



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2024 – 01:36 AM EST

PDB ID : 2HC0  
Title : Structure of HIV protease 6X mutant in complex with AB-2.  
Authors : Heaslet, H.; Brik, A.; Lin, Y.-C.; Elder, J.H.; Stout, C.D.  
Deposited on : 2006-06-14  
Resolution : 1.30 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 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

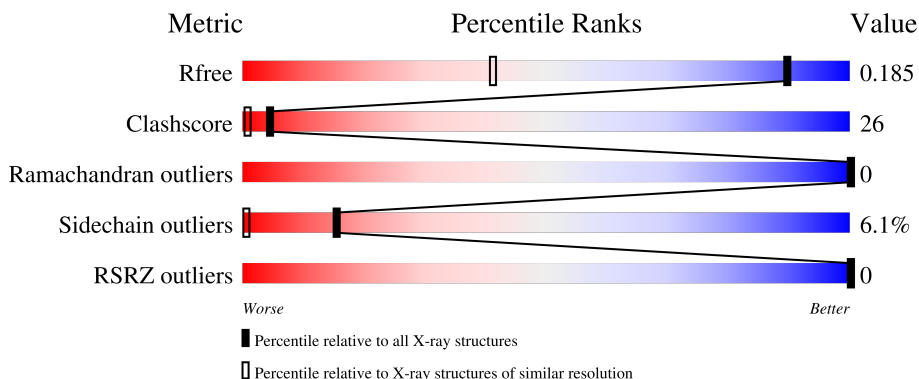
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.30 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))
$R_{free}$	164625	1387 (1.30-1.30)
Clashscore	180529	1497 (1.30-1.30)
Ramachandran outliers	177936	1455 (1.30-1.30)
Sidechain outliers	177891	1455 (1.30-1.30)
RSRZ outliers	164620	1384 (1.30-1.30)

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  $\geq 3$ , 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	99	
1	B	99	

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
2	BR	A	4011[A]	-	-	X	-
3	AB2	A	3500[A]	X	-	-	-
3	AB2	A	3500[B]	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2013 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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	6	0
			804	521	138	142	3			
1	B	99	Total	C	N	O	S	0	7	0
			807	523	139	142	3			

There are 14 discrepancies between the modelled and reference sequences:

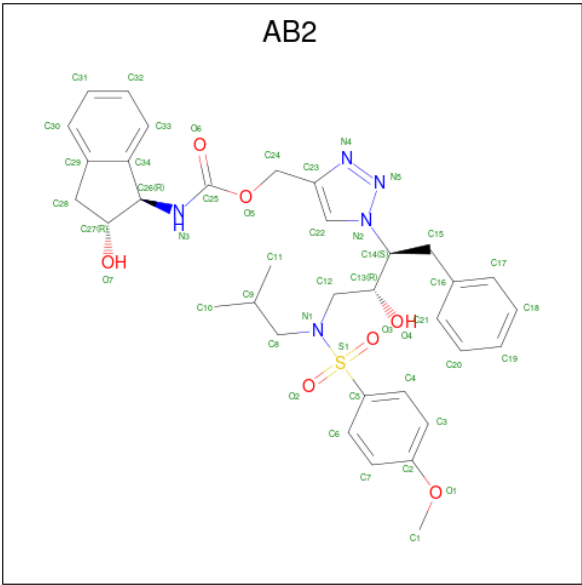
Chain	Residue	Modelled	Actual	Comment	Reference
A	1007	LYS	GLN	engineered mutation	UNP P03367
A	1024	ILE	LEU	engineered mutation	UNP P03367
A	1046	ILE	MET	engineered mutation	UNP P03367
A	1053	LEU	PHE	engineered mutation	UNP P03367
A	1063	PRO	LEU	engineered mutation	UNP P03367
A	1077	ILE	VAL	engineered mutation	UNP P03367
A	1082	ALA	VAL	engineered mutation	UNP P03367
B	2107	LYS	GLN	engineered mutation	UNP P03367
B	2124	ILE	LEU	engineered mutation	UNP P03367
B	2146	ILE	MET	engineered mutation	UNP P03367
B	2153	LEU	PHE	engineered mutation	UNP P03367
B	2163	PRO	LEU	engineered mutation	UNP P03367
B	2177	ILE	VAL	engineered mutation	UNP P03367
B	2182	ALA	VAL	engineered mutation	UNP P03367

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Br	0	2
			7	7		
2	B	7	Total	Br	0	0
			7	7		

- Molecule 3 is [1-((1S,2R)-1-BENZYL-2-HYDROXY-3-{ISOBUTYL}[(4-METHOXYPHEN

YL)SULFONYL]AMINO}PROPYL)-1H-1,2,3-TRIAZOL-4-YL]METHYL (1R,2R)-2-HYDROXY-2,3-DIHYDRO-1H-INDEN-1-YLCARBAMATE (three-letter code: AB2) (formula: C<sub>34</sub>H<sub>41</sub>N<sub>5</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	94	68	10	14	2	0	1

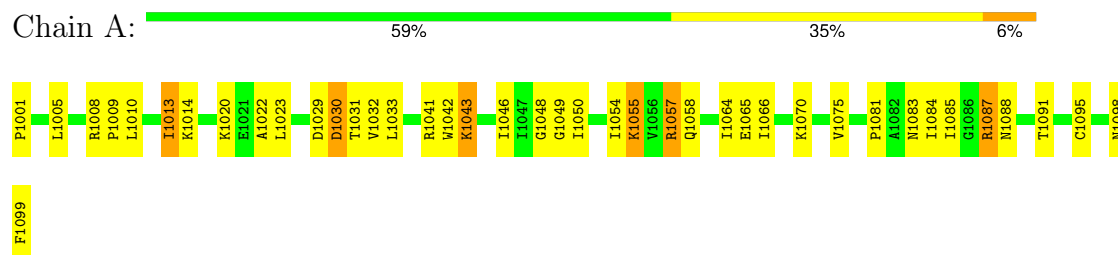
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	146	Total	O	0	1
			147	147		

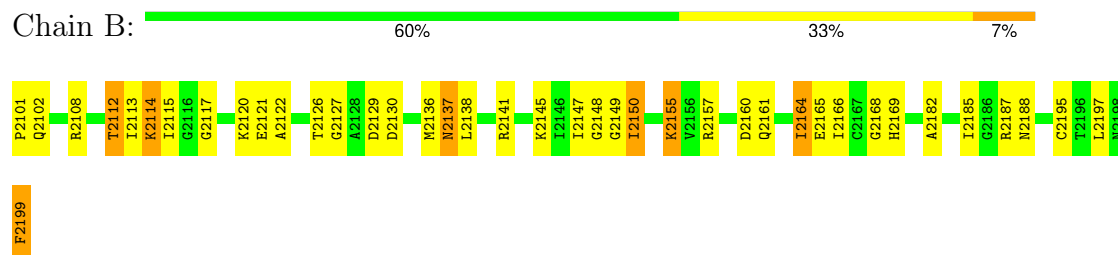
### 3 Residue-property plots

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: Protease



#### • Molecule 1: Protease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.61Å 86.61Å 33.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.00 – 1.30 86.61 – 1.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (87.00-1.30) 92.6 (86.61-1.30)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.30Å)	Xtriage
Refinement program	SHELX, SHELXL	Depositor
R, $R_{free}$	0.142 , 0.168 0.154 , 0.185	Depositor DCC
$R_{free}$ test set	2911 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 79.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BR, AB2

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	0.50	0/818	1.36	8/1107 (0.7%)
1	B	0.58	1/820 (0.1%)	1.33	10/1110 (0.9%)
All	All	0.54	1/1638 (0.1%)	1.35	18/2217 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2199	PHE	C-OXT	5.54	1.33	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	ARG	NE-CZ-NH2	9.15	124.88	120.30
1	A	1041	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	A	1030	ASP	CB-CG-OD2	-7.97	111.12	118.30
1	B	2114	LYS	CB-CG-CD	7.79	131.85	111.60
1	A	1087	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	2141	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	1057	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	A	1087	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	1041	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	2108	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	2157	ARG	CD-NE-CZ	5.98	131.97	123.60
1	B	2129	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	2114	LYS	CD-CE-NZ	5.78	125.00	111.70
1	B	2129	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	2187	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	2108	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	B	2108	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	1008	ARG	NH1-CZ-NH2	-5.11	113.78	119.40



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	804	0	862	50	0
1	B	807	0	869	51	0
2	A	7	0	0	2	0
2	B	7	0	0	0	0
3	A	94	0	77	17	0
4	A	147	0	0	6	0
4	B	147	0	0	6	0
All	All	2013	0	1808	91	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 26.

All (91) 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:B:2126[B]:THR:HG21	1:B:2197:LEU:HD11	1.42	1.01
1:B:2113[B]:ILE:HD12	1:B:2166:ILE:HG12	1.46	0.97
1:B:2115[A]:ILE:HD12	1:B:2164[A]:ILE:HD11	1.58	0.85
1:A:1013[B]:ILE:HD11	1:A:1022:ALA:HB3	1.59	0.83
2:A:4011[A]:BR:BR	4:A:5156:HOH:O	2.51	0.82
1:A:1009:PRO:HG3	1:B:2126[B]:THR:HG22	1.61	0.81
1:A:1013[A]:ILE:HG13	1:A:1064[A]:ILE:HD11	1.62	0.79
1:A:1013[B]:ILE:HD12	1:A:1085:ILE:HD11	1.67	0.77
1:A:1033[B]:LEU:HD12	1:A:1083:ASN:HB3	1.66	0.76
1:A:1020:LYS:HD2	4:A:5216:HOH:O	1.88	0.73
3:A:3500[A]:AB2:H6	1:B:2148:GLY:O	1.89	0.72
1:A:1029:ASP:N	3:A:3500[B]:AB2:H12	2.06	0.70
1:B:2115[B]:ILE:HD11	1:B:2120:LYS:HG3	1.74	0.70
1:B:2115[B]:ILE:HD12	1:B:2115[B]:ILE:O	1.93	0.69
1:B:2115[B]:ILE:HG22	1:B:2164[B]:ILE:HG22	1.76	0.68
1:B:2137:ASN:HA	4:B:5089:HOH:O	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2136:MET:HA	4:B:5161:HOH:O	1.96	0.64
1:A:1030:ASP:O	3:A:3500[B]:AB2:H13A	1.98	0.63
1:A:1032:VAL:O	1:A:1033[B]:LEU:HD13	1.97	0.63
1:A:1081:PRO:HD2	3:A:3500[B]:AB2:H18	1.83	0.60
1:A:1049:GLY:HA2	3:A:3500[A]:AB2:C20	2.31	0.60
1:B:2122:ALA:HB3	1:B:2185:ILE:HD11	1.84	0.60
1:A:1049:GLY:HA3	1:B:2150[A]:ILE:HG22	1.84	0.59
1:B:2101:PRO:HA	4:B:5123:HOH:O	2.05	0.57
1:A:1014[B]:LYS:HB3	1:A:1065[B]:GLU:HB3	1.86	0.57
4:A:5251:HOH:O	1:B:2169:HIS:HE1	1.88	0.56
1:A:1065[B]:GLU:OE1	1:A:1070:LYS:HG2	2.05	0.55
1:A:1013[B]:ILE:CD1	1:A:1085:ILE:HD11	2.37	0.55
1:A:1070:LYS:HE2	4:A:5032:HOH:O	2.07	0.55
1:B:2115[A]:ILE:HD12	1:B:2164[A]:ILE:CD1	2.33	0.55
1:A:1009:PRO:HG3	1:B:2126[B]:THR:CG2	2.34	0.54
3:A:3500[A]:AB2:H11	1:B:2130:ASP:OD2	2.08	0.54
1:A:1048:GLY:O	3:A:3500[A]:AB2:H282	2.09	0.53
3:A:3500[A]:AB2:H113	1:B:2127:GLY:O	2.09	0.52
1:A:1050:ILE:HG13	3:A:3500[A]:AB2:H18	1.91	0.52
1:A:1033[B]:LEU:HD23	1:A:1075:VAL:HG13	1.92	0.52
1:A:1099:PHE:HB3	1:B:2195:CYS:HA	1.91	0.51
1:A:1005:LEU:CD2	1:B:2126[B]:THR:HG23	2.40	0.51
1:A:1095:CYS:HA	1:B:2199:PHE:HB3	1.92	0.51
1:A:1031:THR:HG22	1:A:1033[B]:LEU:HD21	1.93	0.51
1:B:2113[A]:ILE:HD11	1:B:2164[A]:ILE:HG12	1.92	0.51
2:A:4011[A]:BR:BR	1:B:2148:GLY:N	2.92	0.50
1:B:2113[A]:ILE:HD11	1:B:2164[A]:ILE:HD13	1.93	0.50
1:B:2165:GLU:OE2	1:B:2168:GLY:O	2.30	0.50
3:A:3500[A]:AB2:O3	1:B:2149:GLY:HA2	2.12	0.50
1:B:2112:THR:HG23	1:B:2121:GLU:OE1	2.12	0.49
1:A:1048:GLY:O	3:A:3500[A]:AB2:O6	2.30	0.49
1:A:1049:GLY:HA3	1:B:2150[A]:ILE:CG2	2.41	0.49
1:A:1050:ILE:O	1:B:2150[B]:ILE:O	2.30	0.49
1:B:2113[B]:ILE:HG23	1:B:2165:GLU:O	2.13	0.49
1:B:2113[A]:ILE:HD11	1:B:2164[A]:ILE:CG1	2.42	0.48
1:A:1048:GLY:O	3:A:3500[B]:AB2:H6	2.13	0.48
1:B:2112:THR:O	1:B:2113[B]:ILE:HD13	2.14	0.47
1:A:1042:TRP:CE2	1:A:1057:ARG:HD2	2.50	0.47
1:B:2113[A]:ILE:HD11	1:B:2164[A]:ILE:CD1	2.44	0.47
1:A:1013[B]:ILE:HD11	1:A:1022:ALA:CB	2.38	0.47
3:A:3500[B]:AB2:H18	1:B:2150[B]:ILE:HG13	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2113[B]:ILE:HD11	1:B:2185:ILE:CD1	2.46	0.46
1:B:2114:LYS:O	1:B:2115[B]:ILE:HG23	2.16	0.46
1:A:1087:ARG:O	1:A:1091:THR:HG23	2.15	0.46
1:A:1043:LYS:HE2	4:A:5040:HOH:O	2.15	0.45
1:A:1057:ARG:NH2	4:A:5090:HOH:O	2.47	0.45
1:A:1098:ASN:HD21	1:B:2102:GLN:CD	2.19	0.45
1:B:2137:ASN:ND2	4:B:5226:HOH:O	2.50	0.45
1:A:1046:ILE:HG12	1:A:1055:LYS:HD2	1.98	0.45
1:B:2155[B]:LYS:NZ	4:B:5134:HOH:O	2.50	0.44
1:A:1005:LEU:HD22	1:B:2126[B]:THR:HG23	1.98	0.44
1:A:1084:ILE:CD1	3:A:3500[B]:AB2:H4	2.47	0.44
1:A:1013[B]:ILE:HG23	1:A:1066:ILE:HG12	1.99	0.44
1:A:1033[B]:LEU:HD22	1:A:1033[B]:LEU:N	2.32	0.43
1:B:2145:LYS:HE2	1:B:2147:ILE:CG2	2.48	0.43
1:B:2160:ASP:HB3	1:B:2161:GLN:OE1	2.18	0.43
1:A:1046:ILE:HG12	1:A:1055:LYS:CD	2.48	0.42
1:A:1010:LEU:HD12	1:A:1023:LEU:CD2	2.49	0.42
1:B:2115[B]:ILE:CG2	1:B:2164[B]:ILE:HG22	2.45	0.42
1:A:1033[B]:LEU:HD23	1:A:1075:VAL:CG1	2.48	0.42
3:A:3500[B]:AB2:H13A	3:A:3500[B]:AB2:H3	1.36	0.42
1:A:1031:THR:HG22	1:A:1033[B]:LEU:CD2	2.50	0.42
1:A:1033[B]:LEU:HD12	1:A:1083:ASN:CB	2.43	0.42
1:A:1001:PRO:HD2	1:B:2199:PHE:CZ	2.55	0.42
3:A:3500[B]:AB2:H111	1:B:2182:ALA:HB3	2.02	0.41
1:A:1013[A]:ILE:HD12	1:A:1013[A]:ILE:HG21	1.77	0.41
1:B:2114:LYS:HE3	1:B:2117:GLY:HA2	2.01	0.41
1:A:1050:ILE:HD12	3:A:3500[B]:AB2:N4	2.36	0.41
1:B:2112:THR:C	1:B:2113[B]:ILE:HD13	2.40	0.41
1:A:1010:LEU:HD12	1:A:1023:LEU:HD23	2.03	0.41
1:B:2112:THR:HG22	1:B:2120:LYS:O	2.21	0.41
1:A:1043:LYS:NZ	1:A:1058:GLN:NE2	2.69	0.40
1:A:1054:ILE:HD11	1:B:2150[A]:ILE:HD11	2.03	0.40
1:B:2155[A]:LYS:HE2	4:B:5121:HOH:O	2.21	0.40
1:B:2138:LEU:HD23	1:B:2138:LEU:HA	1.94	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	103/99 (104%)	101 (98%)	2 (2%)	0	100	100
1	B	104/99 (105%)	101 (97%)	3 (3%)	0	100	100
All	All	207/198 (104%)	202 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	88/82 (107%)	83 (94%)	5 (6%)	17	1
1	B	88/82 (107%)	79 (90%)	9 (10%)	6	0
All	All	176/164 (107%)	162 (92%)	14 (8%)	15	0

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013[A]	ILE
1	A	1013[B]	ILE
1	A	1043	LYS
1	A	1055	LYS
1	A	1088	ASN
1	B	2112	THR
1	B	2137	ASN
1	B	2150[A]	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	2150[B]	ILE
1	B	2155[A]	LYS
1	B	2155[B]	LYS
1	B	2164[A]	ILE
1	B	2164[B]	ILE
1	B	2188	ASN

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

Mol	Chain	Res	Type
1	A	1018	GLN
1	A	1058	GLN
1	A	1088	ASN
1	B	2137	ASN
1	B	2188	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 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
3	AB2	A	3500[B]	-	50,51,51	2.81	26 (52%)	61,72,72	4.07	29 (47%)
3	AB2	A	3500[A]	-	50,51,51	2.86	27 (54%)	61,72,72	3.80	29 (47%)

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	AB2	A	3500[B]	-	3/3/8/9	8/37/55/55	0/5/5/5
3	AB2	A	3500[A]	-	1/1/8/9	12/37/55/55	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3500[B]	AB2	S1-N1	8.34	1.75	1.63
3	A	3500[A]	AB2	S1-N1	7.38	1.73	1.63
3	A	3500[A]	AB2	C12-C13	-5.44	1.45	1.52
3	A	3500[B]	AB2	C33-C34	5.33	1.46	1.39
3	A	3500[B]	AB2	O5-C25	5.25	1.45	1.35
3	A	3500[B]	AB2	C3-C2	4.98	1.48	1.38
3	A	3500[A]	AB2	C33-C34	4.97	1.45	1.39
3	A	3500[B]	AB2	C6-C5	4.91	1.46	1.38
3	A	3500[A]	AB2	C6-C5	4.68	1.46	1.38
3	A	3500[A]	AB2	C3-C2	4.49	1.47	1.38
3	A	3500[A]	AB2	O5-C25	4.47	1.44	1.35
3	A	3500[B]	AB2	C12-C13	-4.39	1.46	1.52
3	A	3500[A]	AB2	C31-C30	4.28	1.46	1.38
3	A	3500[A]	AB2	O3-S1	-4.14	1.39	1.43
3	A	3500[B]	AB2	C31-C30	4.02	1.45	1.38
3	A	3500[A]	AB2	N4-N5	-4.01	1.27	1.34
3	A	3500[A]	AB2	C13-C14	4.00	1.56	1.53
3	A	3500[B]	AB2	C15-C14	3.98	1.59	1.53
3	A	3500[B]	AB2	N4-N5	-3.82	1.27	1.34
3	A	3500[B]	AB2	C18-C17	3.78	1.45	1.38
3	A	3500[A]	AB2	C15-C14	3.76	1.59	1.53
3	A	3500[A]	AB2	C4-C3	3.56	1.44	1.38
3	A	3500[A]	AB2	C18-C17	3.40	1.44	1.38
3	A	3500[A]	AB2	C27-C26	-3.23	1.51	1.55
3	A	3500[A]	AB2	C20-C21	3.16	1.44	1.38
3	A	3500[A]	AB2	C5-S1	3.15	1.80	1.76

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3500[B]	AB2	C20-C21	3.06	1.44	1.38
3	A	3500[B]	AB2	C7-C6	3.03	1.43	1.38
3	A	3500[B]	AB2	C21-C16	2.97	1.44	1.38
3	A	3500[B]	AB2	C19-C18	2.89	1.44	1.38
3	A	3500[A]	AB2	C26-N3	-2.85	1.40	1.46
3	A	3500[B]	AB2	C17-C16	2.81	1.44	1.38
3	A	3500[A]	AB2	C32-C31	2.77	1.44	1.38
3	A	3500[A]	AB2	C17-C16	2.76	1.44	1.38
3	A	3500[B]	AB2	C27-C26	-2.72	1.52	1.55
3	A	3500[B]	AB2	C32-C33	2.68	1.43	1.38
3	A	3500[A]	AB2	C7-C6	2.66	1.43	1.38
3	A	3500[A]	AB2	C32-C33	2.55	1.43	1.38
3	A	3500[A]	AB2	C21-C16	2.52	1.43	1.38
3	A	3500[B]	AB2	O2-S1	-2.46	1.40	1.43
3	A	3500[B]	AB2	C4-C3	2.43	1.42	1.38
3	A	3500[B]	AB2	C32-C31	2.42	1.43	1.38
3	A	3500[B]	AB2	C29-C34	2.42	1.43	1.39
3	A	3500[B]	AB2	C13-C14	2.41	1.55	1.53
3	A	3500[A]	AB2	C29-C34	2.40	1.43	1.39
3	A	3500[B]	AB2	O1-C2	2.38	1.42	1.37
3	A	3500[B]	AB2	O3-S1	-2.36	1.41	1.43
3	A	3500[A]	AB2	C25-N3	-2.33	1.28	1.34
3	A	3500[A]	AB2	C19-C18	2.27	1.43	1.38
3	A	3500[B]	AB2	O4-C13	-2.26	1.38	1.43
3	A	3500[A]	AB2	C20-C19	2.26	1.43	1.38
3	A	3500[B]	AB2	C4-C5	2.18	1.42	1.38
3	A	3500[A]	AB2	C7-C2	2.10	1.42	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3500[B]	AB2	O2-S1-N1	12.78	118.72	106.69
3	A	3500[A]	AB2	C9-C8-N1	12.48	126.87	112.41
3	A	3500[B]	AB2	C9-C8-N1	12.47	126.86	112.41
3	A	3500[A]	AB2	O2-S1-N1	11.20	117.23	106.69
3	A	3500[A]	AB2	C22-N2-C14	8.20	132.75	125.48
3	A	3500[A]	AB2	C34-C26-N3	-8.03	91.29	114.77
3	A	3500[B]	AB2	O4-C13-C14	7.60	126.74	109.30
3	A	3500[B]	AB2	C1-O1-C2	-7.55	101.31	117.50
3	A	3500[B]	AB2	O7-C27-C28	7.47	127.64	110.81
3	A	3500[B]	AB2	O7-C27-C26	7.42	131.20	110.00
3	A	3500[A]	AB2	C1-O1-C2	6.81	132.09	117.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3500[B]	AB2	C20-C19-C18	6.73	129.08	119.87
3	A	3500[B]	AB2	C22-N2-C14	6.48	131.22	125.48
3	A	3500[B]	AB2	C34-C26-N3	-6.19	96.68	114.77
3	A	3500[B]	AB2	C29-C28-C27	-5.83	98.10	103.43
3	A	3500[B]	AB2	C19-C20-C21	-5.77	113.12	120.24
3	A	3500[A]	AB2	O4-C13-C14	5.76	122.53	109.30
3	A	3500[B]	AB2	C34-C26-C27	-5.75	98.28	102.48
3	A	3500[B]	AB2	C16-C15-C14	-5.69	101.33	113.48
3	A	3500[A]	AB2	C26-N3-C25	5.68	133.47	121.69
3	A	3500[A]	AB2	C8-N1-S1	5.61	129.54	117.32
3	A	3500[A]	AB2	C29-C28-C27	-5.38	98.51	103.43
3	A	3500[A]	AB2	O6-C25-N3	-5.14	116.43	124.86
3	A	3500[A]	AB2	O3-S1-O2	-5.14	111.58	119.59
3	A	3500[B]	AB2	C21-C16-C17	4.67	125.18	118.23
3	A	3500[B]	AB2	C4-C5-S1	-4.51	115.25	119.73
3	A	3500[A]	AB2	O7-C27-C26	4.32	122.35	110.00
3	A	3500[A]	AB2	O5-C25-N3	-4.31	101.25	110.45
3	A	3500[B]	AB2	O3-S1-O2	-4.17	113.08	119.59
3	A	3500[A]	AB2	C28-C29-C34	-3.95	105.49	110.95
3	A	3500[A]	AB2	C16-C15-C14	-3.95	105.05	113.48
3	A	3500[B]	AB2	C18-C17-C16	-3.90	115.12	120.61
3	A	3500[B]	AB2	O4-C13-C12	3.71	125.44	110.20
3	A	3500[A]	AB2	C21-C16-C17	3.69	123.71	118.23
3	A	3500[A]	AB2	C22-C23-N4	-3.63	105.93	111.27
3	A	3500[A]	AB2	O5-C25-O6	3.61	131.19	124.26
3	A	3500[A]	AB2	O5-C24-C23	3.61	118.83	109.61
3	A	3500[A]	AB2	C28-C27-C26	-3.61	100.31	103.70
3	A	3500[B]	AB2	C28-C29-C34	-3.59	105.98	110.95
3	A	3500[A]	AB2	C20-C19-C18	3.42	124.55	119.87
3	A	3500[B]	AB2	C15-C16-C21	-3.32	114.72	120.90
3	A	3500[A]	AB2	O7-C27-C28	3.29	118.23	110.81
3	A	3500[B]	AB2	O3-S1-C5	-3.15	104.19	108.10
3	A	3500[B]	AB2	C7-C2-C3	3.11	124.69	120.16
3	A	3500[A]	AB2	C24-O5-C25	2.99	122.65	115.93
3	A	3500[A]	AB2	O2-S1-C5	-2.98	104.40	108.10
3	A	3500[B]	AB2	C33-C34-C29	-2.89	117.44	120.80
3	A	3500[A]	AB2	O4-C13-C12	2.89	122.09	110.20
3	A	3500[A]	AB2	C19-C20-C21	-2.85	116.72	120.24
3	A	3500[B]	AB2	C28-C27-C26	-2.79	101.07	103.70
3	A	3500[A]	AB2	C18-C17-C16	-2.72	116.78	120.61
3	A	3500[B]	AB2	C19-C18-C17	-2.67	116.94	120.24
3	A	3500[A]	AB2	C34-C26-C27	-2.64	100.55	102.48

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3500[B]	AB2	C22-C23-N4	-2.51	107.57	111.27
3	A	3500[A]	AB2	O3-S1-N1	2.47	109.01	106.69
3	A	3500[B]	AB2	O5-C25-N3	-2.33	105.47	110.45
3	A	3500[B]	AB2	C6-C7-C2	-2.10	117.33	119.73
3	A	3500[B]	AB2	C8-N1-S1	2.08	121.85	117.32

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	3500[A]	AB2	C26
3	A	3500[B]	AB2	C13
3	A	3500[B]	AB2	C27
3	A	3500[B]	AB2	C26

All (20) torsion outliers are listed below:

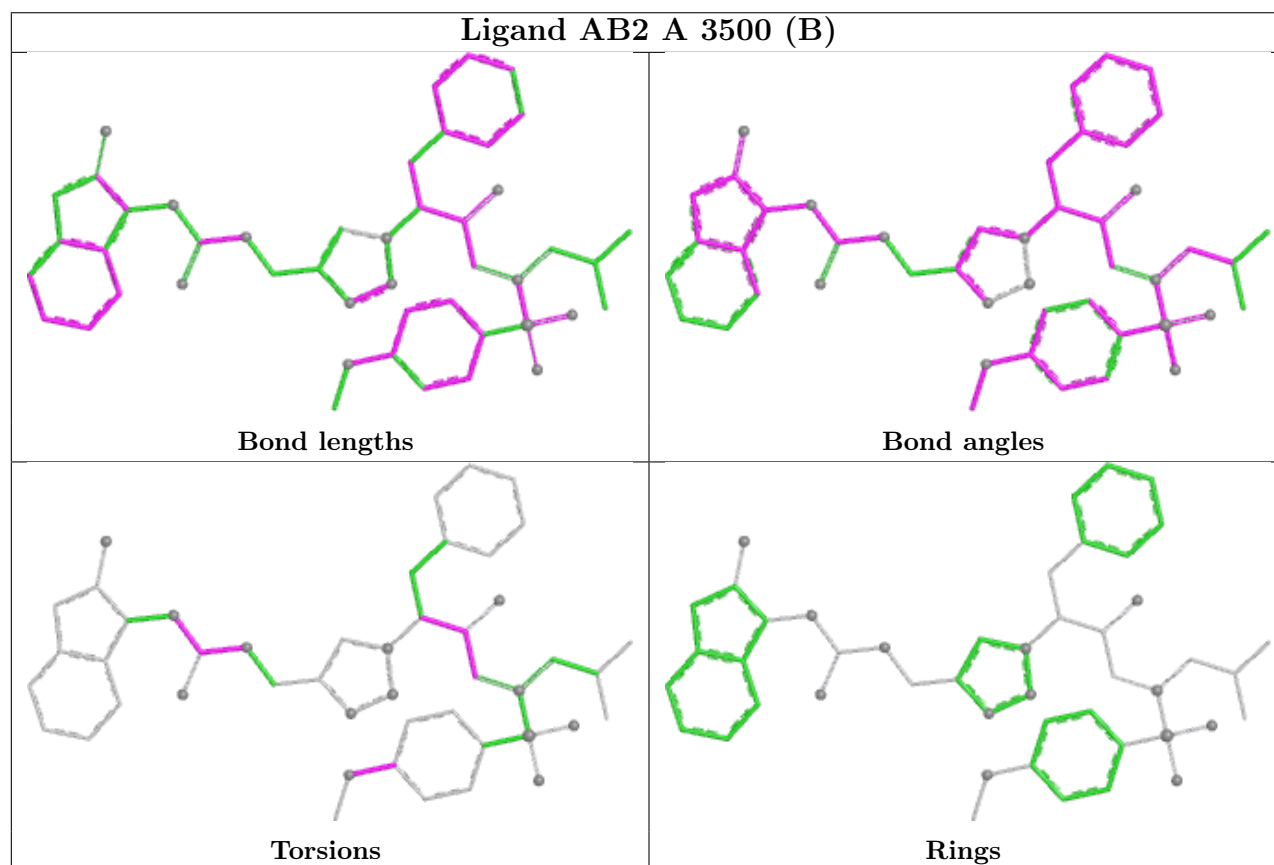
Mol	Chain	Res	Type	Atoms
3	A	3500[A]	AB2	C12-C13-C14-C15
3	A	3500[A]	AB2	C12-C13-C14-N2
3	A	3500[A]	AB2	C27-C26-N3-C25
3	A	3500[B]	AB2	C12-C13-C14-C15
3	A	3500[B]	AB2	C12-C13-C14-N2
3	A	3500[B]	AB2	N3-C25-O5-C24
3	A	3500[A]	AB2	O6-C25-N3-C26
3	A	3500[B]	AB2	O6-C25-N3-C26
3	A	3500[B]	AB2	C7-C2-O1-C1
3	A	3500[A]	AB2	N3-C25-O5-C24
3	A	3500[B]	AB2	C3-C2-O1-C1
3	A	3500[A]	AB2	N1-C8-C9-C11
3	A	3500[B]	AB2	N1-C12-C13-O4
3	A	3500[A]	AB2	C7-C2-O1-C1
3	A	3500[A]	AB2	C3-C2-O1-C1
3	A	3500[A]	AB2	N1-C8-C9-C10
3	A	3500[A]	AB2	C12-N1-S1-O3
3	A	3500[B]	AB2	N1-C12-C13-C14
3	A	3500[A]	AB2	C12-N1-S1-O2
3	A	3500[A]	AB2	C4-C5-S1-O2

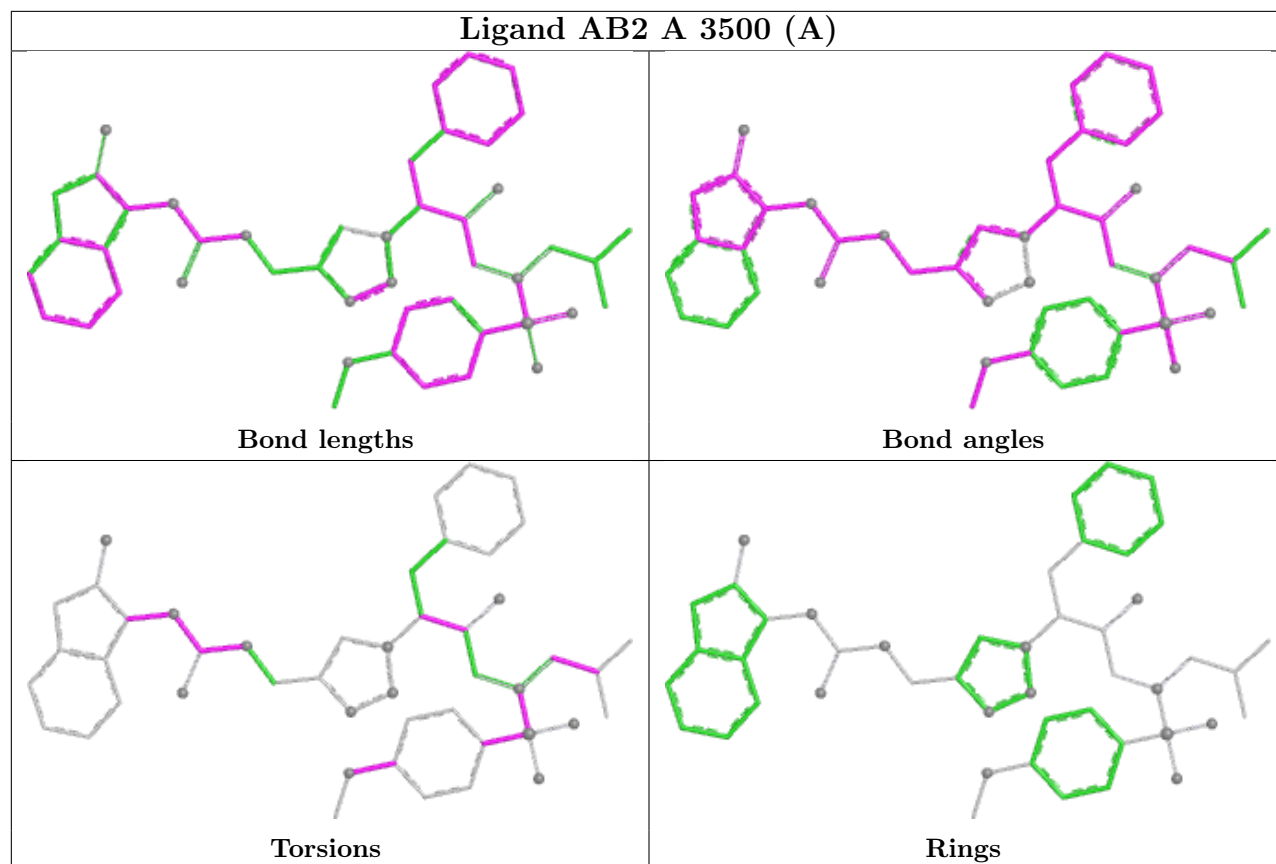
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3500[B]	AB2	9	0
3	A	3500[A]	AB2	8	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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	99/99 (100%)	-0.90	0 100 100	6, 16, 29, 35	6 (6%)
1	B	99/99 (100%)	-0.87	0 100 100	6, 15, 31, 36	8 (8%)
All	All	198/198 (100%)	-0.89	0 100 100	6, 16, 30, 36	14 (7%)

There are no RSRZ outliers to report.

### 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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
3	AB2	A	3500[A]	47/47	0.99	0.05	9,14,21,35	47
3	AB2	A	3500[B]	47/47	0.99	0.05	7,13,18,30	47
2	BR	A	4007	1/1	1.00	0.02	35,35,35,35	0
2	BR	A	4011[A]	1/1	1.00	0.05	22,22,22,22	1
2	BR	A	4011[B]	1/1	1.00	0.05	25,25,25,25	1
2	BR	A	4012[A]	1/1	1.00	0.08	21,21,21,21	1
2	BR	A	4012[B]	1/1	1.00	0.08	23,23,23,23	1

*Continued on next page...*

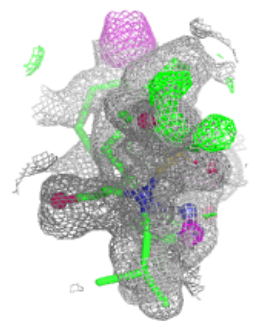
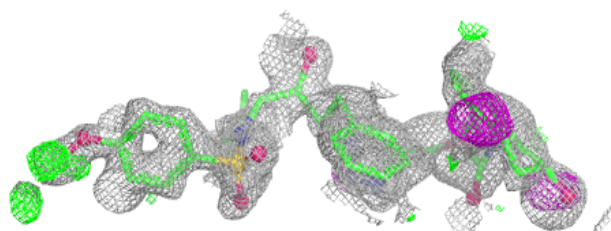
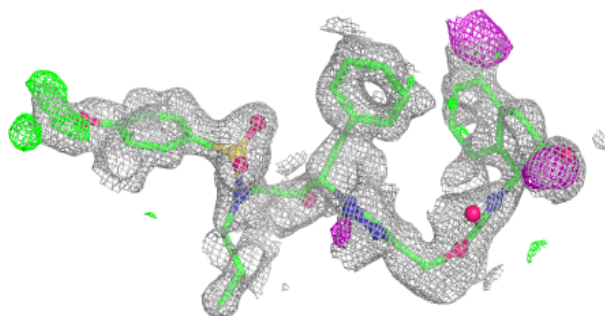
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BR	B	4002	1/1	1.00	0.02	14,14,14,14	0
2	BR	B	4003	1/1	1.00	0.02	18,18,18,18	0
2	BR	B	4004	1/1	1.00	0.02	18,18,18,18	0
2	BR	B	4005	1/1	1.00	0.05	22,22,22,22	0
2	BR	B	4008	1/1	1.00	0.03	38,38,38,38	0
2	BR	B	4009	1/1	1.00	0.01	18,18,18,18	0
2	BR	B	4010	1/1	1.00	0.05	36,36,36,36	0
2	BR	A	4001	1/1	1.00	0.02	14,14,14,14	0
2	BR	A	4006	1/1	1.00	0.04	20,20,20,20	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.

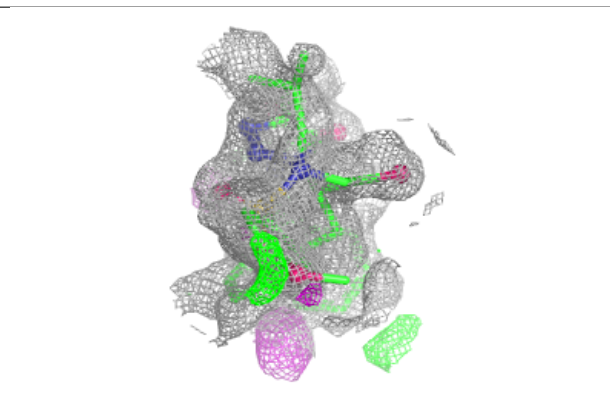
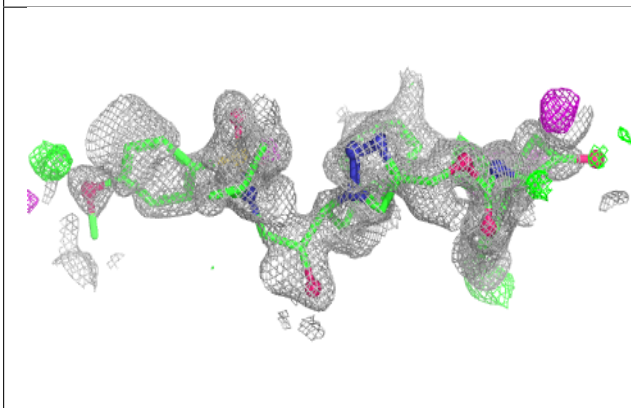
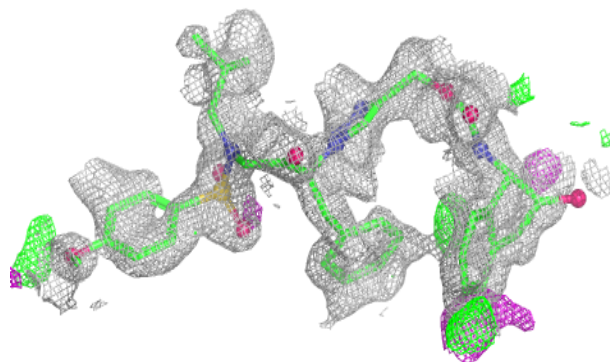
**Electron density around AB2 A 3500 (A):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AB2 A 3500 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.