



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2021 – 12:16 PM JST

PDB ID : 7ECR  
Title : Crystal Structure of Aspergillus terreus Glutamate Dehydrogenase (AtGDH)  
Complexed With Succinate and ADP-ribose  
Authors : Godsora, B.K.J.; Prakash, P.; Puneekar, N.S.; Bhaumik, P.  
Deposited on : 2021-03-13  
Resolution : 1.73 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.

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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 : 2.23.2  
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) : 2.23.2

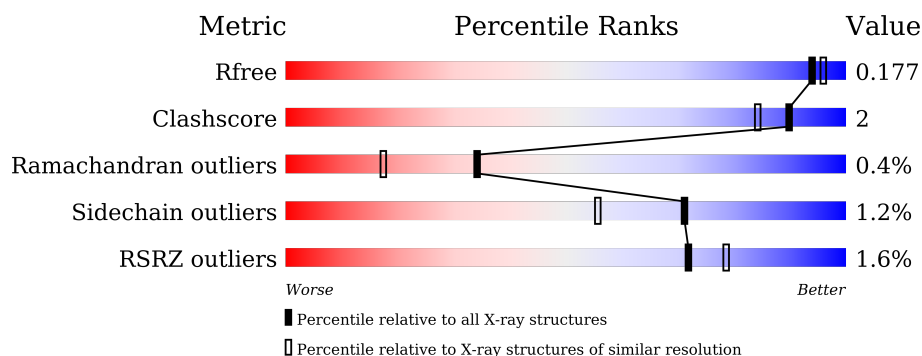
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	460	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>
1	B	460	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	C	460	<div> <div>%</div> <div>93%</div> <div>6%</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
2	GOL	C	505	-	X	-	-
2	GOL	C	506	-	X	-	-

## 2 Entry composition [i](#)

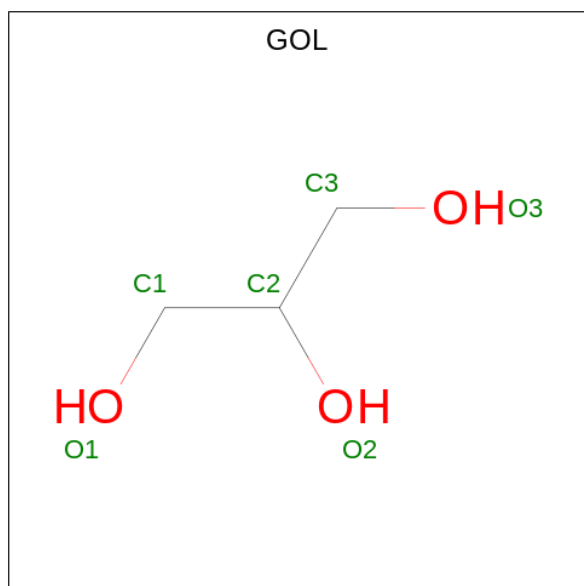
There are 5 unique types of molecules in this entry. The entry contains 12302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	15	0
			3551	2244	615	678	14			
1	B	460	Total	C	N	O	S	0	8	0
			3503	2213	608	668	14			
1	C	460	Total	C	N	O	S	0	9	0
			3508	2216	607	671	14			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



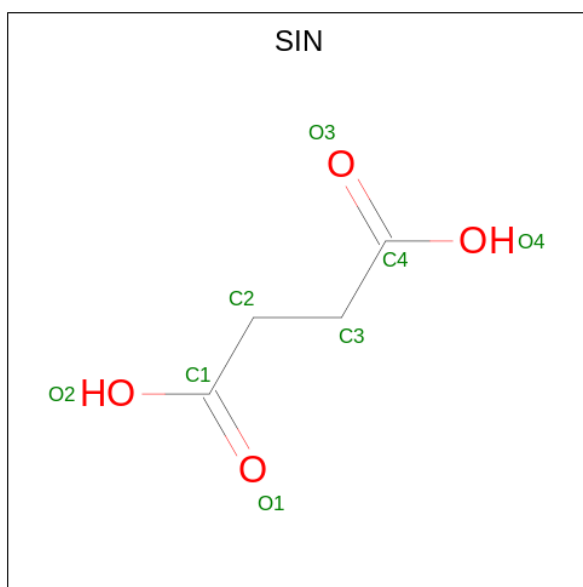
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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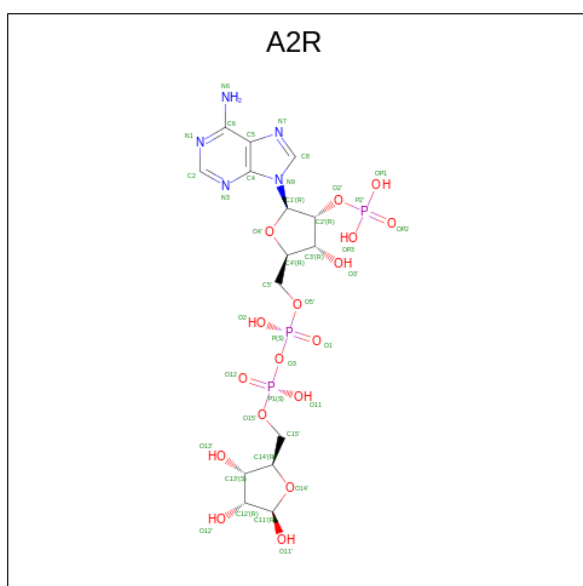
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total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

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 4	O 4	0	0
3	B	1	Total 8	C 4	O 4	0	0
3	C	1	Total 8	C 4	O 4	0	0

- Molecule 4 is [(2R,3R,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3-HYDROXY-4-(PHOSPHONOOXY)TETRAHYDROFURAN-2-YL]METHYL [(2R,3S,4R,5R)-3,4,5-TRIHIDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (three-letter code: A2R) (formula: C<sub>15</sub>H<sub>24</sub>N<sub>5</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	15	5	17	3		
4	B	1	Total	C	N	O	P	0	0
			40	15	5	17	3		
4	C	1	Total	C	N	O	P	0	0
			40	15	5	17	3		

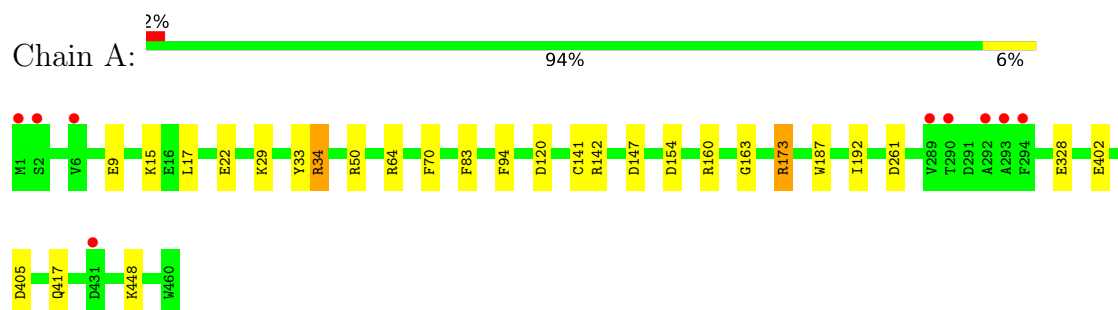
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	491	Total	O	0	0
			491	491		
5	B	476	Total	O	0	0
			476	476		
5	C	509	Total	O	0	0
			509	509		

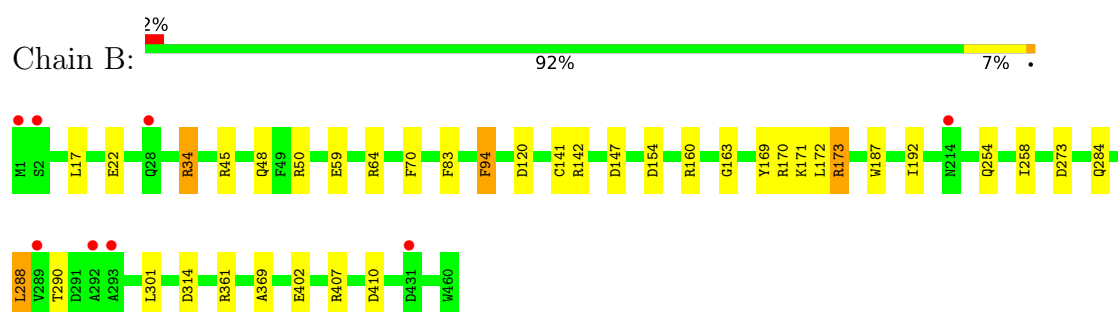
### 3 Residue-property plots [i](#)

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 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.

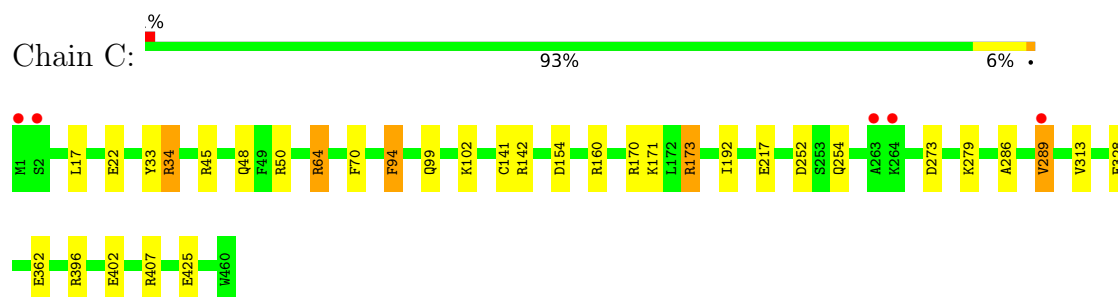
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.88Å 153.75Å 259.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.68 – 1.73 38.68 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.68-1.73) 99.7 (38.68-1.73)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.145 , 0.167 0.157 , 0.177	Depositor DCC
$R_{free}$ test set	12303 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: SIN, GOL, A2R

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	1.16	1/3657 (0.0%)	1.10	20/4942 (0.4%)
1	B	1.20	5/3597 (0.1%)	1.11	20/4864 (0.4%)
1	C	1.14	5/3605 (0.1%)	1.08	18/4875 (0.4%)
All	All	1.17	11/10859 (0.1%)	1.10	58/14681 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	GLU	CD-OE2	8.98	1.35	1.25
1	C	160	ARG	CZ-NH1	6.78	1.41	1.33
1	B	402	GLU	CD-OE1	6.70	1.33	1.25
1	C	362	GLU	CD-OE1	-6.59	1.18	1.25
1	C	217	GLU	CD-OE1	6.14	1.32	1.25
1	B	402	GLU	CG-CD	5.92	1.60	1.51
1	B	170	ARG	CZ-NH2	-5.87	1.25	1.33
1	C	313	VAL	CB-CG2	-5.24	1.41	1.52
1	A	9	GLU	CD-OE2	5.22	1.31	1.25
1	C	425	GLU	CD-OE2	5.17	1.31	1.25
1	B	59	GLU	CD-OE1	-5.07	1.20	1.25

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64[A]	ARG	NE-CZ-NH1	13.66	127.13	120.30
1	A	64[B]	ARG	NE-CZ-NH1	13.66	127.13	120.30
1	C	64[A]	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	C	64[B]	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	A	173	ARG	NE-CZ-NH1	-10.27	115.17	120.30
1	C	173	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	C	34	ARG	NE-CZ-NH1	-9.51	115.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64[A]	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	B	64[B]	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	A	405	ASP	CB-CG-OD1	9.14	126.53	118.30
1	C	50	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	C	160	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	B	64[A]	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	B	64[B]	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	405	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	C	64[A]	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	C	64[B]	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	B	34	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	B	147	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	A	173	ARG	CG-CD-NE	-7.61	95.82	111.80
1	B	314	ASP	CB-CG-OD1	-7.04	111.96	118.30
1	A	142	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	147	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	B	142	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	160	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	33	TYR	CB-CG-CD1	6.54	124.92	121.00
1	B	407	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	261	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	64[A]	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	64[B]	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	170	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	B	120	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	C	33	TYR	CB-CG-CD1	6.02	124.61	121.00
1	B	288	LEU	CB-CA-C	-6.00	98.80	110.20
1	B	273	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	173	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	45	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	407	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	34	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	142	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	173	ARG	CA-CB-CG	-5.70	100.87	113.40
1	A	120	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	50	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	273	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	407	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	170	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	C	252	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	83	PHE	CB-CG-CD1	5.43	124.60	120.80
1	A	83	PHE	CB-CG-CD2	-5.41	117.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	LYS	CD-CE-NZ	-5.39	99.30	111.70
1	C	160	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	50	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	45	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	173	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
1	A	15[A]	LYS	CD-CE-NZ	-5.26	99.59	111.70
1	A	15[B]	LYS	CD-CE-NZ	-5.26	99.59	111.70
1	A	160	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	142	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	3551	0	3526	9	0
1	B	3503	0	3470	16	1
1	C	3508	0	3472	13	1
2	A	36	0	48	1	0
2	B	36	0	48	0	0
2	C	48	0	61	0	0
3	A	8	0	4	0	0
3	B	8	0	4	0	0
3	C	8	0	4	0	0
4	A	40	0	20	0	0
4	B	40	0	20	0	0
4	C	40	0	20	0	0
5	A	491	0	0	4	0
5	B	476	0	0	3	0
5	C	509	0	0	6	0
All	All	12302	0	10697	38	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (38) 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:141[B]:CYS:SG	1:B:173:ARG:HD2	1.83	1.17
1:B:410:ASP:HB3	5:B:956:HOH:O	1.66	0.95
1:B:141[B]:CYS:SG	1:B:173:ARG:CD	2.66	0.80
1:C:254[B]:GLN:NE2	5:C:601:HOH:O	2.16	0.73
1:A:141[B]:CYS:SG	5:A:715:HOH:O	2.50	0.69
1:C:22:GLU:OE2	1:C:34:ARG:NH1	2.23	0.66
1:B:141[B]:CYS:SG	1:B:173:ARG:CG	2.90	0.60
1:C:141[B]:CYS:SG	1:C:173:ARG:CG	2.89	0.60
1:B:141[B]:CYS:SG	1:B:173:ARG:HG3	2.46	0.55
1:C:141[B]:CYS:SG	1:C:173:ARG:HG2	2.47	0.54
1:C:141[B]:CYS:SG	1:C:173:ARG:HG3	2.50	0.52
1:B:171:LYS:HG3	5:B:777:HOH:O	2.10	0.52
1:B:410:ASP:CB	5:B:956:HOH:O	2.41	0.51
1:A:22:GLU:OE1	1:A:34:ARG:NH1	2.30	0.51
1:C:402:GLU:HG3	5:C:883:HOH:O	2.11	0.50
1:A:328:GLU:HG2	5:A:1019:HOH:O	2.12	0.49
1:A:141[A]:CYS:SG	1:A:173:ARG:CG	3.00	0.49
1:A:141[A]:CYS:SG	1:A:173:ARG:HG3	2.54	0.48
1:B:22:GLU:OE2	1:B:34:ARG:NH1	2.26	0.47
1:B:169:TYR:CZ	1:B:173:ARG:HD3	2.50	0.47
1:B:258:ILE:HD12	1:B:301:LEU:HD12	1.96	0.46
1:C:99:GLN:HE22	1:C:102:LYS:HZ2	1.62	0.46
1:C:396:ARG:NH1	5:C:606:HOH:O	2.41	0.46
1:A:402:GLU:HG3	5:A:836:HOH:O	2.16	0.45
1:B:141[A]:CYS:SG	1:B:172:LEU:HD13	2.57	0.44
1:B:254[B]:GLN:OE1	1:B:284:GLN:HG3	2.18	0.44
1:B:361:ARG:HA	1:B:369:ALA:HB1	2.00	0.44
1:B:94:PHE:CD1	1:B:94:PHE:C	2.90	0.44
1:A:163:GLY:HA2	1:A:187:TRP:CH2	2.53	0.43
1:C:34:ARG:HD2	5:C:833:HOH:O	2.18	0.43
1:C:94:PHE:CD1	1:C:94:PHE:C	2.92	0.42
1:B:163:GLY:HA2	1:B:187:TRP:CH2	2.55	0.42
1:A:417[B]:GLN:NE2	5:A:606:HOH:O	2.48	0.42
1:A:448[B]:LYS:HZ1	2:A:503:GOL:C3	2.31	0.41
1:C:328:GLU:HG2	5:C:1043:HOH:O	2.21	0.41
1:C:286:ALA:O	1:C:289:VAL:HB	2.21	0.41
1:C:64[B]:ARG:NH1	5:C:624:HOH:O	2.54	0.41
1:B:288:LEU:HA	1:B:288:LEU:HD23	1.93	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLN:NE2	1:C:48:GLN:NE2[2_455]	1.79	0.41

## 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	473/460 (103%)	465 (98%)	6 (1%)	2 (0%)	34	17
1	B	466/460 (101%)	456 (98%)	8 (2%)	2 (0%)	34	17
1	C	467/460 (102%)	458 (98%)	7 (2%)	2 (0%)	34	17
All	All	1406/1380 (102%)	1379 (98%)	21 (2%)	6 (0%)	34	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	B	192	ILE
1	C	192	ILE
1	C	154	ASP
1	A	154	ASP
1	B	154	ASP

### 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	366/351 (104%)	362 (99%)	4 (1%)	73	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	359/351 (102%)	355 (99%)	4 (1%)	73	59
1	C	360/351 (103%)	355 (99%)	5 (1%)	67	50
All	All	1085/1053 (103%)	1072 (99%)	13 (1%)	71	56

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	29	LYS
1	A	70	PHE
1	A	94	PHE
1	B	17	LEU
1	B	70	PHE
1	B	94	PHE
1	B	290	THR
1	C	17	LEU
1	C	70	PHE
1	C	94	PHE
1	C	171	LYS
1	C	289	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
1	C	99	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 monosaccharides in this entry.

## 5.6 Ligand geometry

26 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
4	A2R	A	507	-	37,43,43	1.27	2 (5%)	46,67,67	1.15	3 (6%)
2	GOL	C	502	-	5,5,5	0.64	0	5,5,5	1.29	1 (20%)
2	GOL	C	506	-	5,5,5	1.96	2 (40%)	5,5,5	3.94	3 (60%)
2	GOL	B	508	-	5,5,5	0.77	0	5,5,5	1.26	1 (20%)
2	GOL	A	502	-	5,5,5	0.65	0	5,5,5	0.87	0
2	GOL	B	504	-	5,5,5	0.81	0	5,5,5	0.75	0
2	GOL	A	503	-	5,5,5	0.98	0	5,5,5	1.02	0
4	A2R	B	506	-	37,43,43	1.35	2 (5%)	46,67,67	1.00	3 (6%)
3	SIN	C	508	-	1,7,7	1.08	0	2,8,8	2.55	2 (100%)
2	GOL	A	501	-	5,5,5	0.80	0	5,5,5	0.84	0
2	GOL	C	510	-	5,5,5	1.07	1 (20%)	5,5,5	1.21	0
2	GOL	C	504	-	5,5,5	0.45	0	5,5,5	0.71	0
2	GOL	C	505	-	5,5,5	1.54	2 (40%)	5,5,5	2.46	3 (60%)
2	GOL	B	503	-	5,5,5	0.44	0	5,5,5	1.17	0
2	GOL	A	504	-	5,5,5	0.37	0	5,5,5	1.40	0
2	GOL	A	505	-	5,5,5	0.82	0	5,5,5	3.47	1 (20%)
2	GOL	A	508	-	5,5,5	0.58	0	5,5,5	1.01	0
2	GOL	B	507	-	5,5,5	1.17	1 (20%)	5,5,5	1.13	0
3	SIN	A	506	-	1,7,7	0.67	0	2,8,8	2.87	1 (50%)
2	GOL	C	507	-	5,5,5	0.78	0	5,5,5	0.95	0
3	SIN	B	505	-	1,7,7	0.86	0	2,8,8	3.58	2 (100%)
2	GOL	B	501	-	5,5,5	0.61	0	5,5,5	1.15	0
4	A2R	C	509	-	37,43,43	1.49	7 (18%)	46,67,67	1.35	6 (13%)
2	GOL	C	501	-	5,5,5	1.08	1 (20%)	5,5,5	0.84	0
2	GOL	B	502	-	5,5,5	0.86	0	5,5,5	0.67	0
2	GOL	C	503	-	5,5,5	0.79	0	5,5,5	0.97	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
4	A2R	A	507	-	-	4/23/59/59	0/4/4/4
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	C	506	-	-	4/4/4/4	-
2	GOL	B	508	-	-	2/4/4/4	-
2	GOL	A	502	-	-	0/4/4/4	-
2	GOL	B	504	-	-	0/4/4/4	-
2	GOL	A	503	-	-	2/4/4/4	-
4	A2R	B	506	-	-	5/23/59/59	0/4/4/4
3	SIN	C	508	-	-	0/1/5/5	-
2	GOL	A	501	-	-	0/4/4/4	-
2	GOL	C	510	-	-	0/4/4/4	-
2	GOL	C	504	-	-	0/4/4/4	-
2	GOL	C	505	-	-	2/4/4/4	-
2	GOL	B	503	-	-	4/4/4/4	-
2	GOL	A	504	-	-	1/4/4/4	-
2	GOL	A	505	-	-	2/4/4/4	-
2	GOL	A	508	-	-	2/4/4/4	-
2	GOL	B	507	-	-	1/4/4/4	-
3	SIN	A	506	-	-	0/1/5/5	-
2	GOL	C	507	-	-	3/4/4/4	-
3	SIN	B	505	-	-	0/1/5/5	-
2	GOL	B	501	-	-	3/4/4/4	-
4	A2R	C	509	-	-	3/23/59/59	0/4/4/4
2	GOL	C	501	-	-	3/4/4/4	-
2	GOL	B	502	-	-	0/4/4/4	-
2	GOL	C	503	-	-	0/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	506	A2R	C2-N3	4.86	1.39	1.32
4	A	507	A2R	C2-N3	4.71	1.39	1.32
4	C	509	A2R	C11'-C12'	3.47	1.56	1.52
4	A	507	A2R	C11'-C12'	3.33	1.56	1.52
4	C	509	A2R	O4'-C1'	3.33	1.45	1.41
4	C	509	A2R	P2'-O2'	3.28	1.65	1.59
2	C	506	GOL	C3-C2	-2.87	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	506	A2R	O14'-C11'	2.80	1.46	1.43
4	C	509	A2R	C4-N3	-2.73	1.31	1.35
4	C	509	A2R	C3'-C2'	-2.56	1.47	1.52
2	B	507	GOL	O1-C1	2.50	1.53	1.42
2	C	505	GOL	O1-C1	-2.39	1.32	1.42
2	C	505	GOL	C1-C2	-2.39	1.41	1.51
2	C	510	GOL	O1-C1	2.31	1.52	1.42
2	C	506	GOL	C1-C2	-2.31	1.42	1.51
4	C	509	A2R	P2'-OP3	-2.20	1.46	1.54
4	C	509	A2R	O13'-C13'	2.12	1.48	1.43
2	C	501	GOL	O3-C3	2.07	1.51	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	GOL	C3-C2-C1	-7.33	83.20	111.70
2	C	506	GOL	C3-C2-C1	-6.88	84.95	111.70
4	C	509	A2R	N6-C6-N1	4.14	127.16	118.57
2	C	506	GOL	O2-C2-C3	3.96	126.57	109.12
3	B	505	SIN	C3-C2-C1	-3.93	106.07	112.67
3	A	506	SIN	C2-C3-C4	3.89	119.20	112.67
2	C	505	GOL	C3-C2-C1	-3.76	97.09	111.70
4	A	507	A2R	N3-C2-N1	-3.67	122.94	128.68
4	C	509	A2R	C5-C6-N6	-3.52	115.00	120.35
2	C	505	GOL	O1-C1-C2	-3.42	93.80	110.20
2	C	506	GOL	O1-C1-C2	-3.25	94.60	110.20
3	B	505	SIN	C2-C3-C4	3.20	118.03	112.67
3	C	508	SIN	C3-C2-C1	-2.74	108.07	112.67
4	A	507	A2R	C11'-C12'-C13'	-2.72	98.90	102.30
4	C	509	A2R	OP1-P2'-OP2	2.52	120.55	110.68
2	B	508	GOL	C3-C2-C1	-2.47	102.11	111.70
4	A	507	A2R	O11'-C11'-O14'	-2.38	108.08	111.13
4	C	509	A2R	O4'-C4'-C3'	2.37	109.81	105.11
3	C	508	SIN	C2-C3-C4	2.34	116.59	112.67
2	C	502	GOL	O3-C3-C2	2.29	121.20	110.20
4	C	509	A2R	O2'-C2'-C3'	2.23	119.76	111.68
4	B	506	A2R	O14'-C11'-C12'	-2.16	101.80	104.46
4	B	506	A2R	O3'-C3'-C4'	-2.11	104.95	111.05
4	B	506	A2R	OP1-P2'-OP2	2.10	118.92	110.68
4	C	509	A2R	OP1-P2'-O2'	-2.09	96.62	105.99
2	C	505	GOL	O3-C3-C2	-2.04	100.43	110.20

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	O1-C1-C2-C3
2	A	504	GOL	C1-C2-C3-O3
2	A	505	GOL	O1-C1-C2-O2
2	A	505	GOL	O1-C1-C2-C3
2	A	508	GOL	C1-C2-C3-O3
2	B	501	GOL	C1-C2-C3-O3
2	B	503	GOL	O1-C1-C2-C3
2	B	503	GOL	C1-C2-C3-O3
2	B	508	GOL	C1-C2-C3-O3
2	C	501	GOL	O1-C1-C2-C3
2	C	502	GOL	O1-C1-C2-O2
2	C	502	GOL	O1-C1-C2-C3
2	C	505	GOL	C1-C2-C3-O3
2	C	505	GOL	O2-C2-C3-O3
2	C	506	GOL	O1-C1-C2-O2
2	C	506	GOL	O1-C1-C2-C3
4	B	506	A2R	C15'-O15'-P1-O12
2	A	503	GOL	O1-C1-C2-O2
2	C	501	GOL	O1-C1-C2-O2
4	A	507	A2R	C3'-C2'-O2'-P2'
4	B	506	A2R	C3'-C2'-O2'-P2'
2	B	507	GOL	C1-C2-C3-O3
2	C	506	GOL	C1-C2-C3-O3
2	C	507	GOL	O1-C1-C2-C3
2	C	507	GOL	C1-C2-C3-O3
4	A	507	A2R	C1'-C2'-O2'-P2'
4	B	506	A2R	C1'-C2'-O2'-P2'
2	A	508	GOL	O2-C2-C3-O3
2	B	501	GOL	O2-C2-C3-O3
2	B	503	GOL	O1-C1-C2-O2
2	B	508	GOL	O2-C2-C3-O3
2	B	503	GOL	O2-C2-C3-O3
2	C	506	GOL	O2-C2-C3-O3
4	C	509	A2R	C3'-C2'-O2'-P2'
2	B	501	GOL	O1-C1-C2-O2
2	C	507	GOL	O1-C1-C2-O2
4	C	509	A2R	C1'-C2'-O2'-P2'
2	C	501	GOL	O2-C2-C3-O3
4	A	507	A2R	C15'-O15'-P1-O3
4	B	506	A2R	C15'-O15'-P1-O3

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Mol	Chain	Res	Type	Atoms
4	B	506	A2R	O4'-C4'-C5'-O5'
4	A	507	A2R	O4'-C4'-C5'-O5'
4	C	509	A2R	O4'-C4'-C5'-O5'

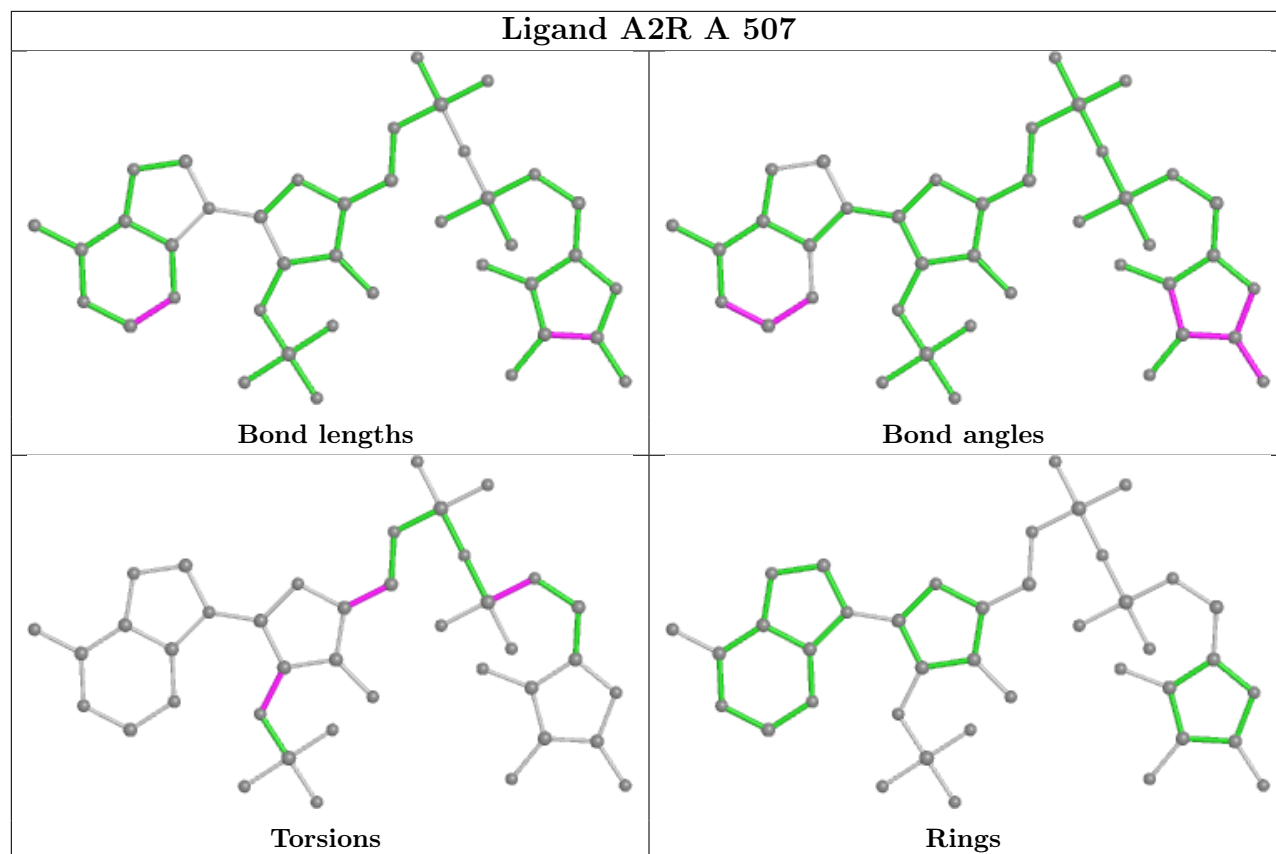
There are no ring outliers.

1 monomer is involved in 1 short contact:

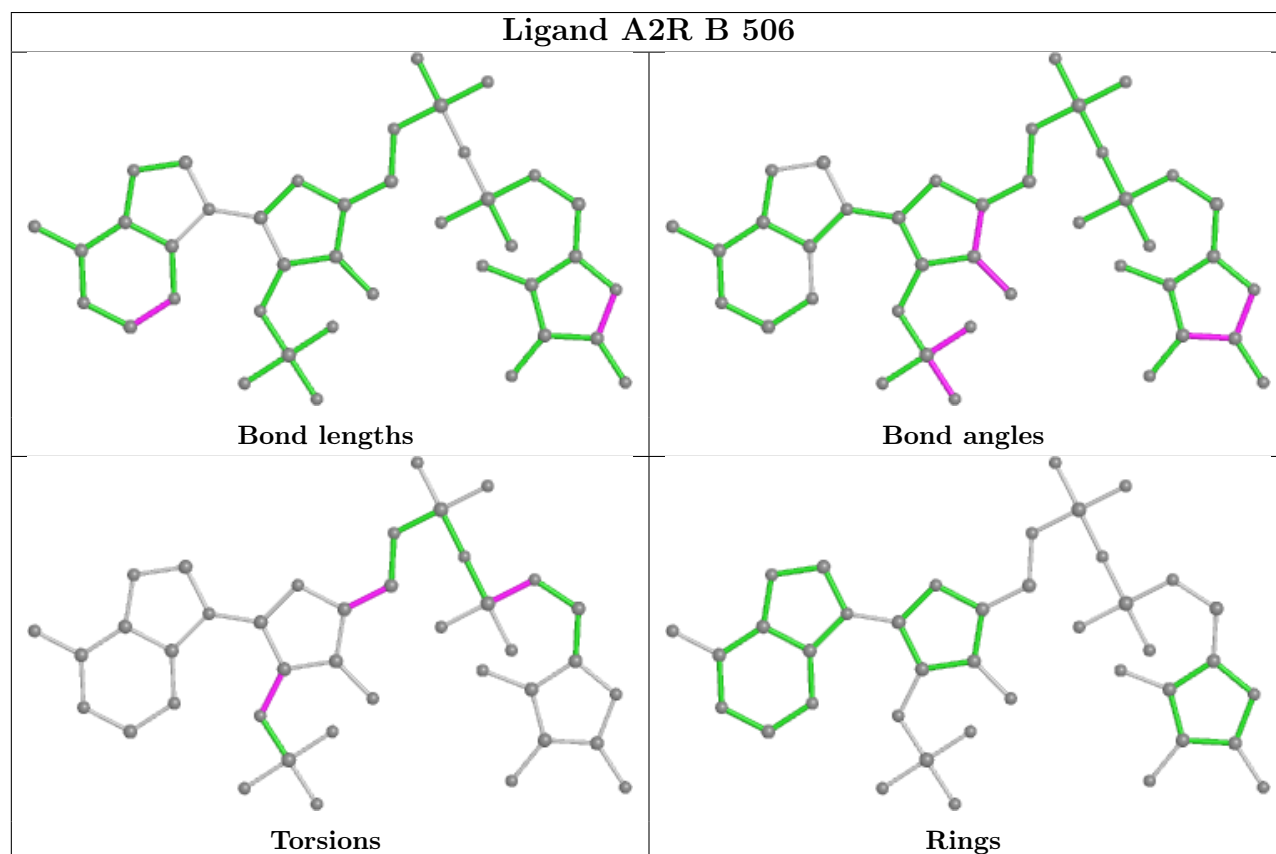
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	1	0

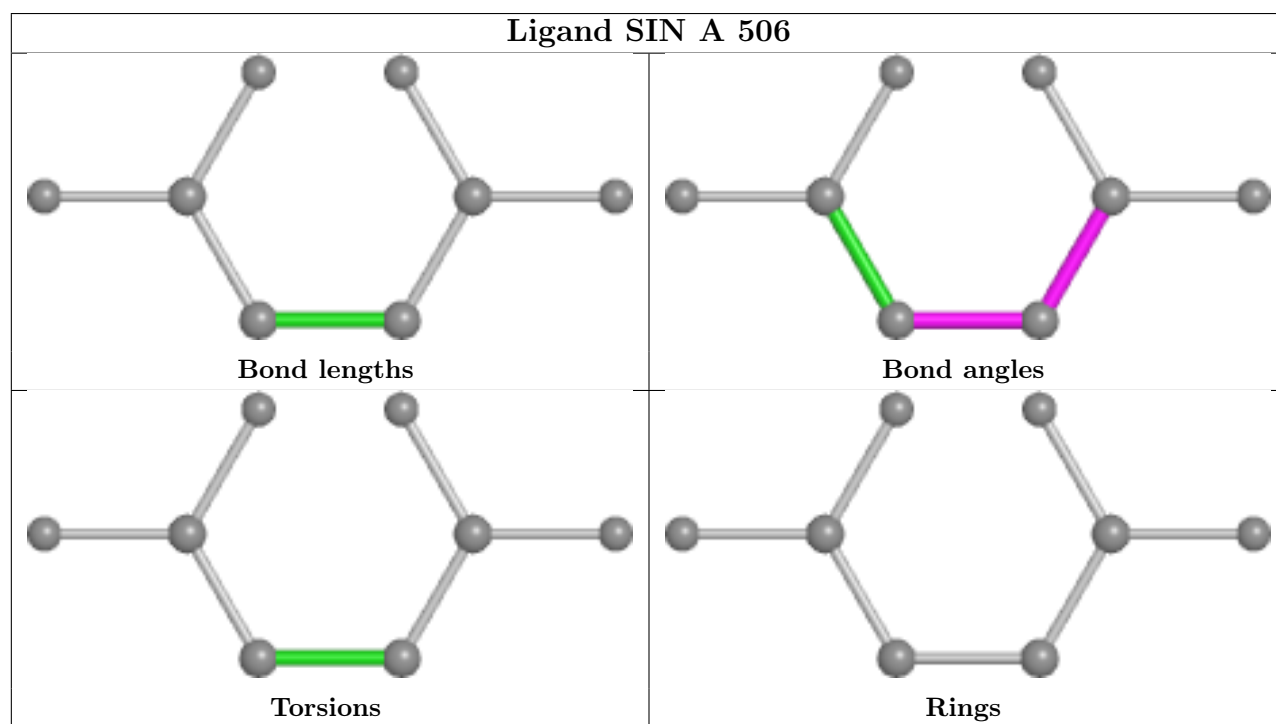
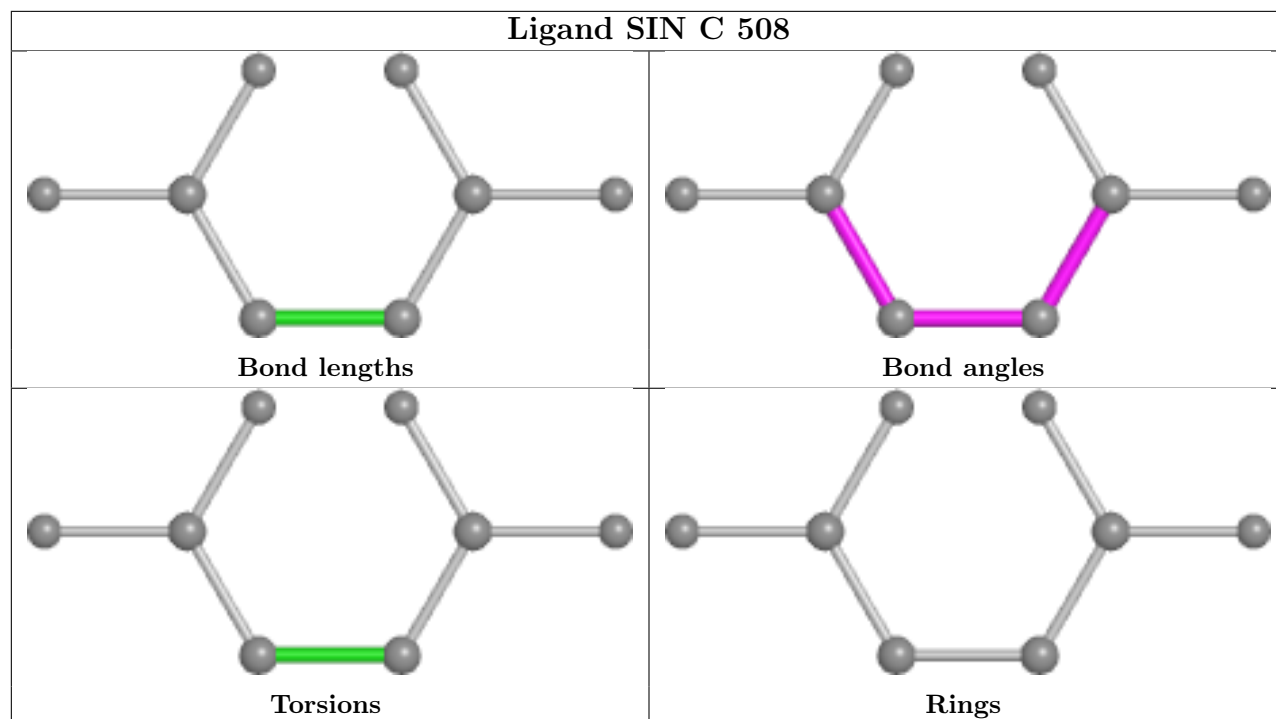
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

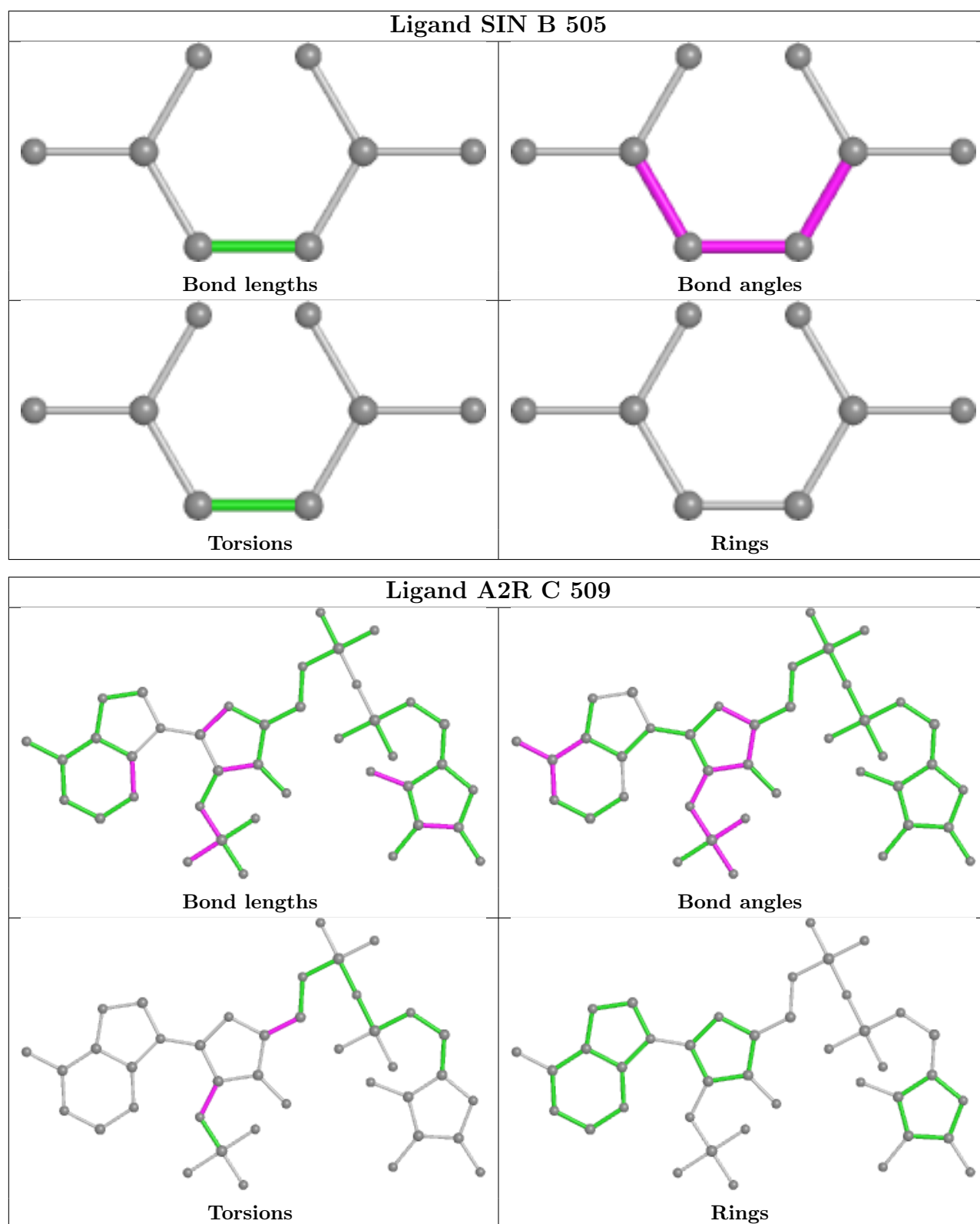
## Ligand A2R A 507



## Ligand A2R B 506







## 5.7 Other polymers [i](#)

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

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	460/460 (100%)	-0.30	9 (1%) 65 71	13, 18, 33, 50	1 (0%)
1	B	460/460 (100%)	-0.27	8 (1%) 70 76	13, 18, 32, 56	4 (0%)
1	C	460/460 (100%)	-0.44	5 (1%) 80 85	12, 16, 29, 49	4 (0%)
All	All	1380/1380 (100%)	-0.34	22 (1%) 72 78	12, 17, 31, 56	9 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	ALA	5.4
1	B	292	ALA	4.7
1	A	2	SER	4.1
1	A	292	ALA	3.5
1	B	293	ALA	3.4
1	C	289	VAL	3.2
1	A	289	VAL	3.1
1	A	290	THR	3.0
1	B	1	MET	3.0
1	A	1	MET	3.0
1	B	2	SER	2.8
1	B	289	VAL	2.7
1	C	2	SER	2.5
1	A	431	ASP	2.5
1	C	1	MET	2.4
1	C	263	ALA	2.3
1	B	28	GLN	2.2
1	B	431	ASP	2.1
1	A	6	VAL	2.1
1	C	264	LYS	2.0
1	A	294	PHE	2.0
1	B	214[A]	ASN	2.0

## 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](#)

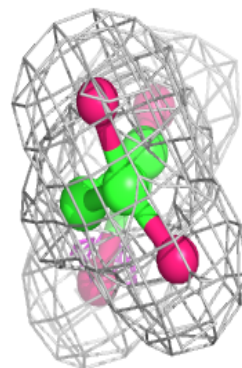
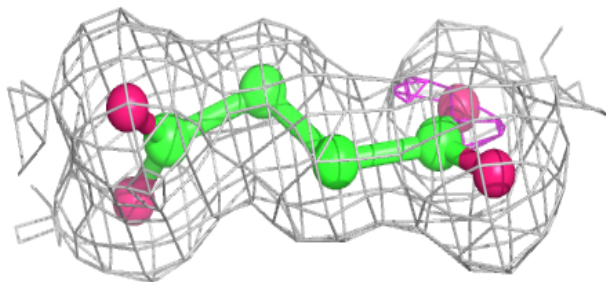
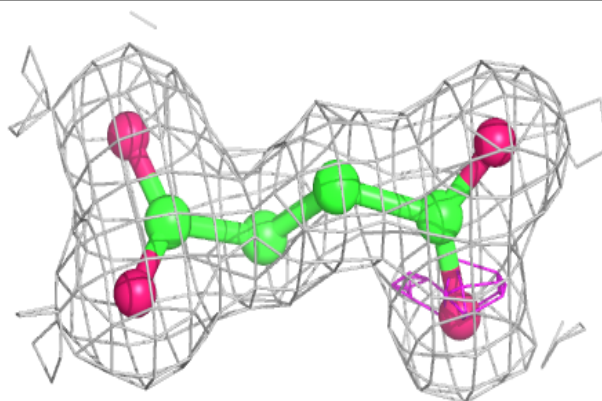
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	505	6/6	0.89	0.29	14,21,23,23	6
2	GOL	B	504	6/6	0.90	0.12	30,37,40,42	0
2	GOL	C	507	6/6	0.90	0.12	40,44,48,49	0
2	GOL	C	501	6/6	0.91	0.12	28,39,40,45	0
2	GOL	B	503	6/6	0.91	0.17	31,34,38,42	0
2	GOL	C	506	6/6	0.91	0.57	5,6,7,9	6
2	GOL	A	503	6/6	0.91	0.10	20,39,42,51	0
2	GOL	C	510	6/6	0.91	0.20	20,46,50,54	0
2	GOL	C	504	6/6	0.92	0.19	30,35,38,40	0
2	GOL	A	501	6/6	0.93	0.10	27,34,35,36	0
2	GOL	A	504	6/6	0.93	0.17	31,34,38,44	0
2	GOL	B	507	6/6	0.93	0.20	22,39,47,52	0
2	GOL	B	508	6/6	0.93	0.22	40,50,55,64	0
2	GOL	A	508	6/6	0.93	0.18	23,45,56,64	0
2	GOL	A	505	6/6	0.94	0.14	15,19,20,22	6
2	GOL	B	502	6/6	0.94	0.10	19,37,45,48	0
2	GOL	C	502	6/6	0.95	0.12	25,29,31,40	0
2	GOL	A	502	6/6	0.95	0.10	28,32,38,39	0
2	GOL	C	503	6/6	0.96	0.08	19,33,37,41	0
2	GOL	B	501	6/6	0.96	0.14	27,30,33,37	0
3	SIN	A	506	8/8	0.98	0.09	16,17,18,19	0
3	SIN	B	505	8/8	0.98	0.08	16,18,18,19	0
3	SIN	C	508	8/8	0.98	0.07	14,16,17,18	0
4	A2R	A	507	40/40	0.98	0.07	14,16,23,24	0
4	A2R	B	506	40/40	0.98	0.07	13,17,22,24	0
4	A2R	C	509	40/40	0.99	0.06	12,15,22,24	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.

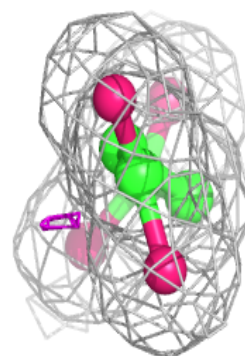
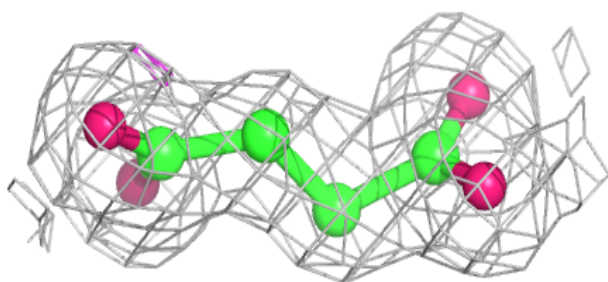
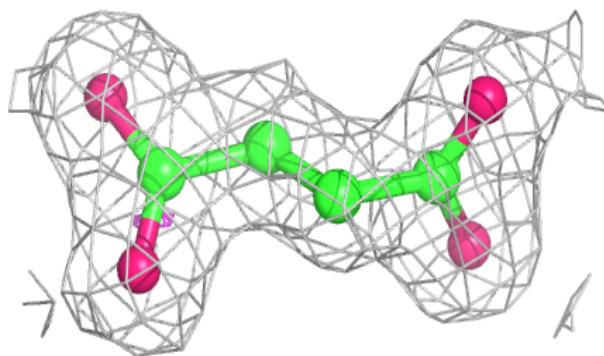
**Electron density around SIN A 506:**

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)

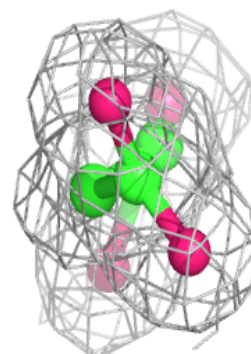
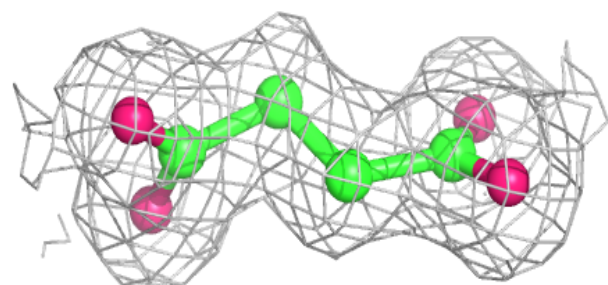
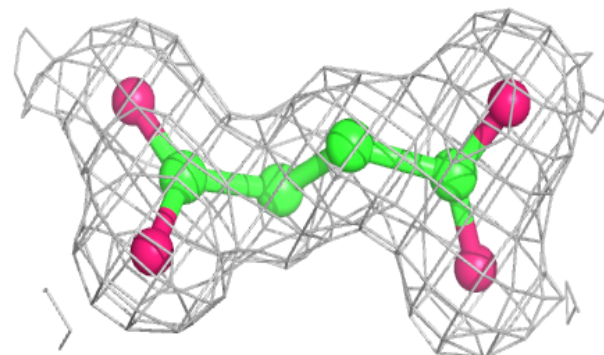


**Electron density around SIN B 505:**

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

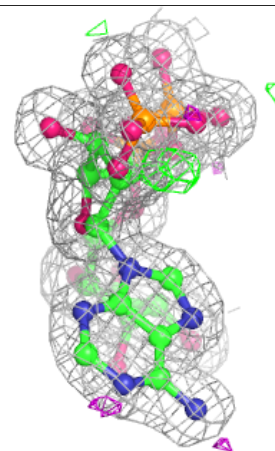
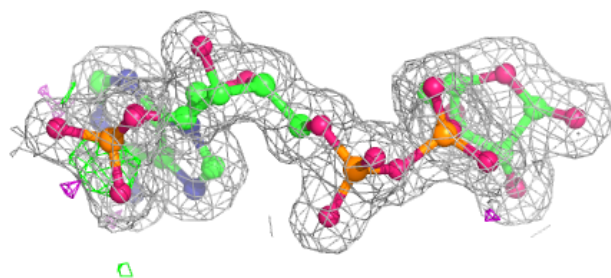
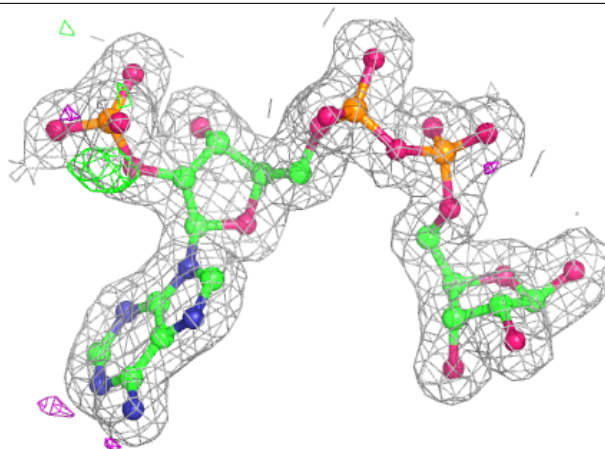
**Electron density around SIN C 508:**

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



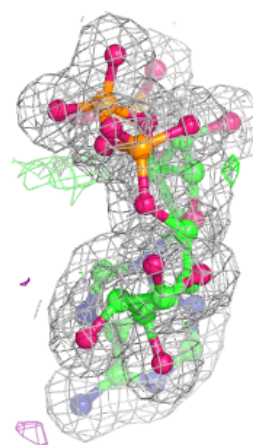
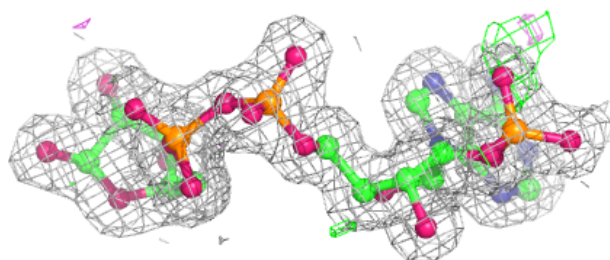
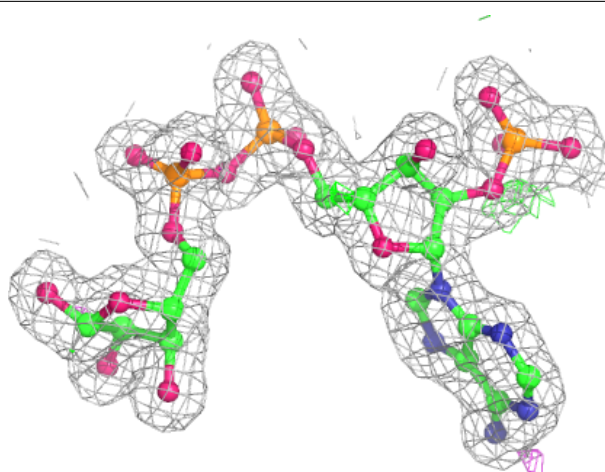
**Electron density around A2R A 507:**

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



**Electron density around A2R B 506:**

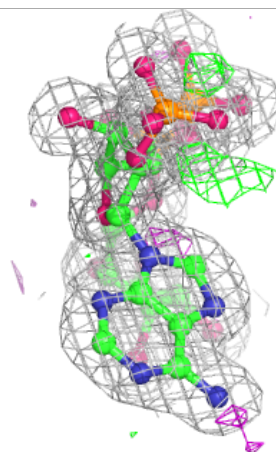
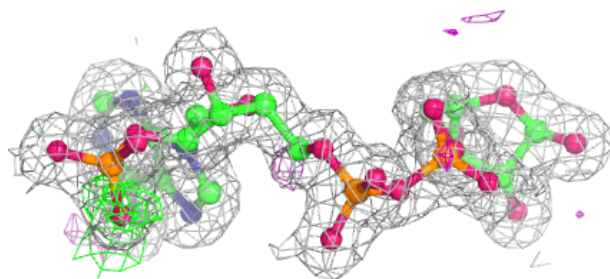
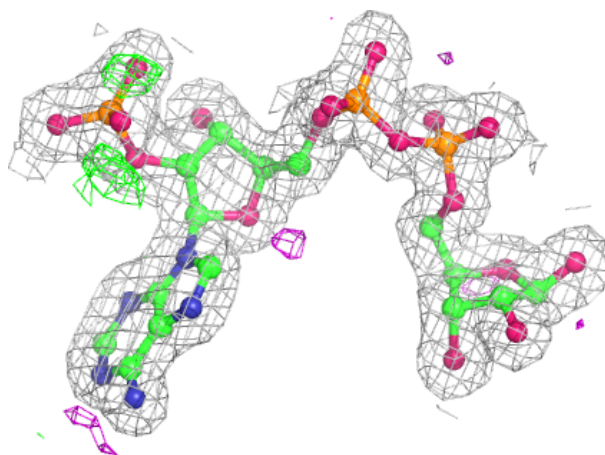
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A2R C 509:**

$2mF_o-DF_c$  (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.