GOL	B	1463	8	-	2/4/4/4	-
7	GOL	A	1453	-	-	4/4/4/4	-
9	NAG	A	3249	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1462	AGG	O2-S1	4.70	1.50	1.43
10	B	1462	AGG	O1-S1	4.34	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1462	AGG	O2-S1-O1	-7.53	108.45	119.35
9	A	3015	NAG	C4-C3-C2	4.44	117.53	111.02
10	B	1462	AGG	O2-S1-N	2.46	110.66	107.12
9	A	3015	NAG	C3-C4-C5	2.12	114.02	110.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1462	AGG	C3-C4-S1-N
10	B	1462	AGG	N-CA-CB-CG

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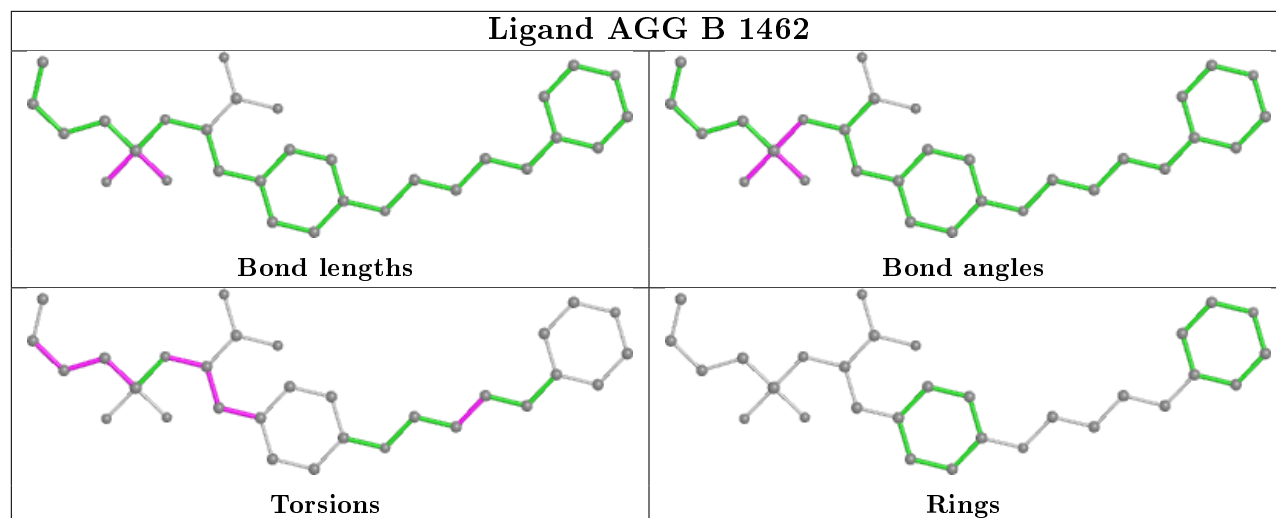
Mol	Chain	Res	Type	Atoms
10	B	1462	AGG	C-CA-CB-CG
9	A	3015	NAG	O5-C5-C6-O6
10	B	1462	AGG	C11-C12-C13-C14
10	B	1462	AGG	C2-C3-C4-S1
9	B	3099	NAG	C4-C5-C6-O6
10	B	1462	AGG	C-CA-N-S1
9	A	3015	NAG	C4-C5-C6-O6
7	A	1453	GOL	O1-C1-C2-C3
10	B	1462	AGG	C1-C2-C3-C4
7	A	1453	GOL	O1-C1-C2-O2
10	B	1462	AGG	CA-CB-CG-CD2
9	B	3099	NAG	O5-C5-C6-O6
10	B	1462	AGG	CA-CB-CG-CD1
7	B	1463	GOL	C1-C2-C3-O3
7	A	1453	GOL	C1-C2-C3-O3
7	A	1453	GOL	O2-C2-C3-O3
7	B	1463	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1462	AGG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/452 (100%)	-0.02	4 (0%) 84 84	39, 51, 59, 67	1 (0%)
2	B	456/461 (98%)	0.54	51 (11%) 5 4	38, 50, 60, 70	1 (0%)
3	H	219/221 (99%)	-0.00	3 (1%) 75 75	43, 51, 58, 72	0
4	L	214/214 (100%)	-0.07	1 (0%) 91 91	40, 50, 57, 71	0
All	All	1341/1348 (99%)	0.16	59 (4%) 34 30	38, 51, 59, 72	2 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	453	GLY	7.0
2	B	444	ASN	6.9
2	B	454	THR	5.9
2	B	443	PRO	5.9
2	B	451	GLY	5.6
1	A	337	PRO	5.3
2	B	11	SER	4.8
2	B	452	ASN	4.7
2	B	448	CYS	4.7
3	H	221	PRO	4.6
2	B	460	CYS	4.2
4	L	214	CYS	4.2
3	H	137	THR	3.7
2	B	459	VAL	3.7
2	B	79	GLN	3.5
2	B	450	ASN	3.5
2	B	449	ASN	3.4
2	B	31	LEU	3.4
2	B	441	ALA	3.4
2	B	33	LEU	3.4
2	B	35	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	1	GLY	3.2
2	B	461	ARG	3.2
1	A	320	ARG	3.1
2	B	376	ASN	3.1
2	B	32	PRO	3.1
2	B	9	GLY	3.1
2	B	455	PHE	3.0
2	B	437	CYS	3.0
2	B	447	ARG	3.0
2	B	81	THR	3.0
2	B	34	GLY	2.9
2	B	445	SER	2.9
2	B	446	HIS	2.9
2	B	78	SER	2.9
1	A	319	ASP	2.8
2	B	378	GLU	2.7
2	B	408	GLN	2.7
2	B	29	GLU	2.7
2	B	456	GLU	2.7
2	B	364	GLU	2.6
2	B	36	PRO	2.6
2	B	442	GLU	2.4
2	B	30	ALA	2.4
2	B	48	ASN	2.4
2	B	379	VAL	2.3
2	B	85	PRO	2.2
2	B	70	SER	2.2
2	B	14	GLN	2.2
2	B	439	ALA	2.2
2	B	434	ASP	2.2
2	B	24	ALA	2.1
2	B	365	GLU	2.1
2	B	426	ILE	2.0
2	B	80	VAL	2.0
2	B	405	GLY	2.0
2	B	409	GLU	2.0
1	A	336	GLY	2.0
3	H	211	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	C	3	11/12	0.79	0.39	93,98,104,108	0
5	MAN	C	5	11/12	0.82	0.41	109,110,111,111	0
5	NAG	C	2	14/15	0.86	0.33	73,77,83,89	0
6	MAN	D	3	11/12	0.87	0.23	83,89,90,90	0
6	MAN	D	7	11/12	0.88	0.23	85,86,88,88	11
6	NAG	D	2	14/15	0.88	0.26	78,86,88,89	0
5	MAN	C	4	11/12	0.88	0.33	92,94,97,97	0
6	NAG	D	1	14/15	0.90	0.24	72,75,79,82	0
6	MAN	D	6	11/12	0.90	0.32	87,88,90,92	0
6	MAN	D	5	11/12	0.91	0.15	68,70,72,72	0
6	MAN	D	4	11/12	0.94	0.23	74,78,81,85	0
5	NAG	C	1	14/15	0.97	0.14	46,54,61,68	0

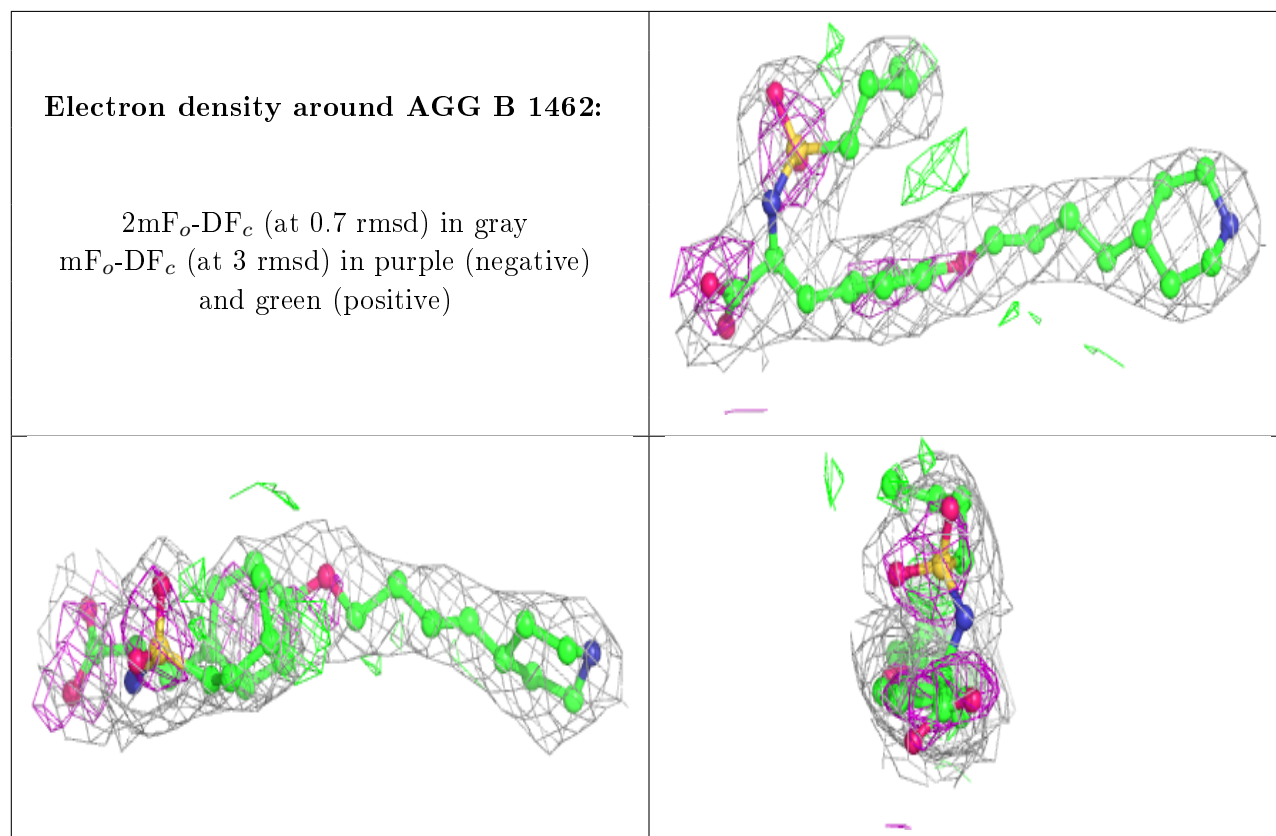
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	A	3249	14/15	0.73	0.45	82,84,85,85	14
9	NAG	A	3015	14/15	0.75	0.54	90,94,96,96	0
9	NAG	B	3099	14/15	0.82	0.40	88,93,95,95	0
7	GOL	A	1453	6/6	0.91	0.22	61,62,63,64	0
7	GOL	B	1463	6/6	0.93	0.20	53,57,59,59	0
8	CA	A	2004	1/1	0.96	0.05	60,60,60,60	0
11	MG	B	2001	1/1	0.96	0.04	37,37,37,37	0
8	CA	A	2006	1/1	0.97	0.03	68,68,68,68	0
8	CA	A	2005	1/1	0.97	0.05	58,58,58,58	0
10	AGG	B	1462	30/30	0.97	0.13	39,44,49,51	0
8	CA	B	2003	1/1	0.98	0.04	38,38,38,38	0
8	CA	A	2007	1/1	0.98	0.07	59,59,59,59	0
8	CA	B	2002	1/1	0.99	0.04	38,38,38,38	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.