



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:52 AM UTC

PDB ID : 8BGI / pdb_00008bgi
Title : GABA-A receptor $\alpha 5$ homomer - $\alpha 5V1$ - Flumazenil
Authors : Miller, P.S.; Malinauskas, T.M.; Omari, K.E.; Aricescu, A.R.
Deposited on : 2022-10-27
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

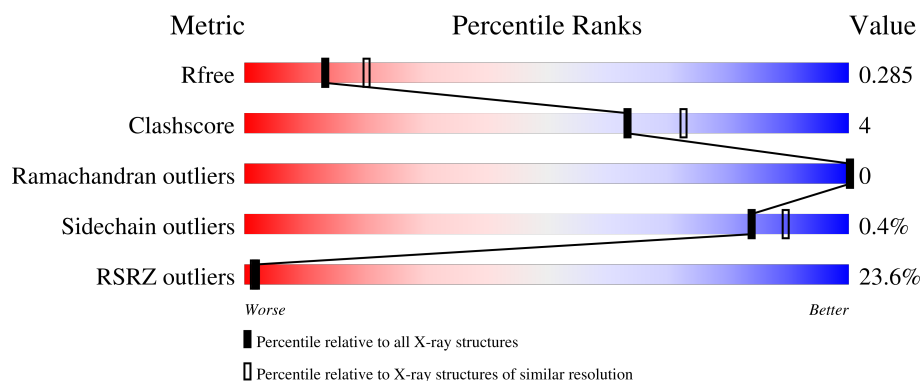
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	361	
1	B	361	
1	C	361	
1	D	361	
1	E	361	

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	SO4	C	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27623 atoms, of which 13621 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 Gamma-aminobutyric acid receptor subunit alpha-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	335	Total	C	H	N	O	S	0	0	0
			5366	1746	2661	448	493	18			
1	B	335	Total	C	H	N	O	S	0	0	0
			5364	1746	2659	448	493	18			
1	C	335	Total	C	H	N	O	S	0	0	0
			5366	1746	2661	448	493	18			
1	D	335	Total	C	H	N	O	S	0	0	0
			5366	1746	2661	448	493	18			
1	E	335	Total	C	H	N	O	S	0	0	0
			5366	1746	2661	448	493	18			

There are 215 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	MET	ILE	conflict	UNP P31644
A	51	ASN	THR	conflict	UNP P31644
A	67	ILE	VAL	conflict	UNP P31644
A	70	ALA	ARG	conflict	UNP P31644
A	72	THR	SER	conflict	UNP P31644
A	90	ASP	ASN	conflict	UNP P31644
A	92	ARG	LEU	conflict	UNP P31644
A	93	VAL	LEU	conflict	UNP P31644
A	95	ASP	SER	conflict	UNP P31644
A	96	GLN	LYS	conflict	UNP P31644
A	107	ASP	GLY	conflict	UNP P31644
A	111	PHE	ILE	conflict	UNP P31644
A	114	GLY	ASN	conflict	UNP P31644
A	121	MET	LEU	conflict	UNP P31644
A	124	ILE	LEU	conflict	UNP P31644
A	125	TRP	GLU	conflict	UNP P31644
A	126	ASN	ASP	conflict	UNP P31644
A	129	ARG	THR	conflict	UNP P31644
A	130	VAL	LEU	conflict	UNP P31644

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Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ASP	GLN	conflict	UNP P31644
A	153	GLU	ALA	conflict	UNP P31644
A	154	GLN	HIS	conflict	UNP P31644
A	155	ASN	ALA	conflict	UNP P31644
A	316	SER	-	linker	UNP P31644
A	317	GLN	-	linker	UNP P31644
A	318	PRO	-	linker	UNP P31644
A	319	ALA	-	linker	UNP P31644
A	320	ARG	-	linker	UNP P31644
A	321	ALA	-	linker	UNP P31644
A	322	ALA	-	linker	UNP P31644
A	404	ILE	VAL	engineered mutation	UNP P31644
A	420	ARG	-	expression tag	UNP P31644
A	421	GLY	-	expression tag	UNP P31644
A	422	THR	-	expression tag	UNP P31644
A	423	THR	-	expression tag	UNP P31644
A	424	GLU	-	expression tag	UNP P31644
A	425	THR	-	expression tag	UNP P31644
A	426	SER	-	expression tag	UNP P31644
A	427	GLN	-	expression tag	UNP P31644
A	428	VAL	-	expression tag	UNP P31644
A	429	ALA	-	expression tag	UNP P31644
A	430	PRO	-	expression tag	UNP P31644
A	431	ALA	-	expression tag	UNP P31644
B	48	MET	ILE	conflict	UNP P31644
B	51	ASN	THR	conflict	UNP P31644
B	67	ILE	VAL	conflict	UNP P31644
B	70	ALA	ARG	conflict	UNP P31644
B	72	THR	SER	conflict	UNP P31644
B	90	ASP	ASN	conflict	UNP P31644
B	92	ARG	LEU	conflict	UNP P31644
B	93	VAL	LEU	conflict	UNP P31644
B	95	ASP	SER	conflict	UNP P31644
B	96	GLN	LYS	conflict	UNP P31644
B	107	ASP	GLY	conflict	UNP P31644
B	111	PHE	ILE	conflict	UNP P31644
B	114	GLY	ASN	conflict	UNP P31644
B	121	MET	LEU	conflict	UNP P31644
B	124	ILE	LEU	conflict	UNP P31644
B	125	TRP	GLU	conflict	UNP P31644
B	126	ASN	ASP	conflict	UNP P31644
B	129	ARG	THR	conflict	UNP P31644

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Chain	Residue	Modelled	Actual	Comment	Reference
B	130	VAL	LEU	conflict	UNP P31644
B	145	ASP	GLN	conflict	UNP P31644
B	153	GLU	ALA	conflict	UNP P31644
B	154	GLN	HIS	conflict	UNP P31644
B	155	ASN	ALA	conflict	UNP P31644
B	316	SER	-	linker	UNP P31644
B	317	GLN	-	linker	UNP P31644
B	318	PRO	-	linker	UNP P31644
B	319	ALA	-	linker	UNP P31644
B	320	ARG	-	linker	UNP P31644
B	321	ALA	-	linker	UNP P31644
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B	421	GLY	-	expression tag	UNP P31644
B	422	THR	-	expression tag	UNP P31644
B	423	THR	-	expression tag	UNP P31644
B	424	GLU	-	expression tag	UNP P31644
B	425	THR	-	expression tag	UNP P31644
B	426	SER	-	expression tag	UNP P31644
B	427	GLN	-	expression tag	UNP P31644
B	428	VAL	-	expression tag	UNP P31644
B	429	ALA	-	expression tag	UNP P31644
B	430	PRO	-	expression tag	UNP P31644
B	431	ALA	-	expression tag	UNP P31644
C	48	MET	ILE	conflict	UNP P31644
C	51	ASN	THR	conflict	UNP P31644
C	67	ILE	VAL	conflict	UNP P31644
C	70	ALA	ARG	conflict	UNP P31644
C	72	THR	SER	conflict	UNP P31644
C	90	ASP	ASN	conflict	UNP P31644
C	92	ARG	LEU	conflict	UNP P31644
C	93	VAL	LEU	conflict	UNP P31644
C	95	ASP	SER	conflict	UNP P31644
C	96	GLN	LYS	conflict	UNP P31644
C	107	ASP	GLY	conflict	UNP P31644
C	111	PHE	ILE	conflict	UNP P31644
C	114	GLY	ASN	conflict	UNP P31644
C	121	MET	LEU	conflict	UNP P31644
C	124	ILE	LEU	conflict	UNP P31644
C	125	TRP	GLU	conflict	UNP P31644
C	126	ASN	ASP	conflict	UNP P31644

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Chain	Residue	Modelled	Actual	Comment	Reference
C	129	ARG	THR	conflict	UNP P31644
C	130	VAL	LEU	conflict	UNP P31644
C	145	ASP	GLN	conflict	UNP P31644
C	153	GLU	ALA	conflict	UNP P31644
C	154	GLN	HIS	conflict	UNP P31644
C	155	ASN	ALA	conflict	UNP P31644
C	316	SER	-	linker	UNP P31644
C	317	GLN	-	linker	UNP P31644
C	318	PRO	-	linker	UNP P31644
C	319	ALA	-	linker	UNP P31644
C	320	ARG	-	linker	UNP P31644
C	321	ALA	-	linker	UNP P31644
C	322	ALA	-	linker	UNP P31644
C	404	ILE	VAL	engineered mutation	UNP P31644
C	420	ARG	-	expression tag	UNP P31644
C	421	GLY	-	expression tag	UNP P31644
C	422	THR	-	expression tag	UNP P31644
C	423	THR	-	expression tag	UNP P31644
C	424	GLU	-	expression tag	UNP P31644
C	425	THR	-	expression tag	UNP P31644
C	426	SER	-	expression tag	UNP P31644
C	427	GLN	-	expression tag	UNP P31644
C	428	VAL	-	expression tag	UNP P31644
C	429	ALA	-	expression tag	UNP P31644
C	430	PRO	-	expression tag	UNP P31644
C	431	ALA	-	expression tag	UNP P31644
D	48	MET	ILE	conflict	UNP P31644
D	51	ASN	THR	conflict	UNP P31644
D	67	ILE	VAL	conflict	UNP P31644
D	70	ALA	ARG	conflict	UNP P31644
D	72	THR	SER	conflict	UNP P31644
D	90	ASP	ASN	conflict	UNP P31644
D	92	ARG	LEU	conflict	UNP P31644
D	93	VAL	LEU	conflict	UNP P31644
D	95	ASP	SER	conflict	UNP P31644
D	96	GLN	LYS	conflict	UNP P31644
D	107	ASP	GLY	conflict	UNP P31644
D	111	PHE	ILE	conflict	UNP P31644
D	114	GLY	ASN	conflict	UNP P31644
D	121	MET	LEU	conflict	UNP P31644
D	124	ILE	LEU	conflict	UNP P31644
D	125	TRP	GLU	conflict	UNP P31644

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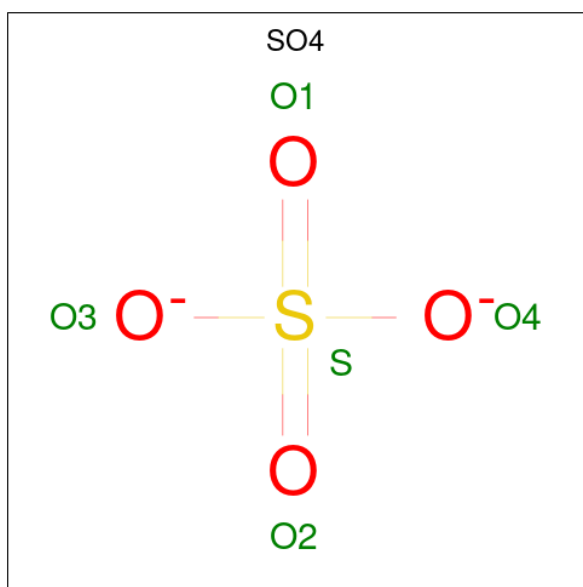
Chain	Residue	Modelled	Actual	Comment	Reference
D	126	ASN	ASP	conflict	UNP P31644
D	129	ARG	THR	conflict	UNP P31644
D	130	VAL	LEU	conflict	UNP P31644
D	145	ASP	GLN	conflict	UNP P31644
D	153	GLU	ALA	conflict	UNP P31644
D	154	GLN	HIS	conflict	UNP P31644
D	155	ASN	ALA	conflict	UNP P31644
D	316	SER	-	linker	UNP P31644
D	317	GLN	-	linker	UNP P31644
D	318	PRO	-	linker	UNP P31644
D	319	ALA	-	linker	UNP P31644
D	320	ARG	-	linker	UNP P31644
D	321	ALA	-	linker	UNP P31644
D	322	ALA	-	linker	UNP P31644
D	404	ILE	VAL	engineered mutation	UNP P31644
D	420	ARG	-	expression tag	UNP P31644
D	421	GLY	-	expression tag	UNP P31644
D	422	THR	-	expression tag	UNP P31644
D	423	THR	-	expression tag	UNP P31644
D	424	GLU	-	expression tag	UNP P31644
D	425	THR	-	expression tag	UNP P31644
D	426	SER	-	expression tag	UNP P31644
D	427	GLN	-	expression tag	UNP P31644
D	428	VAL	-	expression tag	UNP P31644
D	429	ALA	-	expression tag	UNP P31644
D	430	PRO	-	expression tag	UNP P31644
D	431	ALA	-	expression tag	UNP P31644
E	48	MET	ILE	conflict	UNP P31644
E	51	ASN	THR	conflict	UNP P31644
E	67	ILE	VAL	conflict	UNP P31644
E	70	ALA	ARG	conflict	UNP P31644
E	72	THR	SER	conflict	UNP P31644
E	90	ASP	ASN	conflict	UNP P31644
E	92	ARG	LEU	conflict	UNP P31644
E	93	VAL	LEU	conflict	UNP P31644
E	95	ASP	SER	conflict	UNP P31644
E	96	GLN	LYS	conflict	UNP P31644
E	107	ASP	GLY	conflict	UNP P31644
E	111	PHE	ILE	conflict	UNP P31644
E	114	GLY	ASN	conflict	UNP P31644
E	121	MET	LEU	conflict	UNP P31644
E	124	ILE	LEU	conflict	UNP P31644

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Chain	Residue	Modelled	Actual	Comment	Reference
E	125	TRP	GLU	conflict	UNP P31644
E	126	ASN	ASP	conflict	UNP P31644
E	129	ARG	THR	conflict	UNP P31644
E	130	VAL	LEU	conflict	UNP P31644
E	145	ASP	GLN	conflict	UNP P31644
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E	423	THR	-	expression tag	UNP P31644
E	424	GLU	-	expression tag	UNP P31644
E	425	THR	-	expression tag	UNP P31644
E	426	SER	-	expression tag	UNP P31644
E	427	GLN	-	expression tag	UNP P31644
E	428	VAL	-	expression tag	UNP P31644
E	429	ALA	-	expression tag	UNP P31644
E	430	PRO	-	expression tag	UNP P31644
E	431	ALA	-	expression tag	UNP P31644

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



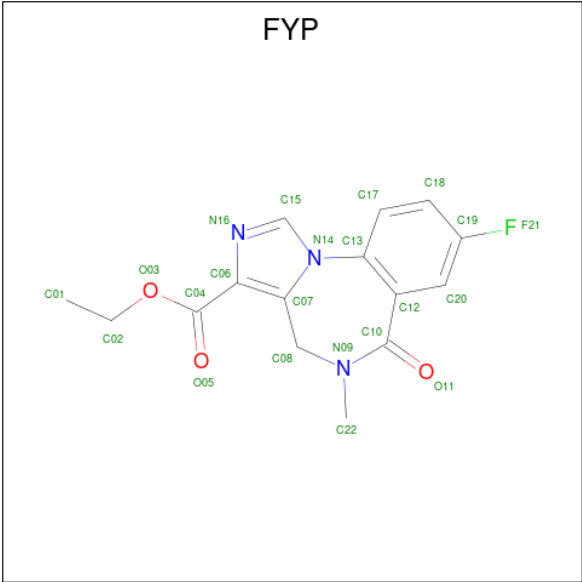
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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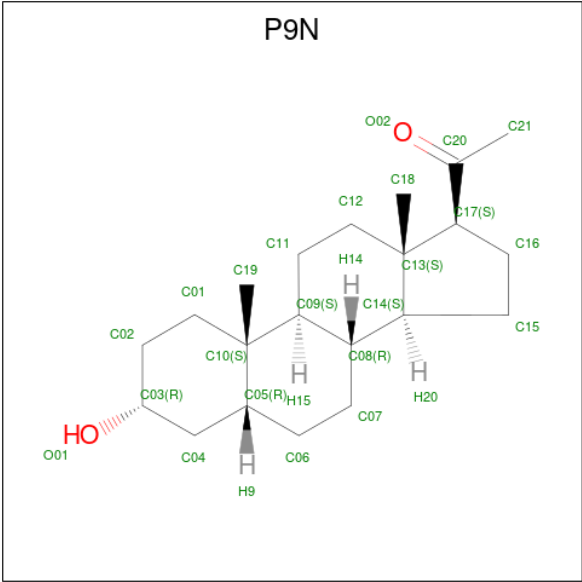
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ethyl 8-fluoro-5-methyl-6-oxo-5,6-dihydro-4H-imidazo[1,5-a][1,4]benzodiazepine-3-carboxylate (CCD ID: FYP) (formula: C₁₅H₁₄FN₃O₃) (labeled as "Ligand of Interest" by depositor).



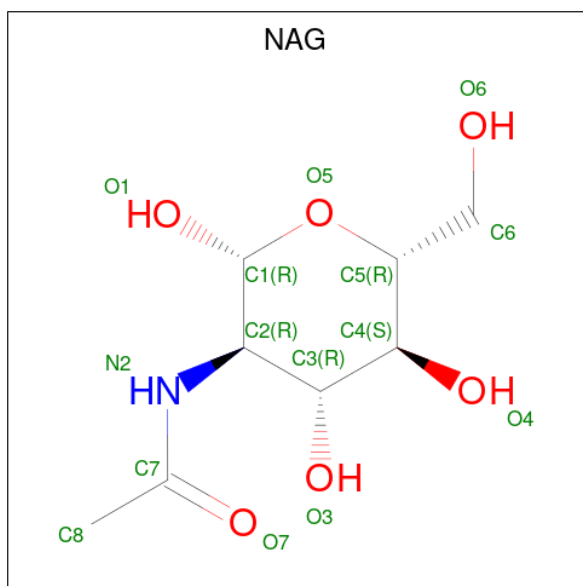
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 36	C 15	F 1	H 14	N 3	O 3	0	0
3	B	1	Total 36	C 15	F 1	H 14	N 3	O 3	0	0
3	C	1	Total 36	C 15	F 1	H 14	N 3	O 3	0	0
3	D	1	Total 36	C 15	F 1	H 14	N 3	O 3	0	0
3	E	1	Total 36	C 15	F 1	H 14	N 3	O 3	0	0

- Molecule 4 is Pregnanolone (CCD ID: P9N) (formula: C₂₁H₃₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			57	21	34	2		
4	B	1	Total	C	H	O	0	0
			57	21	34	2		
4	C	1	Total	C	H	O	0	0
			57	21	34	2		
4	D	1	Total	C	H	O	0	0
			57	21	34	2		
4	E	1	Total	C	H	O	0	0
			57	21	34	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	E	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

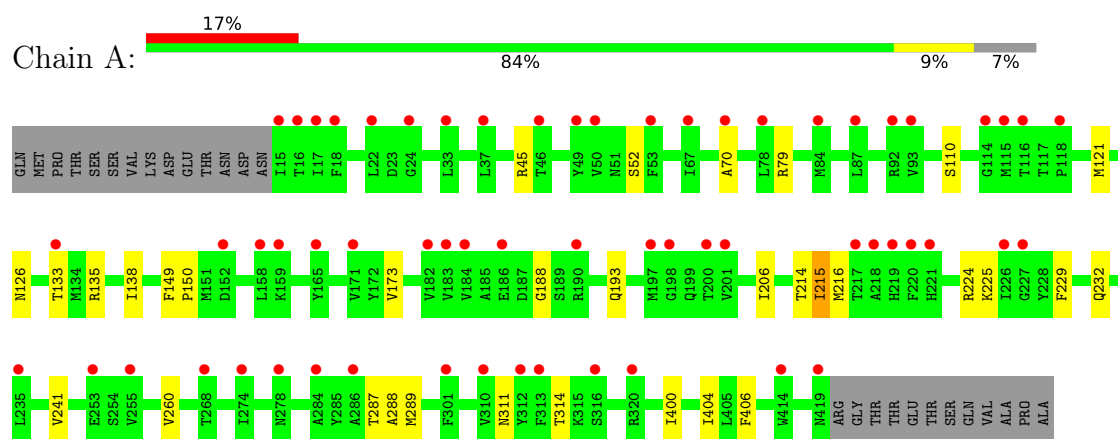
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	B	4	Total 4	O 4	0	0
6	C	5	Total 5	O 5	0	0
6	D	2	Total 2	O 2	0	0
6	E	4	Total 4	O 4	0	0

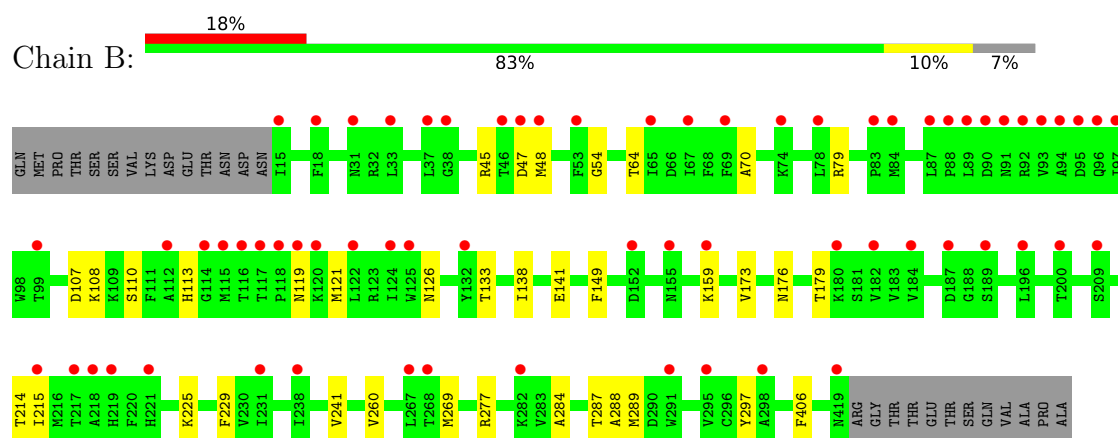
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

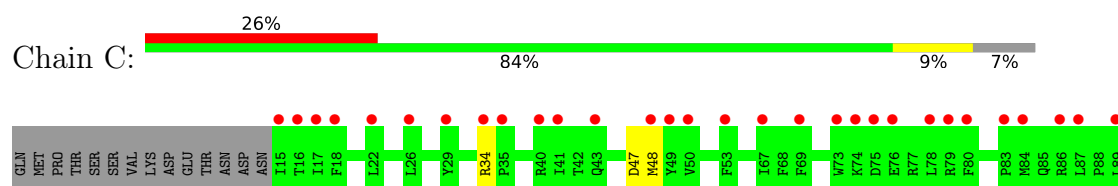
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-5

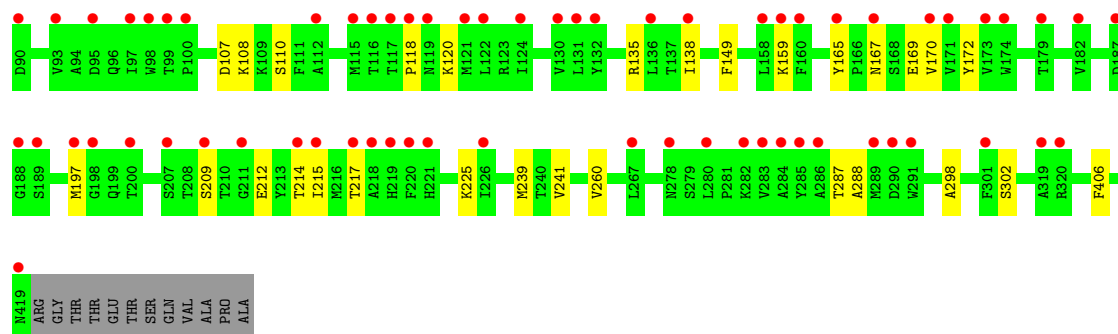


- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-5



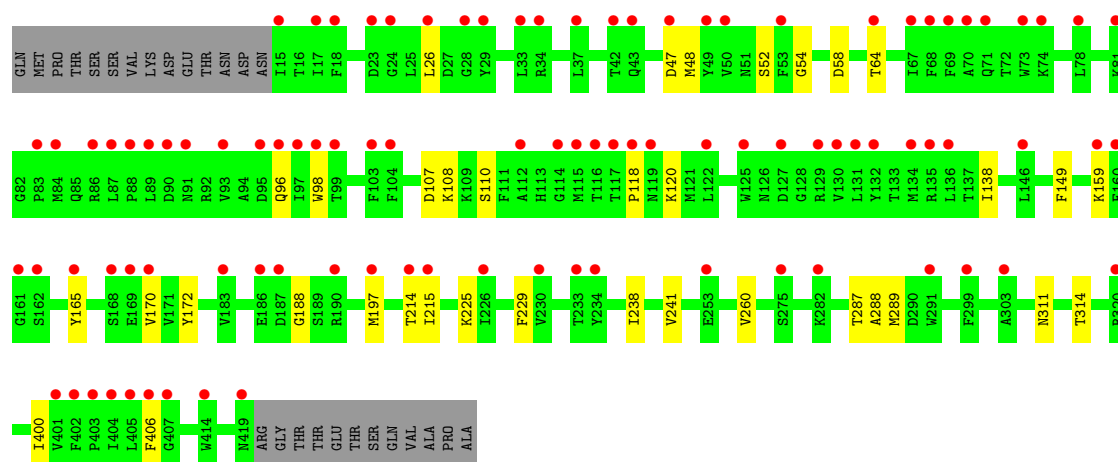
- Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-5





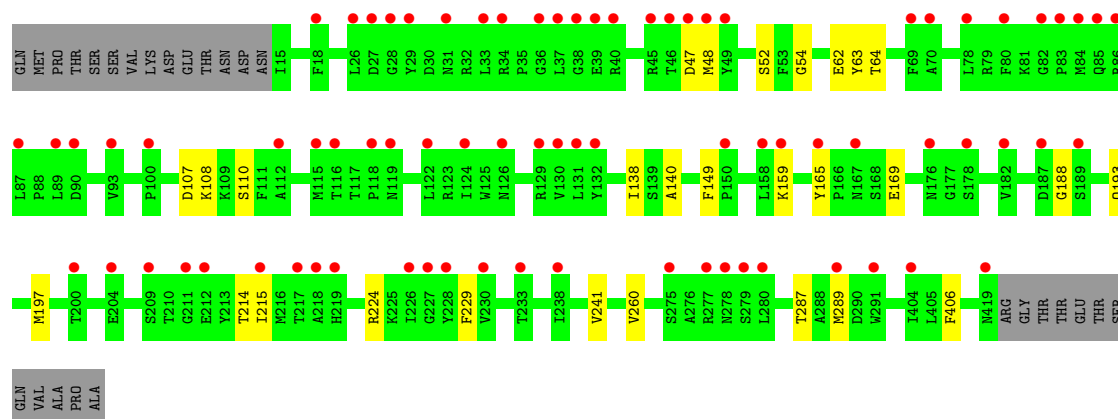
• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-5

Chain D: 27% 83% 10% 7%



• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-5

Chain E: 22% 85% 8% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.77Å 131.64Å 119.17Å 90.00° 100.19° 90.00°	Depositor
Resolution (Å)	47.56 – 2.56 47.56 – 2.57	Depositor EDS
% Data completeness (in resolution range)	92.2 (47.56-2.56) 46.6 (47.56-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.81Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.254 , 0.277 0.263 , 0.285	Depositor DCC
R_{free} test set	1643 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	27623	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: FYP, SO4, NAG, P9N

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	0.12	0/2776	0.29	0/3776
1	B	0.12	0/2776	0.28	0/3776
1	C	0.11	0/2776	0.26	0/3776
1	D	0.15	0/2776	0.27	0/3776
1	E	0.11	0/2776	0.28	0/3776
All	All	0.12	0/13880	0.28	0/18880

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	2705	2661	2667	25	0
1	B	2705	2659	2666	30	0
1	C	2705	2661	2667	23	0
1	D	2705	2661	2667	25	0
1	E	2705	2661	2667	16	0
2	A	30	0	0	0	0
2	B	35	0	0	1	0
2	C	25	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	25	0	0	1	0
2	E	30	0	0	0	0
3	A	22	14	0	0	0
3	B	22	14	0	1	0
3	C	22	14	0	1	0
3	D	22	14	0	0	0
3	E	22	14	0	0	0
4	A	23	34	0	0	0
4	B	23	34	0	0	0
4	C	23	34	0	0	0
4	D	23	34	0	0	0
4	E	23	34	0	0	0
5	A	14	13	13	0	0
5	B	28	26	26	1	0
5	C	14	13	13	0	0
5	D	14	13	13	0	0
5	E	14	13	13	0	0
6	A	8	0	0	0	0
6	B	4	0	0	0	0
6	C	5	0	0	0	0
6	D	2	0	0	0	0
6	E	4	0	0	0	0
All	All	14002	13621	13412	110	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 4.

All (110) 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:206:ILE:HD13	1:A:215:ILE:HD12	1.59	0.84
1:C:225:LYS:NZ	2:C:501:SO4:O2	2.11	0.81
1:D:165:TYR:HD2	1:D:170:VAL:HG21	1.51	0.75
1:C:225:LYS:NZ	2:C:501:SO4:S	2.66	0.67
1:B:149:PHE:HB3	1:B:287:THR:HG23	1.79	0.64
1:A:206:ILE:CD1	1:A:215:ILE:HD12	2.28	0.61
1:A:110:SER:HB2	1:A:138:ILE:HG22	1.84	0.59
1:B:113:HIS:HB2	1:B:119:ASN:HD22	1.71	0.55
1:B:79:ARG:HG3	1:B:126:ASN:O	2.07	0.55
1:A:121:MET:HE2	1:A:133:THR:HG22	1.89	0.55
1:B:107:ASP:OD1	1:B:108:LYS:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:HB3	1:D:287:THR:HG23	1.89	0.54
1:B:110:SER:HB2	1:B:138:ILE:HG22	1.88	0.54
1:A:121:MET:HE2	1:A:133:THR:CG2	2.37	0.54
1:D:260:VAL:HG11	1:E:260:VAL:HG22	1.91	0.53
1:A:229:PHE:HB3	1:A:289:MET:HE1	1.89	0.53
1:B:113:HIS:HB2	1:B:119:ASN:ND2	2.24	0.53
1:A:260:VAL:HG11	1:B:260:VAL:HG22	1.92	0.52
1:A:110:SER:CB	1:A:138:ILE:HG22	2.39	0.52
1:E:54:GLY:N	1:E:64:THR:O	2.43	0.51
1:C:107:ASP:OD1	1:C:108:LYS:N	2.43	0.51
1:E:52:SER:HA	1:E:188:GLY:HA3	1.92	0.51
1:D:225:LYS:NZ	2:D:501:SO4:O2	2.43	0.51
1:B:110:SER:CB	1:B:138:ILE:HG22	2.41	0.51
1:E:149:PHE:HB3	1:E:287:THR:HG23	1.92	0.51
1:D:107:ASP:OD1	1:D:108:LYS:N	2.44	0.50
1:A:149:PHE:HB3	1:A:287:THR:HG23	1.94	0.50
1:B:149:PHE:O	1:B:288:ALA:HB3	2.12	0.50
1:B:229:PHE:HB3	1:B:289:MET:HE1	1.94	0.50
1:D:47:ASP:OD1	1:D:48:MET:N	2.41	0.50
1:B:47:ASP:OD1	1:B:48:MET:N	2.44	0.49
1:B:54:GLY:N	1:B:64:THR:O	2.45	0.49
1:D:98:TRP:HZ2	1:D:165:TYR:HE2	1.61	0.49
1:E:107:ASP:OD1	1:E:108:LYS:N	2.45	0.49
1:E:47:ASP:OD1	1:E:48:MET:N	2.45	0.49
1:D:110:SER:CB	1:D:138:ILE:HG22	2.41	0.49
1:C:110:SER:HB2	1:C:138:ILE:HG22	1.94	0.49
1:D:110:SER:HB2	1:D:138:ILE:HG22	1.95	0.49
1:D:54:GLY:N	1:D:64:THR:O	2.47	0.47
1:E:110:SER:CB	1:E:138:ILE:HG22	2.44	0.47
1:C:34:ARG:NE	1:C:169:GLU:OE1	2.45	0.47
1:A:225:LYS:HE2	1:B:284:ALA:HB3	1.96	0.47
1:B:45:ARG:HG2	1:B:173:VAL:HG23	1.96	0.47
1:E:241:VAL:HG21	1:E:406:PHE:CZ	2.49	0.47
1:B:241:VAL:HG21	1:B:406:PHE:CZ	2.50	0.47
1:C:110:SER:CB	1:C:138:ILE:HG22	2.44	0.47
1:A:311:ASN:O	1:A:314:THR:HG22	2.15	0.46
1:C:172:TYR:H	1:C:214:THR:HG21	1.80	0.46
1:E:229:PHE:HB3	1:E:289:MET:HE1	1.98	0.46
1:C:47:ASP:OD1	1:C:48:MET:N	2.46	0.46
1:A:70:ALA:HB2	3:B:508:FYP:O05	2.16	0.46
1:D:172:TYR:H	1:D:214:THR:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:SER:HB2	1:E:138:ILE:HG22	1.96	0.46
1:A:79:ARG:HG3	1:A:126:ASN:O	2.15	0.45
1:D:260:VAL:CG1	1:E:260:VAL:HG22	2.45	0.45
1:A:135:ARG:NH2	1:B:107:ASP:O	2.49	0.45
1:B:70:ALA:HB2	3:C:506:FYP:O05	2.17	0.45
1:B:225:LYS:NZ	2:B:501:SO4:O4	2.49	0.45
1:C:165:TYR:HD2	1:C:170:VAL:HG21	1.81	0.45
1:A:52:SER:HA	1:A:188:GLY:HA3	1.99	0.45
1:D:58:ASP:OD1	1:D:58:ASP:N	2.49	0.45
1:C:135:ARG:NH1	2:C:504:SO4:O3	2.50	0.45
1:C:239:MET:HA	1:C:239:MET:HE2	1.99	0.45
1:C:165:TYR:CD2	1:C:170:VAL:HG21	2.51	0.44
1:A:214:THR:O	1:A:214:THR:HG23	2.18	0.44
1:A:400:ILE:HG22	1:A:404:ILE:HD12	1.99	0.44
1:C:159:LYS:HG2	1:C:217:THR:HG22	1.99	0.44
1:C:149:PHE:HB3	1:C:287:THR:HG23	1.99	0.44
1:D:238:ILE:O	1:D:241:VAL:HG22	2.18	0.44
1:D:26:LEU:HD13	1:D:96:GLN:OE1	2.18	0.44
1:E:159:LYS:HB3	1:E:215:ILE:HD11	2.00	0.43
1:A:260:VAL:CG1	1:B:260:VAL:HG22	2.49	0.43
1:B:47:ASP:HB3	1:B:70:ALA:HB3	1.99	0.43
1:C:159:LYS:HB3	1:C:215:ILE:HD11	2.00	0.43
1:D:165:TYR:CD2	1:D:170:VAL:HG21	2.41	0.43
1:C:214:THR:HG23	1:C:214:THR:O	2.18	0.43
1:A:241:VAL:HG21	1:A:406:PHE:CZ	2.54	0.43
1:D:214:THR:HG23	1:D:214:THR:O	2.18	0.43
1:D:311:ASN:O	1:D:314:THR:HG22	2.19	0.43
1:A:149:PHE:O	1:A:288:ALA:HB3	2.19	0.43
1:D:52:SER:HA	1:D:188:GLY:HA3	2.00	0.42
1:A:193:GLN:OE1	1:A:224:ARG:NH1	2.52	0.42
1:C:149:PHE:O	1:C:288:ALA:HB3	2.20	0.42
1:D:241:VAL:HG21	1:D:406:PHE:CZ	2.54	0.42
1:C:167:ASN:N	1:C:212:GLU:O	2.46	0.42
1:B:214:THR:O	1:B:214:THR:HG23	2.18	0.42
1:D:98:TRP:CZ2	1:D:165:TYR:HE2	2.38	0.42
1:B:108:LYS:HE3	1:B:141:GLU:HG2	2.02	0.41
1:B:121:MET:HE2	1:B:133:THR:CG2	2.49	0.41
1:A:173:VAL:C	1:A:216:MET:HE1	2.46	0.41
1:B:121:MET:HE2	1:B:133:THR:HG22	2.02	0.41
1:B:159:LYS:HB3	1:B:215:ILE:HD11	2.03	0.41
1:D:118:PRO:O	1:D:120:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:O	1:D:288:ALA:HB3	2.20	0.41
1:B:179:THR:HG22	1:C:209:SER:HB2	2.02	0.41
1:D:229:PHE:HB3	1:D:289:MET:HE1	2.03	0.41
1:E:63:TYR:CE1	1:E:140:ALA:HB3	2.56	0.41
1:B:269:MET:HG2	1:B:297:TYR:HA	2.03	0.41
1:C:118:PRO:O	1:C:120:LYS:N	2.53	0.41
1:B:260:VAL:HG11	1:C:260:VAL:HG22	2.01	0.41
1:A:150:PRO:HG3	1:A:289:MET:HE3	2.02	0.41
1:A:232:GLN:HG3	1:B:277:ARG:HG2	2.03	0.41
1:B:176:ASN:ND2	5:B:510:NAG:O7	2.54	0.41
1:D:159:LYS:HB3	1:D:215:ILE:HD11	2.02	0.41
1:E:165:TYR:HD1	1:E:169:GLU:OE1	2.04	0.41
1:E:214:THR:O	1:E:214:THR:HG23	2.21	0.41
1:E:193:GLN:OE1	1:E:224:ARG:NH1	2.54	0.40
1:A:45:ARG:HG2	1:A:173:VAL:HG23	2.03	0.40
1:C:241:VAL:HG21	1:C:406:PHE:CZ	2.57	0.40
1:C:298:ALA:O	1:C:302:SER:OG	2.32	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	333/361 (92%)	323 (97%)	10 (3%)	0	100	100
1	B	333/361 (92%)	323 (97%)	10 (3%)	0	100	100
1	C	333/361 (92%)	323 (97%)	10 (3%)	0	100	100
1	D	333/361 (92%)	322 (97%)	11 (3%)	0	100	100
1	E	333/361 (92%)	323 (97%)	10 (3%)	0	100	100
All	All	1665/1805 (92%)	1614 (97%)	51 (3%)	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	298/321 (93%)	297 (100%)	1 (0%)	86	91
1	B	298/321 (93%)	298 (100%)	0	100	100
1	C	298/321 (93%)	297 (100%)	1 (0%)	86	91
1	D	298/321 (93%)	296 (99%)	2 (1%)	76	84
1	E	298/321 (93%)	296 (99%)	2 (1%)	76	84
All	All	1490/1605 (93%)	1484 (100%)	6 (0%)	84	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ILE
1	C	197	MET
1	D	197	MET
1	D	400	ILE
1	E	62	GLU
1	E	197	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	71	GLN
1	B	119	ASN
1	B	245	GLN
1	C	71	GLN
1	C	245	GLN
1	D	71	GLN
1	D	245	GLN
1	E	71	GLN
1	E	195	HIS

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Mol	Chain	Res	Type
1	E	245	GLN
1	E	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

45 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	$\# Z > 2$
2	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	C	504	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	502	-	4,4,4	0.25	0	6,6,6	0.08	0
4	P9N	A	508	-	26,26,26	0.13	0	42,42,42	0.28	0
3	FYP	D	506	-	23,24,24	0.24	0	27,35,35	0.33	0
2	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.15	0
3	FYP	B	508	-	23,24,24	0.22	0	27,35,35	0.38	0
3	FYP	C	506	-	23,24,24	0.20	0	27,35,35	0.39	0
3	FYP	A	507	-	23,24,24	0.28	0	27,35,35	0.34	0
2	SO4	E	507	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	P9N	B	509	-	26,26,26	0.14	0	42,42,42	0.29	0
4	P9N	C	507	-	26,26,26	0.16	0	42,42,42	0.28	0
2	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.21	0
4	P9N	D	507	-	26,26,26	0.14	0	42,42,42	0.27	0
2	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.15	0
5	NAG	A	509	1	14,14,15	0.45	0	17,19,21	0.85	1 (5%)
2	SO4	B	506	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.12	0
5	NAG	B	511	1	14,14,15	0.49	0	17,19,21	0.88	1 (5%)
5	NAG	C	508	1	14,14,15	0.48	0	17,19,21	0.78	0
2	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.19	0
2	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.13	0
4	P9N	E	508	-	26,26,26	0.19	0	42,42,42	0.31	0
5	NAG	D	508	1	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
2	SO4	E	503	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	E	506	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	507	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	B	502	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	E	504	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	B	510	1	14,14,15	0.49	0	17,19,21	0.78	1 (5%)
2	SO4	E	505	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	E	502	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	505	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	505	-	4,4,4	0.24	0	6,6,6	0.07	0
3	FYP	E	501	-	23,24,24	0.28	0	27,35,35	0.41	0
2	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	E	509	1	14,14,15	0.47	0	17,19,21	0.75	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
3	FYP	A	507	-	-	4/7/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	510	1	-	1/6/23/26	0/1/1/1
5	NAG	B	511	1	-	1/6/23/26	0/1/1/1
4	P9N	B	509	-	-	0/4/62/62	0/4/4/4
4	P9N	E	508	-	-	0/4/62/62	0/4/4/4
5	NAG	C	508	1	-	1/6/23/26	0/1/1/1
4	P9N	C	507	-	-	0/4/62/62	0/4/4/4
5	NAG	D	508	1	-	1/6/23/26	0/1/1/1
4	P9N	D	507	-	-	0/4/62/62	0/4/4/4
3	FYP	E	501	-	-	2/7/23/23	0/3/3/3
3	FYP	D	506	-	-	0/7/23/23	0/3/3/3
4	P9N	A	508	-	-	0/4/62/62	0/4/4/4
5	NAG	A	509	1	-	1/6/23/26	0/1/1/1
5	NAG	E	509	1	-	0/6/23/26	0/1/1/1
3	FYP	B	508	-	-	0/7/23/23	0/3/3/3
3	FYP	C	506	-	-	0/7/23/23	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	509	NAG	C1-O5-C5	2.30	115.27	112.19
5	D	508	NAG	C1-O5-C5	2.25	115.21	112.19
5	B	511	NAG	C1-O5-C5	2.09	114.99	112.19
5	B	510	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

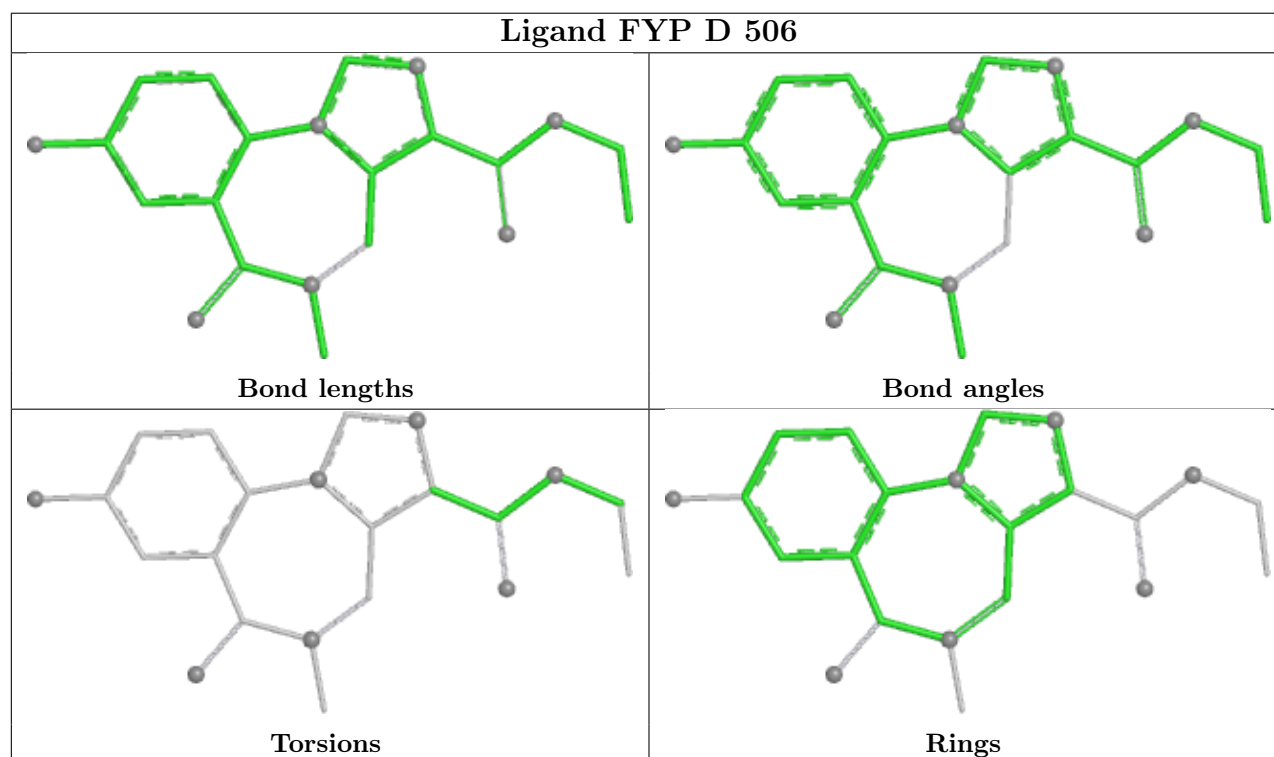
Mol	Chain	Res	Type	Atoms
3	E	501	FYP	C06-C04-O03-C02
5	B	511	NAG	O5-C5-C6-O6
5	D	508	NAG	O5-C5-C6-O6
5	B	510	NAG	O5-C5-C6-O6
5	C	508	NAG	O5-C5-C6-O6
3	E	501	FYP	O05-C04-O03-C02
3	A	507	FYP	O03-C04-C06-N16
3	A	507	FYP	O05-C04-C06-N16
3	A	507	FYP	O05-C04-C06-C07
5	A	509	NAG	C4-C5-C6-O6
3	A	507	FYP	O03-C04-C06-C07

There are no ring outliers.

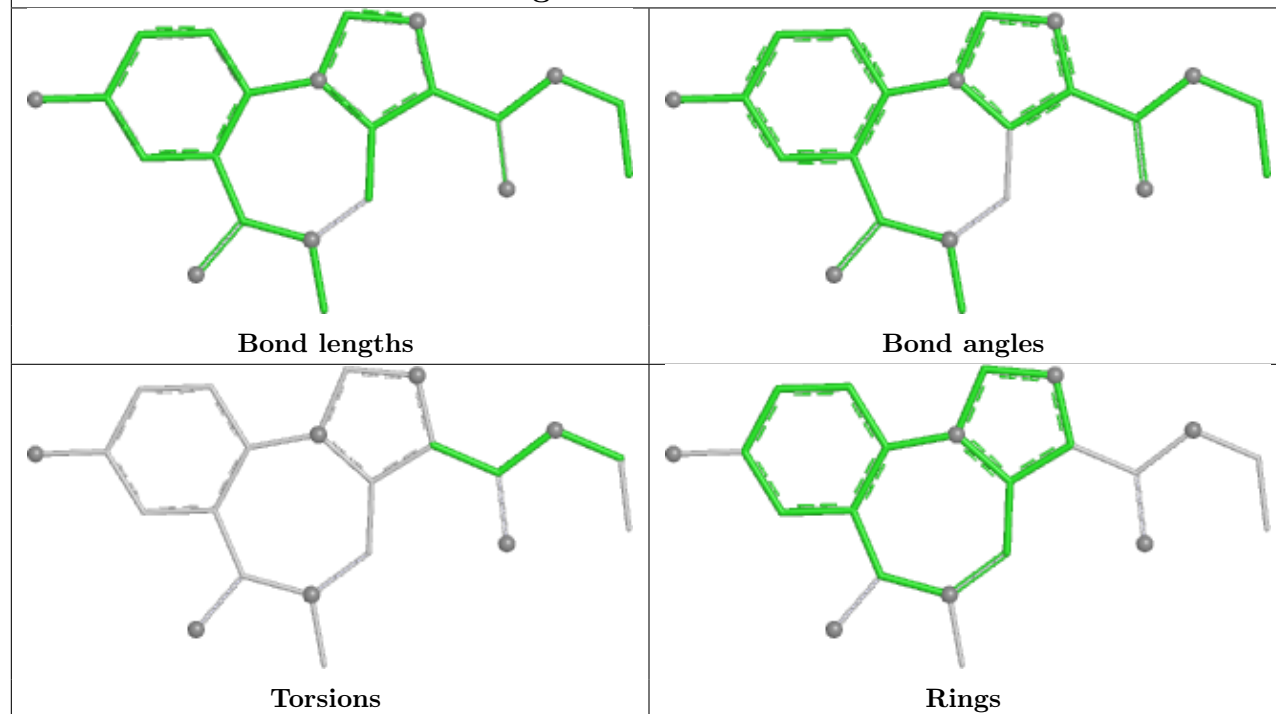
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	504	SO4	1	0
3	B	508	FYP	1	0
3	C	506	FYP	1	0
2	B	501	SO4	1	0
5	B	510	NAG	1	0
2	C	501	SO4	2	0
2	D	501	SO4	1	0

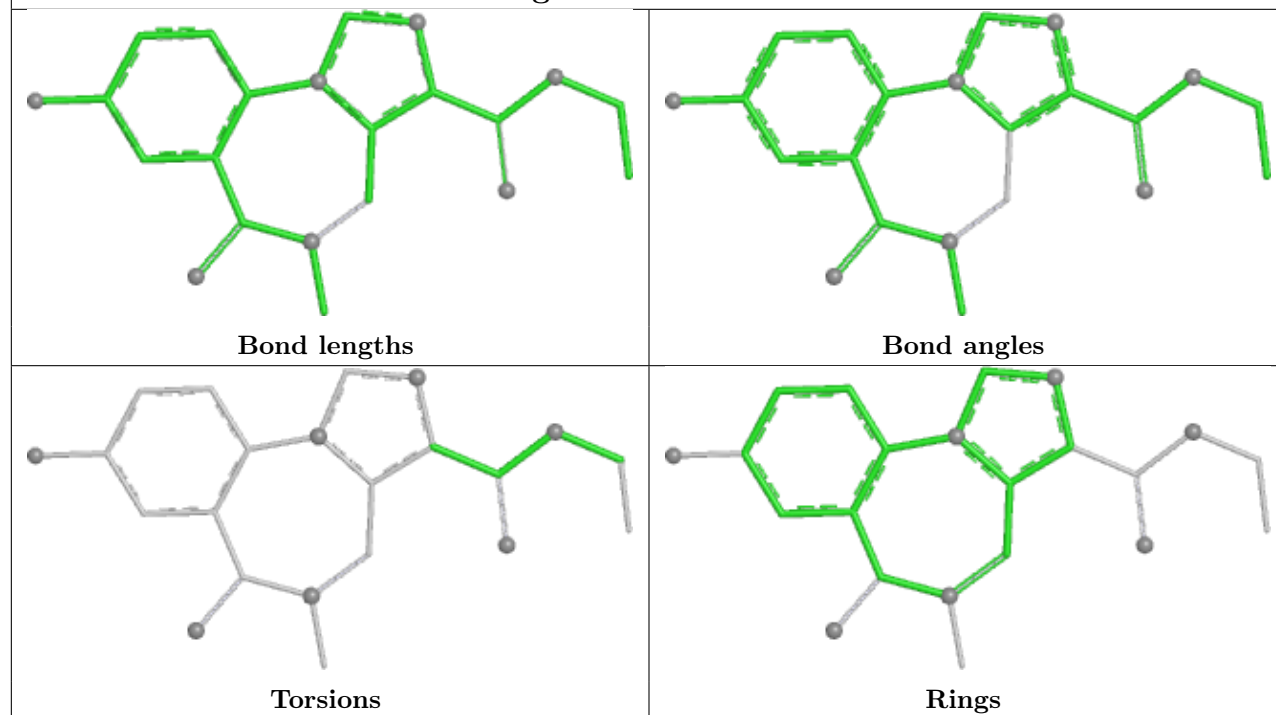
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

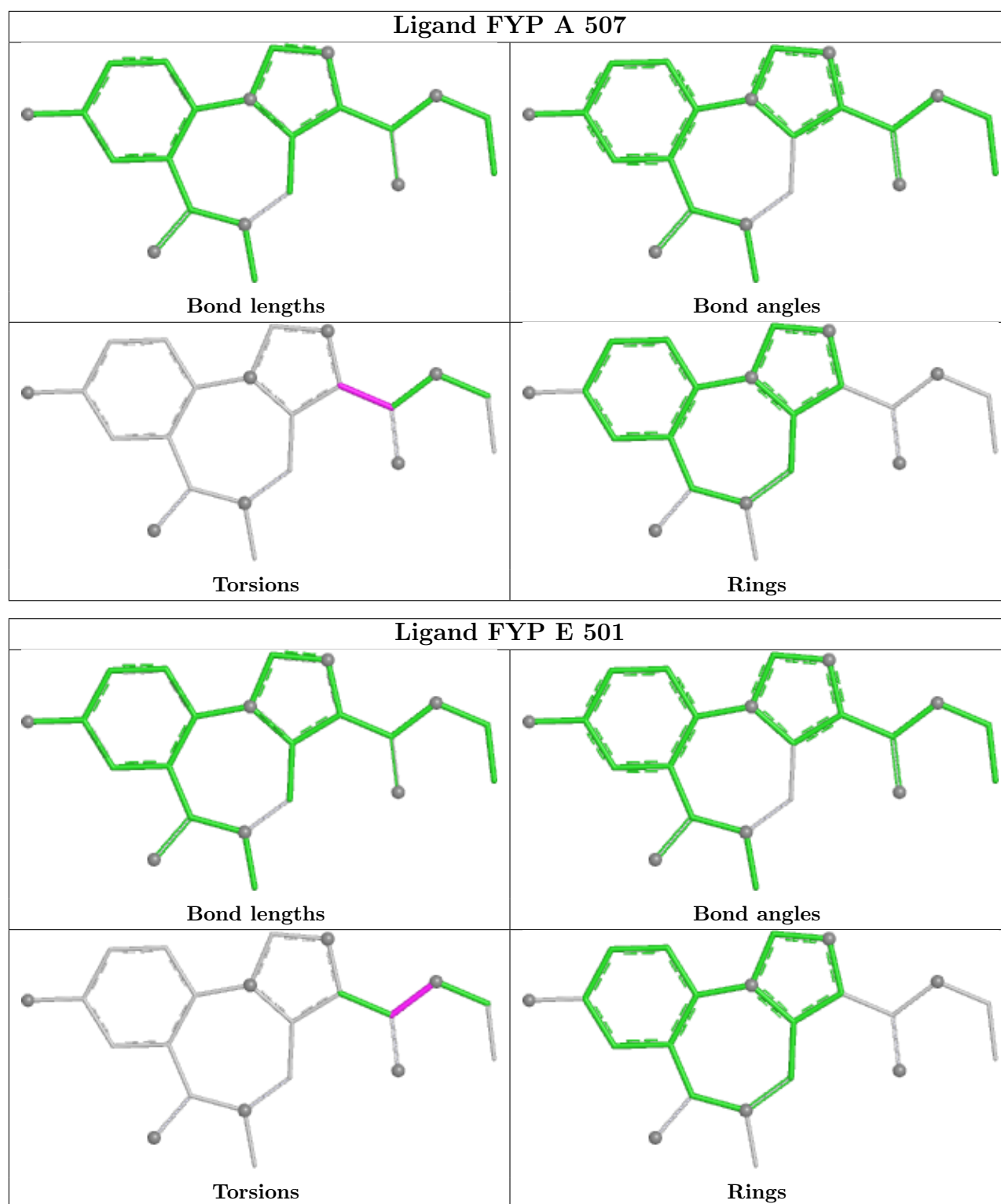


Ligand FYP B 508



Ligand FYP C 506





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	335/361 (92%)	1.22	61 (18%) 3 3	30, 63, 100, 125	0
1	B	335/361 (92%)	1.36	66 (19%) 3 2	32, 68, 110, 142	0
1	C	335/361 (92%)	1.54	94 (28%) 1 1	34, 84, 140, 164	0
1	D	335/361 (92%)	1.59	96 (28%) 1 1	33, 82, 130, 148	0
1	E	335/361 (92%)	1.43	78 (23%) 2 2	29, 71, 121, 142	0
All	All	1675/1805 (92%)	1.43	395 (23%) 2 1	29, 71, 127, 164	0

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	THR	13.5
1	D	18	PHE	8.5
1	D	84	MET	8.0
1	D	116	THR	7.8
1	D	187	ASP	7.7
1	A	218	ALA	7.6
1	B	117	THR	7.5
1	B	94	ALA	7.4
1	B	91	ASN	7.2
1	A	15	ILE	7.1
1	D	186	GLU	7.1
1	C	99	THR	7.0
1	C	158	LEU	6.8
1	C	116	THR	6.8
1	E	84	MET	6.7
1	B	93	VAL	6.6
1	B	122	LEU	6.5
1	B	89	LEU	6.5
1	C	73	TRP	6.5
1	B	90	ASP	6.4

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Mol	Chain	Res	Type	RSRZ
1	E	46	THR	6.3
1	E	87	LEU	6.3
1	C	78	LEU	6.2
1	E	38	GLY	5.9
1	D	122	LEU	5.8
1	C	93	VAL	5.8
1	C	118	PRO	5.7
1	B	78	LEU	5.7
1	A	50	VAL	5.6
1	C	98	TRP	5.6
1	E	189	SER	5.5
1	B	92	ARG	5.5
1	A	84	MET	5.4
1	E	37	LEU	5.4
1	A	18	PHE	5.3
1	C	165	TYR	5.2
1	D	165	TYR	5.2
1	C	89	LEU	5.1
1	C	122	LEU	4.9
1	D	17	ILE	4.9
1	B	95	ASP	4.9
1	E	39	GLU	4.9
1	C	100	PRO	4.8
1	A	184	VAL	4.8
1	B	115	MET	4.8
1	D	89	LEU	4.7
1	D	50	VAL	4.7
1	D	88	PRO	4.7
1	A	220	PHE	4.7
1	B	196	LEU	4.6
1	C	218	ALA	4.6
1	B	33	LEU	4.6
1	A	200	THR	4.6
1	C	18	PHE	4.5
1	C	220	PHE	4.5
1	E	280	LEU	4.5
1	D	87	LEU	4.5
1	C	132	TYR	4.5
1	C	200	THR	4.5
1	E	218	ALA	4.5
1	A	217	THR	4.5
1	D	230	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	158	LEU	4.4
1	E	47	ASP	4.4
1	C	74	LYS	4.4
1	B	37	LEU	4.3
1	E	89	LEU	4.2
1	B	221	HIS	4.2
1	B	118	PRO	4.2
1	E	215	ILE	4.1
1	E	226	ILE	4.1
1	A	53	PHE	4.1
1	B	291	TRP	4.1
1	E	132	TYR	4.1
1	C	83	PRO	4.0
1	C	198	GLY	4.0
1	A	87	LEU	4.0
1	A	284	ALA	4.0
1	E	112	ALA	4.0
1	E	124	ILE	4.0
1	D	118	PRO	4.0
1	C	130	VAL	3.9
1	D	49	TYR	3.9
1	B	18	PHE	3.9
1	C	84	MET	3.9
1	C	124	ILE	3.9
1	E	131	LEU	3.9
1	B	84	MET	3.8
1	C	167	ASN	3.8
1	D	119	ASN	3.8
1	C	217	THR	3.8
1	E	119	ASN	3.8
1	D	404	ILE	3.8
1	E	291	TRP	3.8
1	B	31	ASN	3.8
1	A	116	THR	3.8
1	C	16	THR	3.7
1	E	279	SER	3.7
1	C	119	ASN	3.7
1	A	92	ARG	3.7
1	B	189	SER	3.7
1	E	28	GLY	3.7
1	B	119	ASN	3.7
1	E	70	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	112	ALA	3.6
1	D	215	ILE	3.6
1	D	90	ASP	3.6
1	C	117	THR	3.6
1	D	42	THR	3.6
1	B	155	ASN	3.6
1	E	27	ASP	3.6
1	D	170	VAL	3.6
1	D	136	LEU	3.6
1	D	161	GLY	3.6
1	A	183	VAL	3.6
1	D	99	THR	3.6
1	C	207	SER	3.6
1	B	83	PRO	3.6
1	D	132	TYR	3.5
1	C	320	ARG	3.5
1	D	115	MET	3.5
1	C	87	LEU	3.5
1	B	38	GLY	3.5
1	E	204	GLU	3.5
1	C	15	ILE	3.5
1	E	69	PHE	3.5
1	A	24	GLY	3.4
1	D	15	ILE	3.4
1	E	18	PHE	3.4
1	A	182	VAL	3.4
1	D	405	LEU	3.4
1	D	53	PHE	3.4
1	C	419	ASN	3.4
1	A	159	LYS	3.4
1	E	33	LEU	3.4
1	E	158	LEU	3.3
1	A	46	THR	3.3
1	E	36	GLY	3.3
1	E	80	PHE	3.3
1	C	290	ASP	3.3
1	D	125	TRP	3.3
1	C	86	ARG	3.3
1	D	69	PHE	3.3
1	D	26	LEU	3.3
1	B	46	THR	3.3
1	B	97	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	69	PHE	3.3
1	E	200	THR	3.3
1	B	112	ALA	3.3
1	D	299	PHE	3.2
1	B	182	VAL	3.2
1	D	401	VAL	3.2
1	E	93	VAL	3.2
1	C	226	ILE	3.2
1	C	284	ALA	3.2
1	E	116	THR	3.2
1	E	187	ASP	3.2
1	D	33	LEU	3.2
1	C	285	TYR	3.2
1	A	227	GLY	3.2
1	D	407	GLY	3.2
1	D	47	ASP	3.1
1	D	114	GLY	3.1
1	D	320	ARG	3.1
1	D	78	LEU	3.1
1	A	133	THR	3.0
1	B	180	LYS	3.0
1	B	217	THR	3.0
1	C	286	ALA	3.0
1	D	168	SER	3.0
1	A	201	VAL	3.0
1	B	67	ILE	3.0
1	E	48	MET	3.0
1	E	165	TYR	3.0
1	C	136	LEU	3.0
1	E	26	LEU	3.0
1	E	78	LEU	3.0
1	E	277	ARG	3.0
1	B	215	ILE	3.0
1	C	67	ILE	3.0
1	C	170	VAL	3.0
1	E	118	PRO	3.0
1	A	165	TYR	3.0
1	E	178	SER	3.0
1	E	182	VAL	2.9
1	E	217	THR	2.9
1	C	95	ASP	2.9
1	E	90	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	114	GLY	2.9
1	C	115	MET	2.9
1	D	403	PRO	2.9
1	A	49	TYR	2.9
1	D	104	PHE	2.9
1	C	97	ILE	2.9
1	E	230	VAL	2.9
1	C	291	TRP	2.9
1	C	49	TYR	2.9
1	E	159	LYS	2.9
1	B	53	PHE	2.9
1	C	197	MET	2.9
1	D	402	PHE	2.9
1	E	211	GLY	2.9
1	C	215	ILE	2.8
1	B	200	THR	2.8
1	B	218	ALA	2.8
1	C	90	ASP	2.8
1	B	282	LYS	2.8
1	D	129	ARG	2.8
1	C	75	ASP	2.8
1	C	267	LEU	2.8
1	C	43	GLN	2.8
1	B	419	ASN	2.8
1	D	130	VAL	2.8
1	B	120	LYS	2.8
1	B	187	ASP	2.8
1	E	278	ASN	2.7
1	D	197	MET	2.7
1	A	186	GLU	2.7
1	C	219	HIS	2.7
1	D	406	PHE	2.7
1	A	118	PRO	2.7
1	B	132	TYR	2.7
1	E	176	ASN	2.7
1	A	219	HIS	2.7
1	D	159	LYS	2.7
1	E	167	ASN	2.7
1	D	37	LEU	2.7
1	D	93	VAL	2.7
1	C	319	ALA	2.7
1	D	64	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	67	ILE	2.6
1	D	68	PHE	2.6
1	C	131	LEU	2.6
1	E	122	LEU	2.6
1	C	209	SER	2.6
1	B	152	ASP	2.6
1	C	182	VAL	2.6
1	D	169	GLU	2.6
1	D	183	VAL	2.6
1	E	29	TYR	2.6
1	E	228	TYR	2.6
1	D	98	TRP	2.6
1	D	414	TRP	2.6
1	A	226	ILE	2.6
1	A	274	ILE	2.6
1	C	280	LEU	2.6
1	E	126	ASN	2.6
1	C	189	SER	2.6
1	C	282	LYS	2.6
1	A	197	MET	2.6
1	C	289	MET	2.6
1	C	53	PHE	2.6
1	B	238	ILE	2.5
1	C	17	ILE	2.5
1	D	214	THR	2.5
1	D	275	SER	2.5
1	D	190	ARG	2.5
1	E	115	MET	2.5
1	D	146	LEU	2.5
1	B	96	GLN	2.5
1	A	115	MET	2.5
1	D	134	MET	2.5
1	D	127	ASP	2.5
1	D	91	ASN	2.5
1	D	303	ALA	2.5
1	C	188	GLY	2.5
1	D	234	TYR	2.5
1	C	174	TRP	2.5
1	A	419	ASN	2.5
1	C	278	ASN	2.5
1	C	211	GLY	2.4
1	C	301	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	291	TRP	2.4
1	E	40	ARG	2.4
1	D	419	ASN	2.4
1	E	419	ASN	2.4
1	D	28	GLY	2.4
1	D	29	TYR	2.4
1	E	219	HIS	2.4
1	D	103	PHE	2.4
1	E	289	MET	2.4
1	D	70	ALA	2.4
1	D	117	THR	2.4
1	E	150	PRO	2.4
1	E	209	SER	2.4
1	C	159	LYS	2.4
1	A	78	LEU	2.4
1	B	267	LEU	2.4
1	D	43	GLN	2.4
1	B	48	MET	2.4
1	C	214	THR	2.4
1	E	83	PRO	2.4
1	E	238	ILE	2.4
1	B	47	ASP	2.4
1	C	22	LEU	2.4
1	D	160	PHE	2.4
1	A	171	VAL	2.4
1	A	255	VAL	2.4
1	B	99	THR	2.3
1	C	179	THR	2.3
1	A	198	GLY	2.3
1	E	129	ARG	2.3
1	A	268	THR	2.3
1	A	33	LEU	2.3
1	B	124	ILE	2.3
1	C	187	ASP	2.3
1	B	295	VAL	2.3
1	A	278	ASN	2.3
1	A	16	THR	2.3
1	A	22	LEU	2.3
1	D	74	LYS	2.3
1	C	173	VAL	2.3
1	C	112	ALA	2.3
1	D	86	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	45	ARG	2.3
1	A	114	GLY	2.3
1	C	138	ILE	2.3
1	C	48	MET	2.3
1	B	69	PHE	2.3
1	D	24	GLY	2.2
1	E	82	GLY	2.2
1	B	15	ILE	2.2
1	C	26	LEU	2.2
1	D	81	LYS	2.2
1	E	275	SER	2.2
1	A	310	VAL	2.2
1	B	88	PRO	2.2
1	C	171	VAL	2.2
1	D	34	ARG	2.2
1	D	135	ARG	2.2
1	B	219	HIS	2.2
1	C	221	HIS	2.2
1	E	404	ILE	2.2
1	C	40	ARG	2.2
1	A	313	PHE	2.2
1	C	35	PRO	2.2
1	B	268	THR	2.2
1	A	152	ASP	2.2
1	D	95	ASP	2.2
1	A	301	PHE	2.2
1	E	31	ASN	2.2
1	A	312	TYR	2.2
1	E	233	THR	2.2
1	E	227	GLY	2.2
1	C	41	ILE	2.2
1	A	253	GLU	2.2
1	D	83	PRO	2.2
1	D	282	LYS	2.2
1	C	283	VAL	2.1
1	E	85	GLN	2.1
1	A	316	SER	2.1
1	A	320	ARG	2.1
1	B	209	SER	2.1
1	C	34	ARG	2.1
1	D	162	SER	2.1
1	E	34	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	184	VAL	2.1
1	C	50	VAL	2.1
1	D	131	LEU	2.1
1	C	76	GLU	2.1
1	D	23	ASP	2.1
1	C	80	PHE	2.1
1	A	93	VAL	2.1
1	A	37	LEU	2.1
1	B	87	LEU	2.1
1	E	86	ARG	2.1
1	A	17	ILE	2.1
1	B	65	ILE	2.1
1	D	97	ILE	2.1
1	D	226	ILE	2.1
1	E	49	TYR	2.1
1	B	159	LYS	2.1
1	A	221	HIS	2.1
1	C	160	PHE	2.1
1	A	286	ALA	2.1
1	A	414	TRP	2.1
1	A	190	ARG	2.1
1	C	79	ARG	2.1
1	B	74	LYS	2.1
1	E	130	VAL	2.0
1	A	70	ALA	2.0
1	B	125	TRP	2.0
1	D	67	ILE	2.0
1	D	233	THR	2.0
1	C	29	TYR	2.0
1	E	100	PRO	2.0
1	C	121	MET	2.0
1	D	71	GLN	2.0
1	D	96	GLN	2.0
1	A	235	LEU	2.0
1	B	298	ALA	2.0
1	D	253	GLU	2.0
1	E	212	GLU	2.0
1	B	231	ILE	2.0
1	D	73	TRP	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
5	NAG	C	508	14/15	0.40	0.20	92,101,121,123	0
5	NAG	D	508	14/15	0.58	0.17	102,107,129,129	0
2	SO4	A	505	5/5	0.63	0.16	92,96,101,102	0
2	SO4	B	501	5/5	0.64	0.16	74,77,81,84	0
2	SO4	E	507	5/5	0.65	0.19	76,77,83,88	0
2	SO4	E	503	5/5	0.71	0.15	64,67,72,76	0
2	SO4	D	505	5/5	0.71	0.24	79,82,86,92	0
2	SO4	B	505	5/5	0.73	0.13	89,90,92,92	0
2	SO4	D	502	5/5	0.74	0.20	58,63,68,70	0
5	NAG	A	509	14/15	0.74	0.18	74,81,96,97	0
2	SO4	A	502	5/5	0.74	0.13	62,70,74,77	0
2	SO4	C	505	5/5	0.74	0.20	81,83,95,98	0
2	SO4	D	503	5/5	0.75	0.16	68,70,77,78	0
2	SO4	E	502	5/5	0.76	0.17	79,83,88,93	0
2	SO4	C	502	5/5	0.77	0.13	63,65,70,73	0
2	SO4	B	507	5/5	0.78	0.14	85,86,89,91	0
5	NAG	B	510	14/15	0.79	0.14	74,83,98,103	0
2	SO4	B	502	5/5	0.80	0.12	59,60,64,67	0
5	NAG	B	511	14/15	0.80	0.14	72,79,94,95	0
2	SO4	D	501	5/5	0.81	0.20	85,86,89,91	0
2	SO4	C	501	5/5	0.81	0.15	88,90,96,99	0
2	SO4	A	504	5/5	0.82	0.11	68,71,75,76	0
2	SO4	A	501	5/5	0.83	0.14	70,74,78,83	0
2	SO4	C	503	5/5	0.83	0.16	74,78,83,84	0
2	SO4	B	506	5/5	0.83	0.15	66,68,73,75	0
2	SO4	A	506	5/5	0.84	0.22	67,70,85,88	0
5	NAG	E	509	14/15	0.84	0.12	93,97,116,116	0

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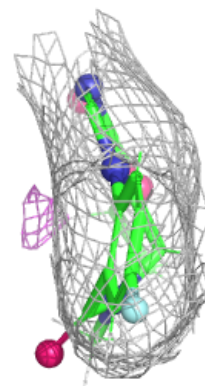
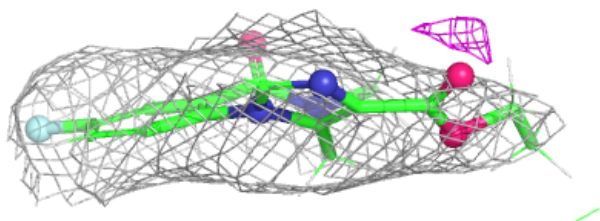
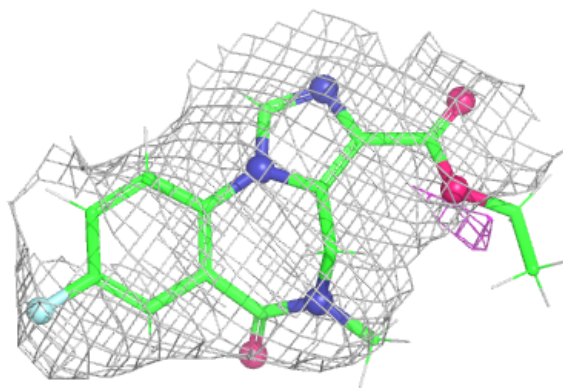
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	E	505	5/5	0.85	0.13	67,68,73,76	0
3	FYP	E	501	22/22	0.85	0.19	82,86,105,105	0
3	FYP	B	508	22/22	0.86	0.17	61,65,80,80	0
2	SO4	E	506	5/5	0.87	0.20	68,70,78,83	0
2	SO4	E	504	5/5	0.88	0.21	66,69,72,76	0
2	SO4	B	504	5/5	0.89	0.14	77,80,81,84	0
2	SO4	A	503	5/5	0.89	0.15	58,59,65,69	0
3	FYP	C	506	22/22	0.90	0.17	61,73,87,90	0
4	P9N	E	508	23/23	0.90	0.12	39,48,51,55	0
2	SO4	D	504	5/5	0.91	0.11	83,83,88,91	0
4	P9N	A	508	23/23	0.91	0.12	31,39,44,46	0
2	SO4	B	503	5/5	0.91	0.15	66,67,72,75	0
3	FYP	D	506	22/22	0.92	0.12	88,89,111,111	0
2	SO4	C	504	5/5	0.92	0.13	88,89,92,93	0
4	P9N	D	507	23/23	0.93	0.10	37,47,51,52	0
4	P9N	C	507	23/23	0.93	0.11	33,40,46,46	0
4	P9N	B	509	23/23	0.94	0.09	33,42,46,47	0
3	FYP	A	507	22/22	0.94	0.13	58,62,77,77	0

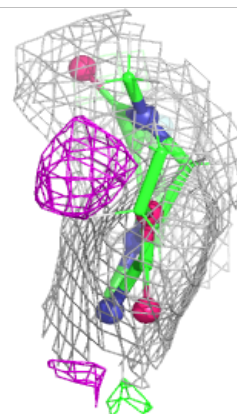
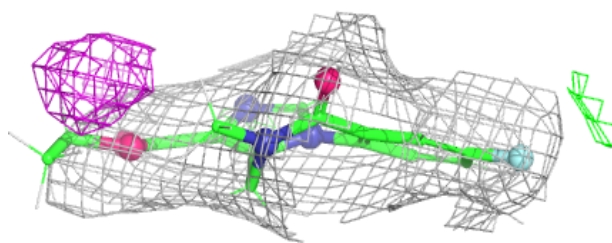
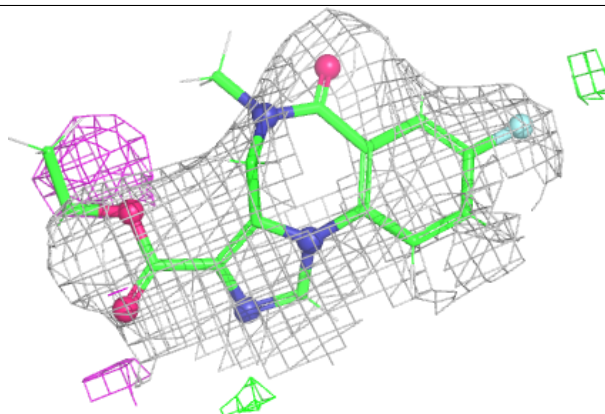
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FYP E 501:

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

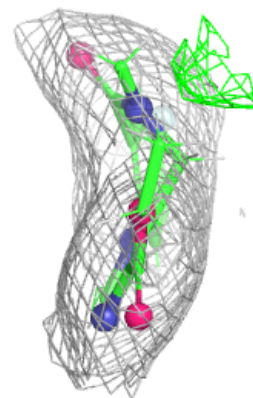
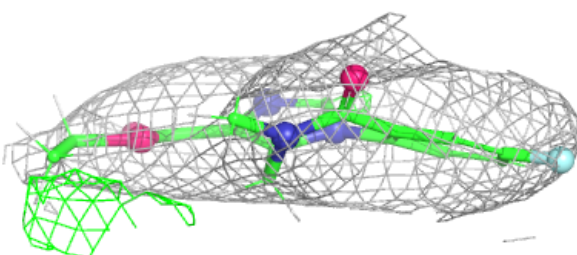
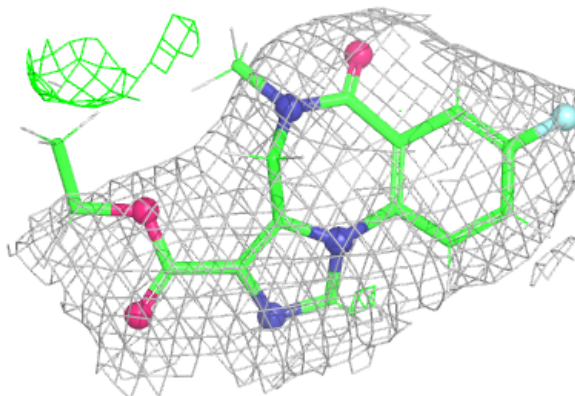
**Electron density around FYP B 508:**

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

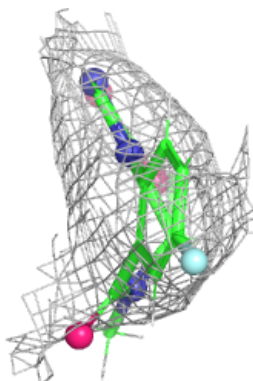
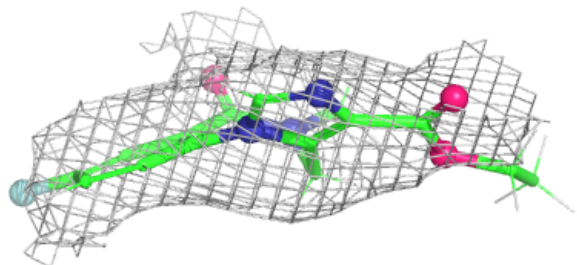
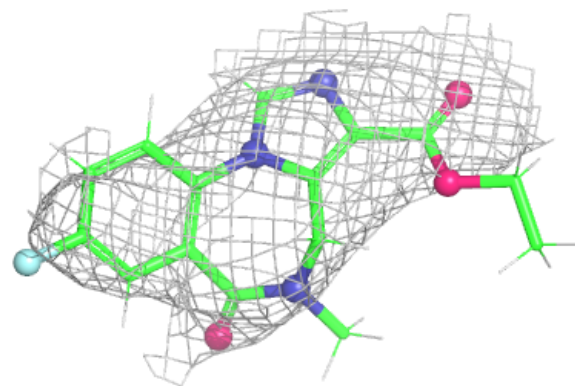


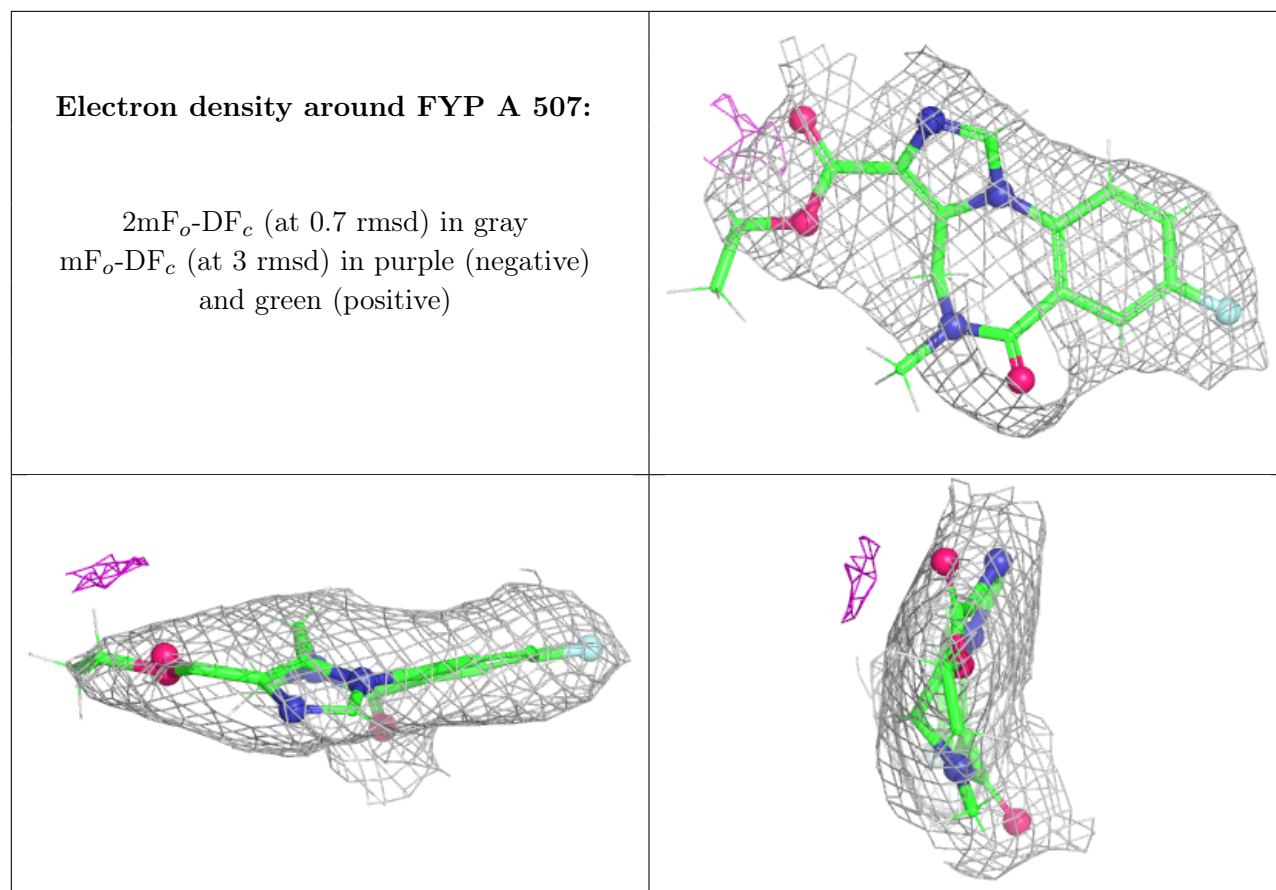
Electron density around FYP C 506:

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

**Electron density around FYP D 506:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.