



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:25 PM UTC

PDB ID : 9XYL / pdb_00009xyl
Title : Human prolyl endopeptidase (PREP) - complex with S17092
Authors : Fucci, I.J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-26
Resolution : 1.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

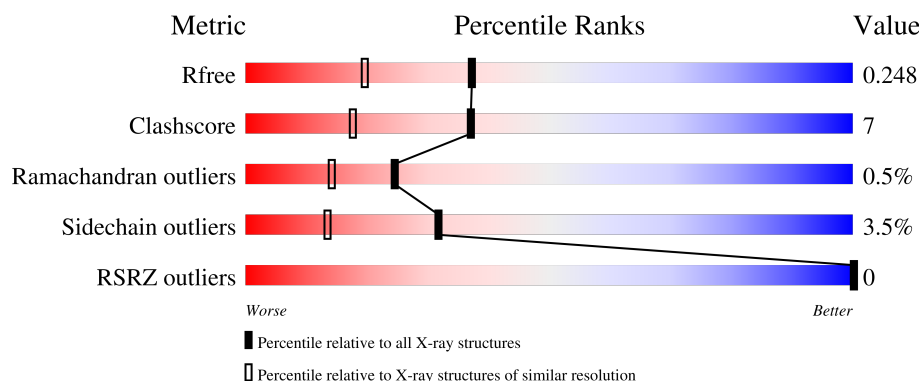
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	711	 77% 19% ...
1	B	711	 75% 20% ...
1	C	711	 76% 20% ...
1	D	711	 74% 22% ...
1	E	711	 72% 23% 5% ...

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Mol	Chain	Length	Quality of chain
1	F	711	 74% 21%

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
4	SCN	A	805	-	-	X	-
4	SCN	C	805	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 69507 atoms, of which 33414 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.

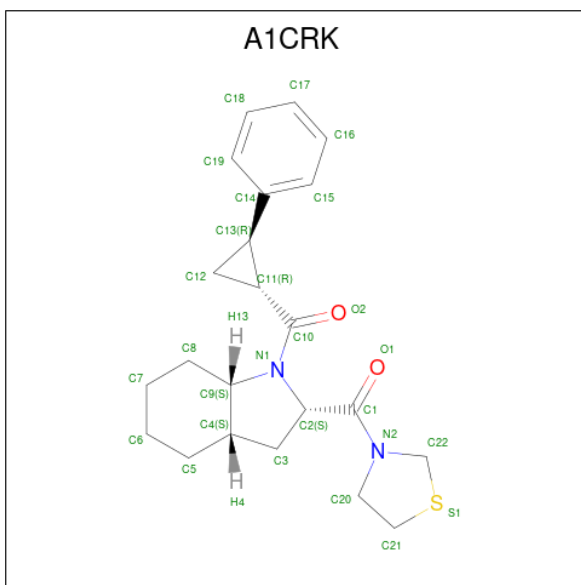
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	707	Total	C	H	N	O	S	178	3	0
			11229	3651	5538	943	1070	27			
1	B	707	Total	C	H	N	O	S	177	0	0
			11187	3639	5514	941	1066	27			
1	C	707	Total	C	H	N	O	S	177	0	0
			11187	3639	5514	941	1066	27			
1	D	707	Total	C	H	N	O	S	177	1	0
			11199	3643	5520	941	1068	27			
1	E	707	Total	C	H	N	O	S	177	0	0
			11187	3639	5514	941	1066	27			
1	F	707	Total	C	H	N	O	S	177	0	0
			11187	3639	5514	941	1066	27			

There are 6 discrepancies between the modelled and reference sequences:

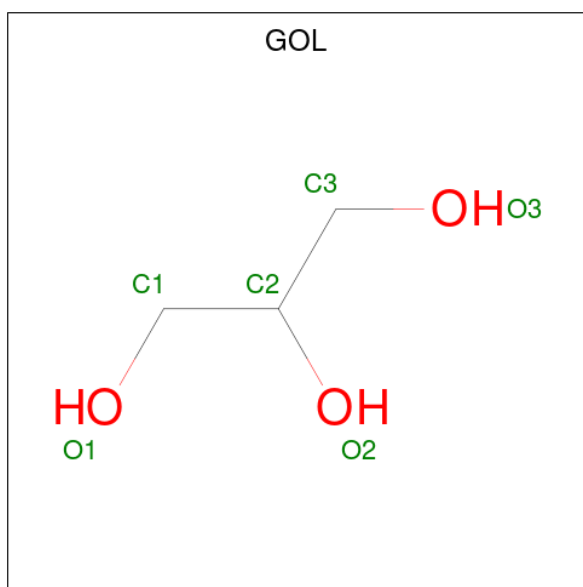
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P48147
B	1	GLY	-	expression tag	UNP P48147
C	1	GLY	-	expression tag	UNP P48147
D	1	GLY	-	expression tag	UNP P48147
E	1	GLY	-	expression tag	UNP P48147
F	1	GLY	-	expression tag	UNP P48147

- Molecule 2 is {(2S,3aS,7aS)-1-[(1R,2R)-2-phenylcyclopropane-1-carbonyl]octahydro-1H-indol-2-yl}(1,3-thiazolidin-3-yl)methanone (CCD ID: A1CRK) (formula: C₂₂H₂₈N₂O₂S) (labeled as "Ligand of Interest" by depositor).



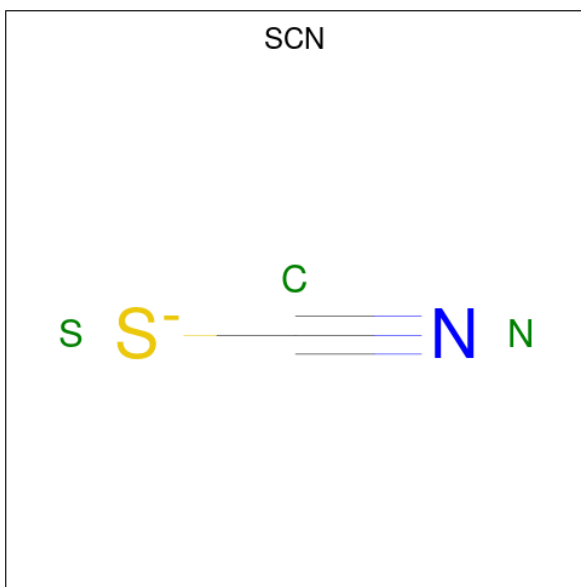
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			55	22	28	2	2	1		
2	B	1	Total	C	H	N	O	S	0	0
			55	22	28	2	2	1		
2	C	1	Total	C	H	N	O	S	0	0
			55	22	28	2	2	1		
2	D	1	Total	C	H	N	O	S	0	0
			55	22	28	2	2	1		
2	E	1	Total	C	H	N	O	S	0	0
			55	22	28	2	2	1		
2	F	1	Total	C	H	N	O	S	0	0
			55	22	28	2	2	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



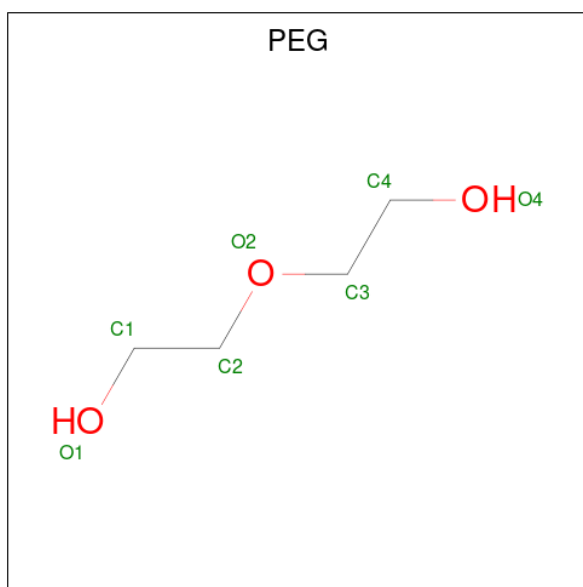
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	C	1	Total	C	H	O	3	0
			14	3	8	3		
3	C	1	Total	C	H	O	3	0
			14	3	8	3		
3	D	1	Total	C	H	O	3	0
			14	3	8	3		
3	E	1	Total	C	H	O	3	0
			14	3	8	3		
3	E	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 4 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



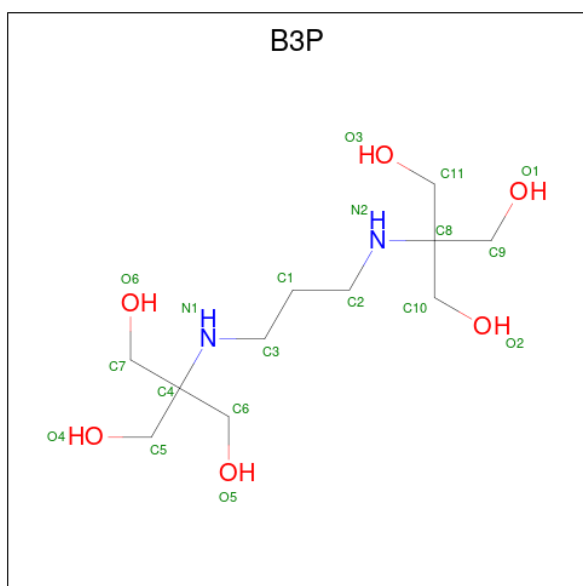
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		
4	C	1	Total	C	N	S	0	0
			3	1	1	1		
4	C	1	Total	C	N	S	0	0
			3	1	1	1		
4	D	1	Total	C	N	S	0	0
			3	1	1	1		
4	E	1	Total	C	N	S	0	0
			3	1	1	1		
4	E	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	2	0
			17	4	10	3		

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	8	0
			45	11	26	2	6		

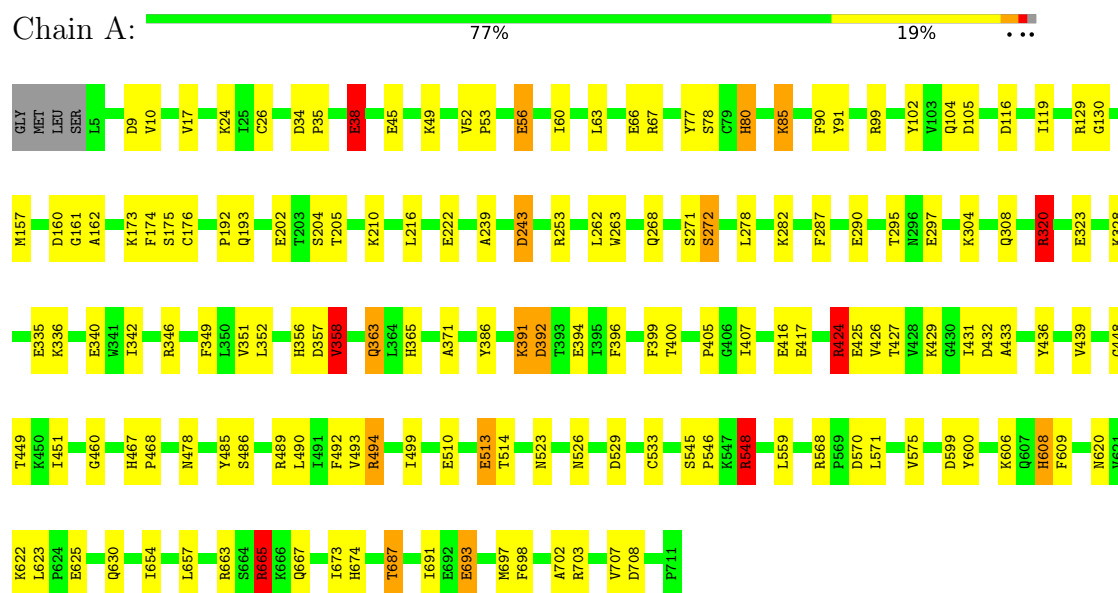
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	343	Total 345	O 345	0	2
7	B	328	Total 328	O 328	0	0
7	C	325	Total 325	O 325	0	0
7	D	246	Total 246	O 246	0	0
7	E	226	Total 226	O 226	0	0
7	F	279	Total 280	O 280	0	1

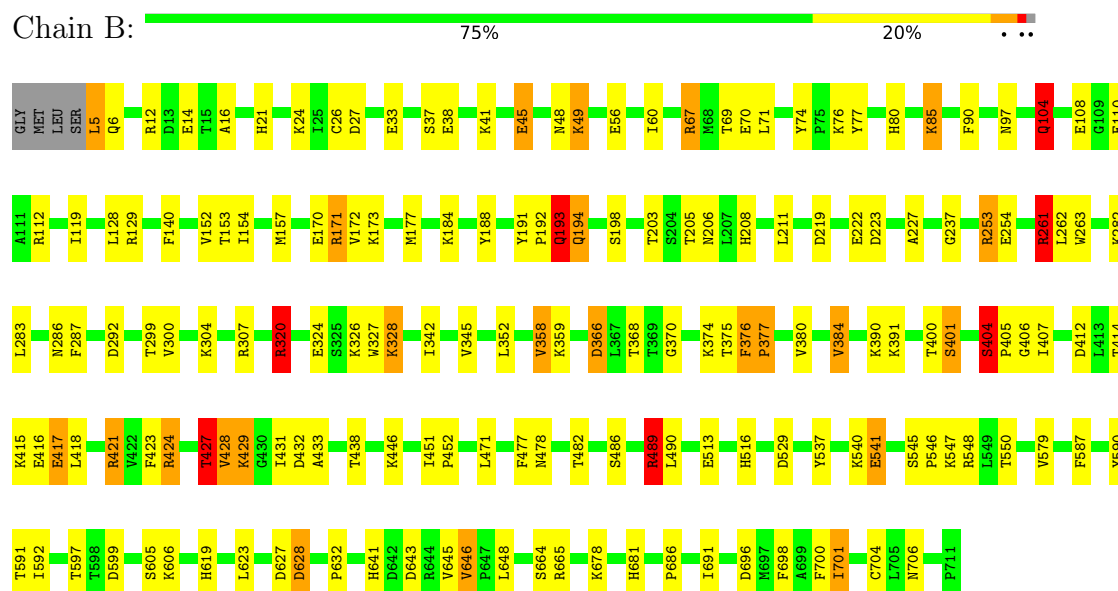
3 Residue-property plots

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: Prolyl endopeptidase

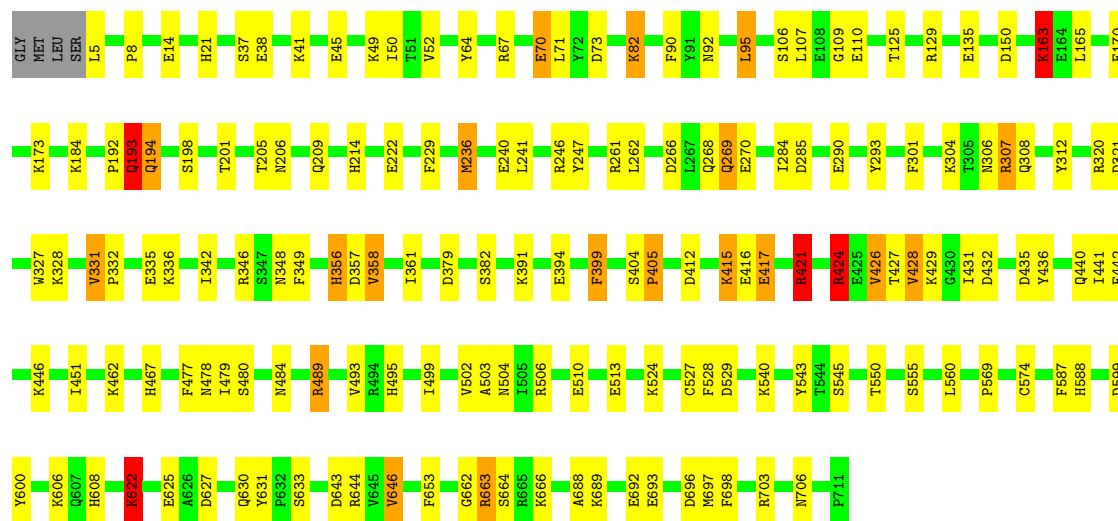


• Molecule 1: Prolyl endopeptidase



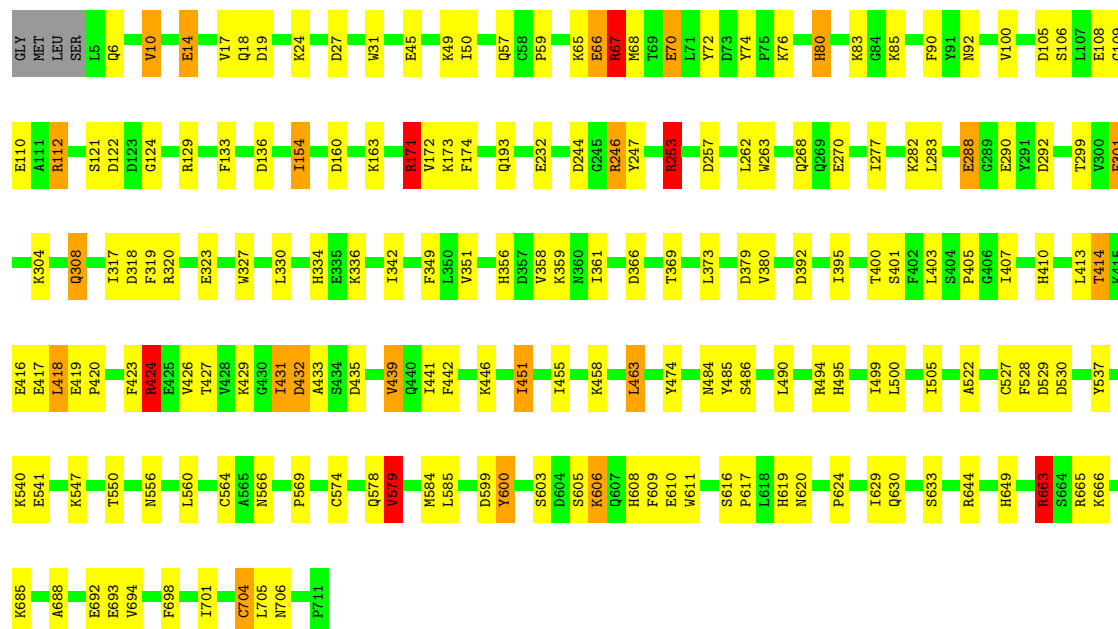
- Molecule 1: Prolyl endopeptidase

Chain C:  76% 20% . . .



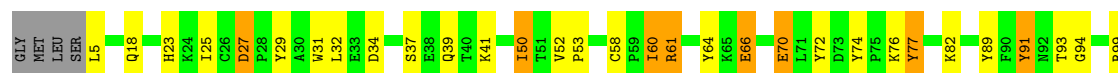
- Molecule 1: Prolyl endopeptidase

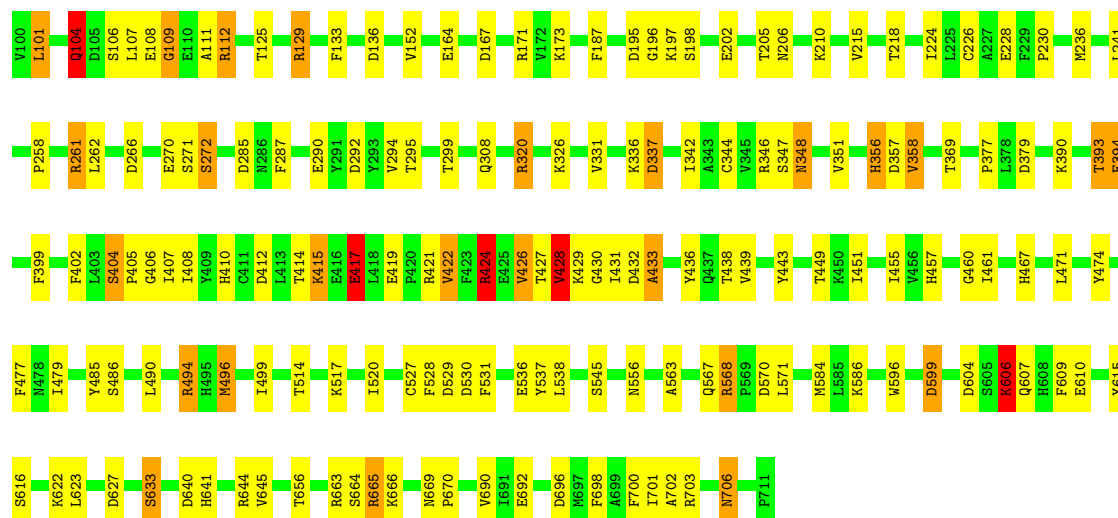
Chain D:  74% 22% . . .



- Molecule 1: Prolyl endopeptidase

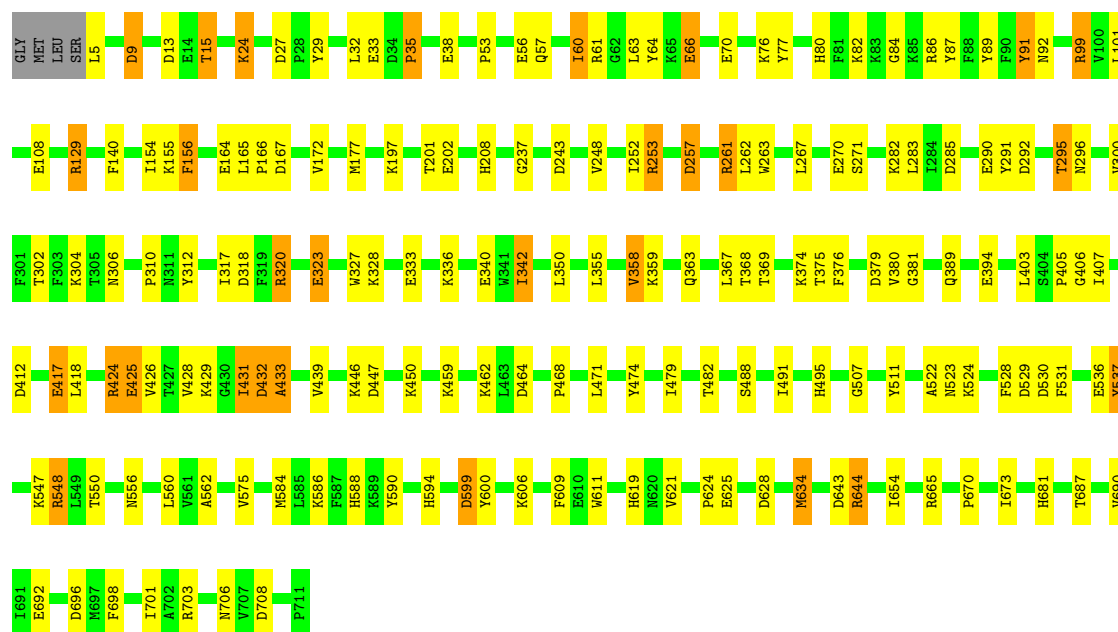
Chain E:  72% 23% 5% . . .





● Molecule 1: Prolyl endopeptidase

Chain F: 74% 21% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.19Å 105.73Å 155.67Å 81.78° 89.79° 89.70°	Depositor
Resolution (Å)	29.68 – 1.81 29.68 – 1.81	Depositor EDS
% Data completeness (in resolution range)	74.1 (29.68-1.81) 74.1 (29.68-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.191 , 0.249 0.190 , 0.248	Depositor DCC
R_{free} test set	16444 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.135 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	69507	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% 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: PEG, GOL, SCN, B3P, A1CRK

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	1.08	3/5849 (0.1%)	1.62	69/7929 (0.9%)
1	B	1.12	5/5825 (0.1%)	1.68	96/7897 (1.2%)
1	C	1.07	6/5825 (0.1%)	1.67	85/7897 (1.1%)
1	D	1.00	4/5834 (0.1%)	1.63	68/7909 (0.9%)
1	E	0.98	4/5825 (0.1%)	1.63	86/7897 (1.1%)
1	F	1.02	3/5825 (0.1%)	1.67	95/7897 (1.2%)
All	All	1.04	25/34983 (0.1%)	1.65	499/47426 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	7
1	D	0	8
1	E	0	8
1	F	0	5
All	All	0	44

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	SER	CA-CB	-7.53	1.43	1.53
1	B	681	HIS	CE1-NE2	-7.48	1.25	1.32
1	D	649	HIS	ND1-CE1	7.01	1.39	1.32
1	A	467	HIS	CG-CD2	6.97	1.43	1.35
1	C	480	SER	CA-CB	-6.84	1.43	1.53

The worst 5 of 499 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	GLN	N-CA-CB	-13.77	87.80	109.69
1	B	193	GLN	CB-CA-C	12.26	134.83	110.42
1	A	548	ARG	CG-CD-NE	-10.81	88.22	112.00
1	D	424	ARG	CB-CA-C	-10.71	92.44	110.43
1	D	193	GLN	CB-CA-C	10.51	126.63	109.70

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain
1	A	239	ALA	Peptide
1	A	253	ARG	Sidechain
1	A	320	ARG	Sidechain
1	A	548	ARG	Sidechain

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	5691	5538	5515	72	0
1	B	5673	5514	5491	69	0
1	C	5673	5514	5491	71	1
1	D	5679	5520	5497	81	0
1	E	5673	5514	5491	107	0
1	F	5673	5514	5491	85	1
2	A	27	28	0	0	0
2	B	27	28	0	0	0
2	C	27	28	0	1	0
2	D	27	28	0	0	0
2	E	27	28	0	2	0
2	F	27	28	0	0	0
3	A	24	32	32	3	0
3	B	18	24	24	1	0
3	C	12	16	16	3	0
3	D	6	8	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	12	16	16	0	0
4	A	3	0	0	2	0
4	B	3	0	0	0	0
4	C	6	0	0	2	0
4	D	3	0	0	0	0
4	E	6	0	0	1	0
5	A	7	10	10	3	0
6	C	19	26	26	0	0
7	A	345	0	0	10	0
7	B	328	0	0	6	0
7	C	325	0	0	7	0
7	D	246	0	0	5	0
7	E	226	0	0	7	0
7	F	280	0	0	7	0
All	All	36093	33414	33108	478	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 7.

The worst 5 of 478 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:C:67:ARG:HD2	7:C:1090:HOH:O	1.50	1.12
1:E:58:CYS:HB3	7:E:1059:HOH:O	1.55	1.05
1:B:85:LYS:HB2	7:B:1085:HOH:O	1.63	0.98
1:C:67:ARG:CD	7:C:1090:HOH:O	2.09	0.91
1:E:346:ARG:HH21	1:E:348:ASN:HD21	1.17	0.90

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:C:198:SER:HG	1:F:24:LYS:HZ3[1_636]	1.31	0.29

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	708/711 (100%)	680 (96%)	27 (4%)	1 (0%)	48	38
1	B	705/711 (99%)	680 (96%)	21 (3%)	4 (1%)	21	11
1	C	705/711 (99%)	672 (95%)	29 (4%)	4 (1%)	21	11
1	D	706/711 (99%)	669 (95%)	32 (4%)	5 (1%)	18	8
1	E	705/711 (99%)	664 (94%)	37 (5%)	4 (1%)	21	11
1	F	705/711 (99%)	671 (95%)	31 (4%)	3 (0%)	30	19
All	All	4234/4266 (99%)	4036 (95%)	177 (4%)	21 (0%)	24	14

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	VAL
1	C	193	GLN
1	E	109	GLY
1	F	433	ALA
1	B	358	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	617/617 (100%)	589 (96%)	28 (4%)	24	8
1	B	614/617 (100%)	593 (97%)	21 (3%)	32	14
1	C	614/617 (100%)	597 (97%)	17 (3%)	38	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	615/617 (100%)	588 (96%)	27 (4%)	25 9
1	E	614/617 (100%)	590 (96%)	24 (4%)	28 11
1	F	614/617 (100%)	599 (98%)	15 (2%)	43 27
All	All	3688/3702 (100%)	3556 (96%)	132 (4%)	32 13

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	665	ARG
1	F	60	ILE
1	F	547	LYS
1	B	678	LYS
1	B	605	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	552	ASN
1	E	478	ASN
1	D	556	ASN
1	E	194	GLN
1	F	80	HIS

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

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	806	-	5,5,5	0.19	0	5,5,5	0.45	0
3	GOL	E	804	-	5,5,5	0.23	0	5,5,5	0.55	0
2	A1CRK	B	801	-	31,31,31	0.87	1 (3%)	42,45,45	1.27	8 (19%)
3	GOL	C	804	-	5,5,5	0.60	0	5,5,5	1.28	1 (20%)
3	GOL	B	805	-	5,5,5	0.30	0	5,5,5	0.47	0
2	A1CRK	A	801	-	31,31,31	0.77	0	42,45,45	1.04	2 (4%)
3	GOL	E	805	-	5,5,5	0.31	0	5,5,5	0.61	0
3	GOL	C	803	-	5,5,5	0.70	0	5,5,5	1.87	1 (20%)
4	SCN	E	802	-	1,2,2	0.59	0	0,1,1	-	-
3	GOL	A	803	-	5,5,5	0.48	0	5,5,5	0.82	0
4	SCN	B	803	-	1,2,2	2.95	1 (100%)	0,1,1	-	-
4	SCN	D	803	-	1,2,2	0.78	0	0,1,1	-	-
3	GOL	A	802	-	5,5,5	0.29	0	5,5,5	0.46	0
2	A1CRK	D	801	-	31,31,31	0.90	1 (3%)	42,45,45	1.50	7 (16%)
6	B3P	C	801	-	18,18,18	0.96	1 (5%)	23,23,23	0.94	2 (8%)
4	SCN	A	805	-	1,2,2	0.45	0	0,1,1	-	-
2	A1CRK	E	801	-	31,31,31	0.90	1 (3%)	42,45,45	1.40	6 (14%)
4	SCN	E	803	-	1,2,2	0.13	0	0,1,1	-	-
4	SCN	C	806	-	1,2,2	0.63	0	0,1,1	-	-
2	A1CRK	C	802	-	31,31,31	1.22	4 (12%)	42,45,45	1.84	7 (16%)
3	GOL	D	802	-	5,5,5	0.21	0	5,5,5	0.34	0
5	PEG	A	807	-	6,6,6	1.06	1 (16%)	5,5,5	0.76	0
3	GOL	B	804	-	5,5,5	0.12	0	5,5,5	0.32	0
2	A1CRK	F	801	-	31,31,31	1.23	2 (6%)	42,45,45	1.29	4 (9%)
3	GOL	A	804	-	5,5,5	0.33	0	5,5,5	0.93	0
3	GOL	B	802	-	5,5,5	0.26	0	5,5,5	0.61	0
4	SCN	C	805	-	1,2,2	0.20	0	0,1,1	-	-

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	GOL	A	806	-	-	2/4/4/4	-
3	GOL	E	804	-	-	0/4/4/4	-
2	A1CRK	B	801	-	-	0/20/55/55	0/5/5/5
3	GOL	C	804	-	-	4/4/4/4	-
3	GOL	B	805	-	-	3/4/4/4	-
2	A1CRK	A	801	-	-	0/20/55/55	0/5/5/5
3	GOL	E	805	-	-	4/4/4/4	-
3	GOL	C	803	-	-	3/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
2	A1CRK	D	801	-	-	0/20/55/55	0/5/5/5
6	B3P	C	801	-	-	3/28/28/28	-
2	A1CRK	E	801	-	-	4/20/55/55	0/5/5/5
2	A1CRK	C	802	-	-	1/20/55/55	0/5/5/5
3	GOL	D	802	-	-	2/4/4/4	-
5	PEG	A	807	-	-	4/4/4/4	-
3	GOL	B	804	-	-	2/4/4/4	-
2	A1CRK	F	801	-	-	0/20/55/55	0/5/5/5
3	GOL	A	804	-	-	2/4/4/4	-
3	GOL	B	802	-	-	0/4/4/4	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	A1CRK	O1-C1	5.04	1.31	1.22
2	C	802	A1CRK	C21-C20	-4.19	1.39	1.51
2	F	801	A1CRK	O2-C10	-3.02	1.17	1.22
4	B	803	SCN	C-N	2.95	1.25	1.15
2	C	802	A1CRK	O2-C10	2.78	1.27	1.22

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	A1CRK	S1-C22-N2	-7.23	96.20	105.51
2	C	802	A1CRK	C20-N2-C1	-4.86	107.16	124.03
2	F	801	A1CRK	C6-C7-C8	-4.49	102.19	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	801	A1CRK	S1-C22-N2	-4.44	99.79	105.51
2	D	801	A1CRK	C21-C20-N2	3.90	114.90	107.13

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	802	A1CRK	O1-C1-N2-C22
2	E	801	A1CRK	O1-C1-N2-C20
2	E	801	A1CRK	O1-C1-N2-C22
2	E	801	A1CRK	C2-C1-N2-C20
2	E	801	A1CRK	C2-C1-N2-C22

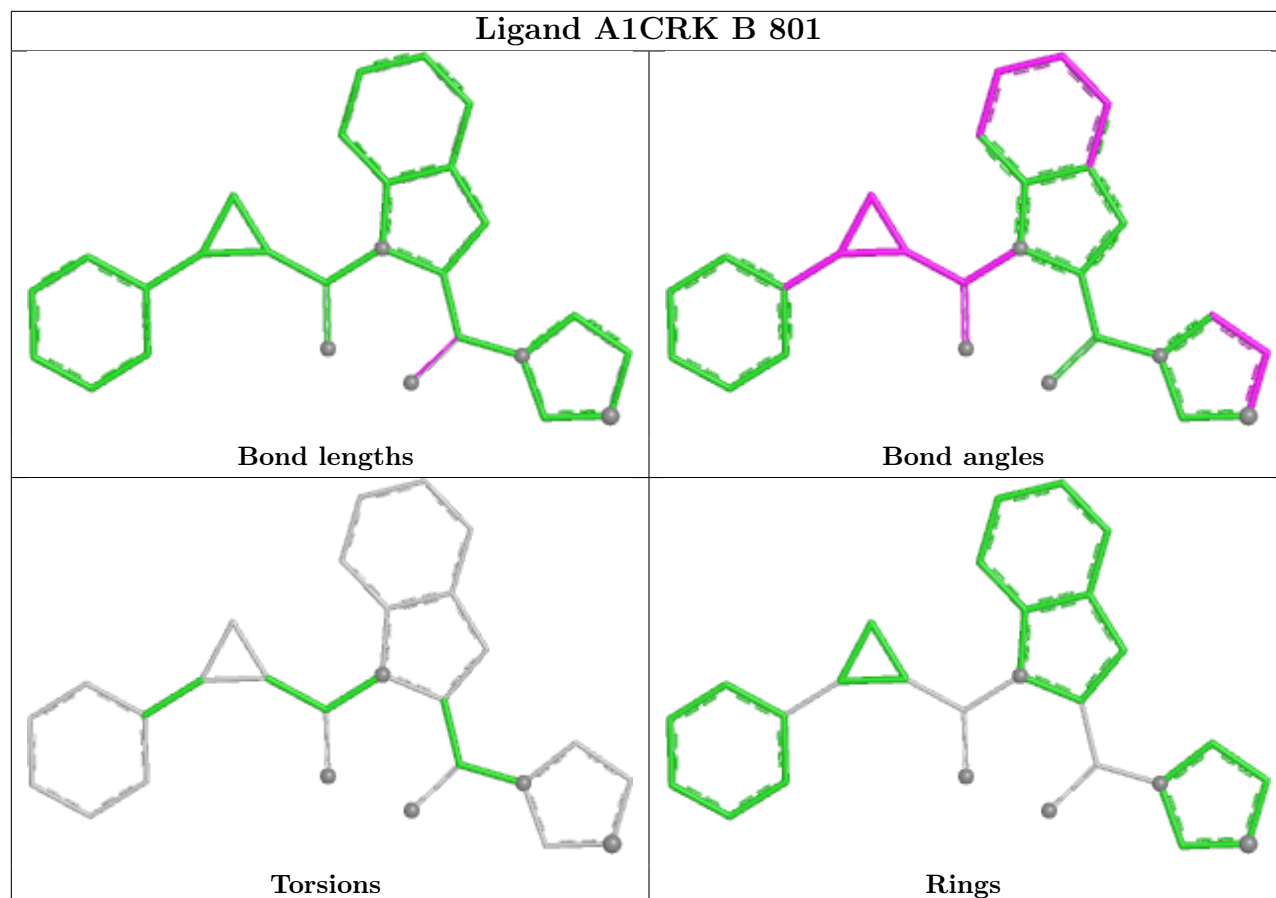
There are no ring outliers.

11 monomers are involved in 21 short contacts:

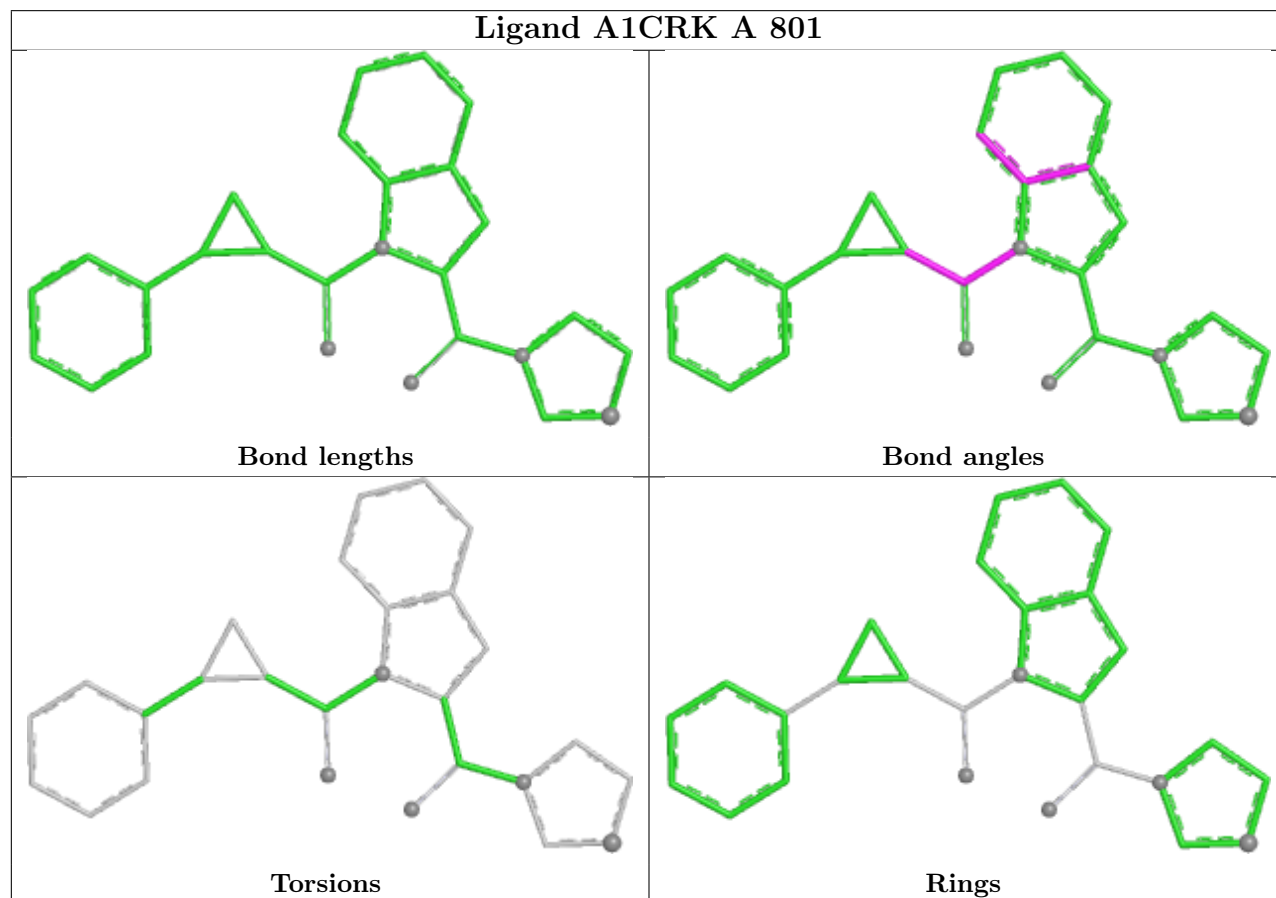
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	805	GOL	1	0
3	C	803	GOL	3	0
3	A	803	GOL	1	0
4	A	805	SCN	2	0
2	E	801	A1CRK	2	0
4	E	803	SCN	1	0
2	C	802	A1CRK	1	0
3	D	802	GOL	3	0
5	A	807	PEG	3	0
3	A	804	GOL	2	0
4	C	805	SCN	2	0

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.

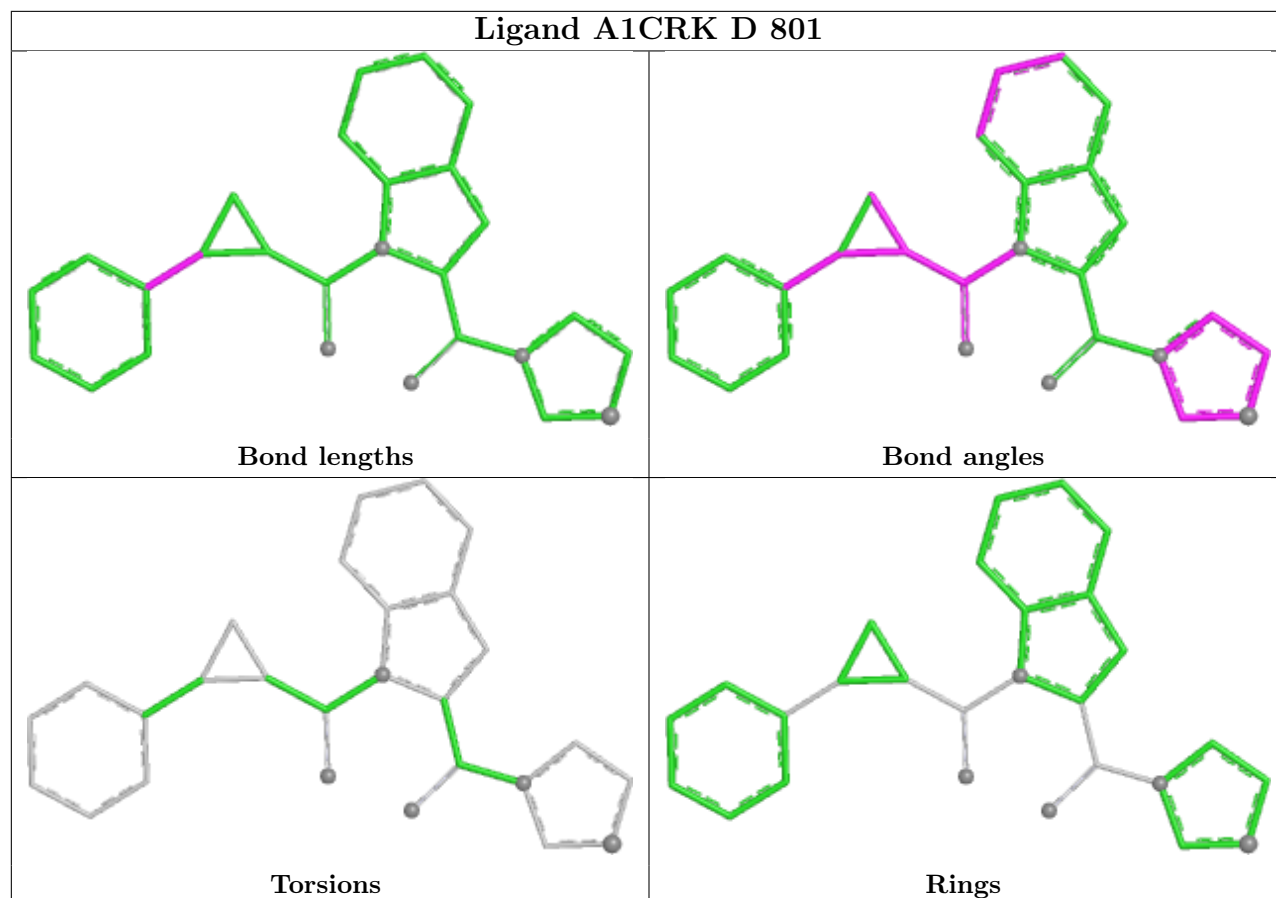
Ligand A1CRK B 801



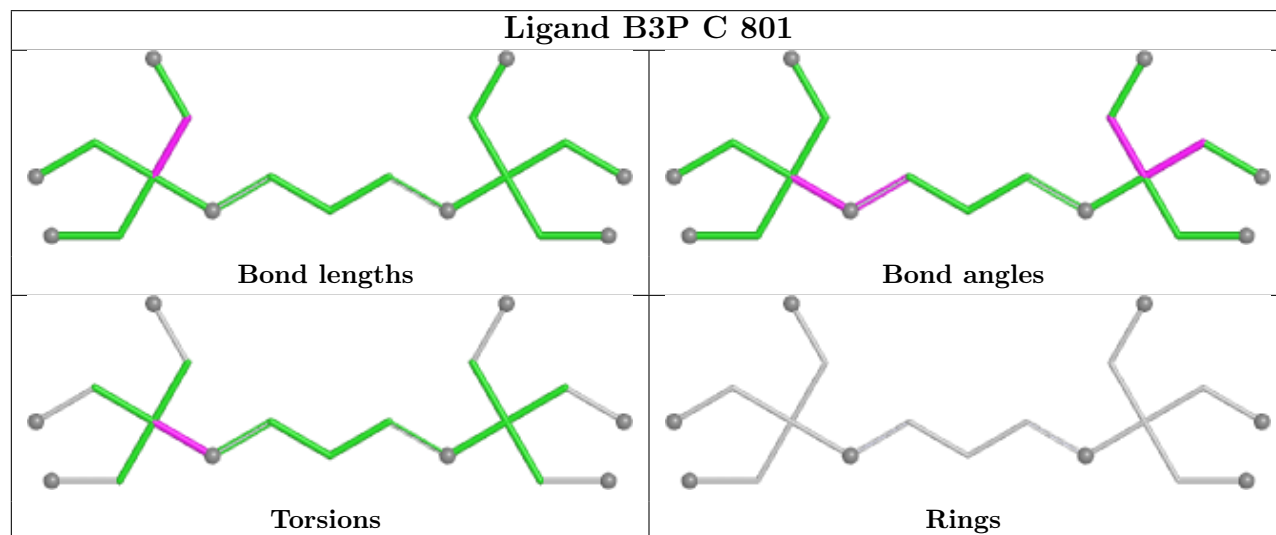
Ligand A1CRK A 801



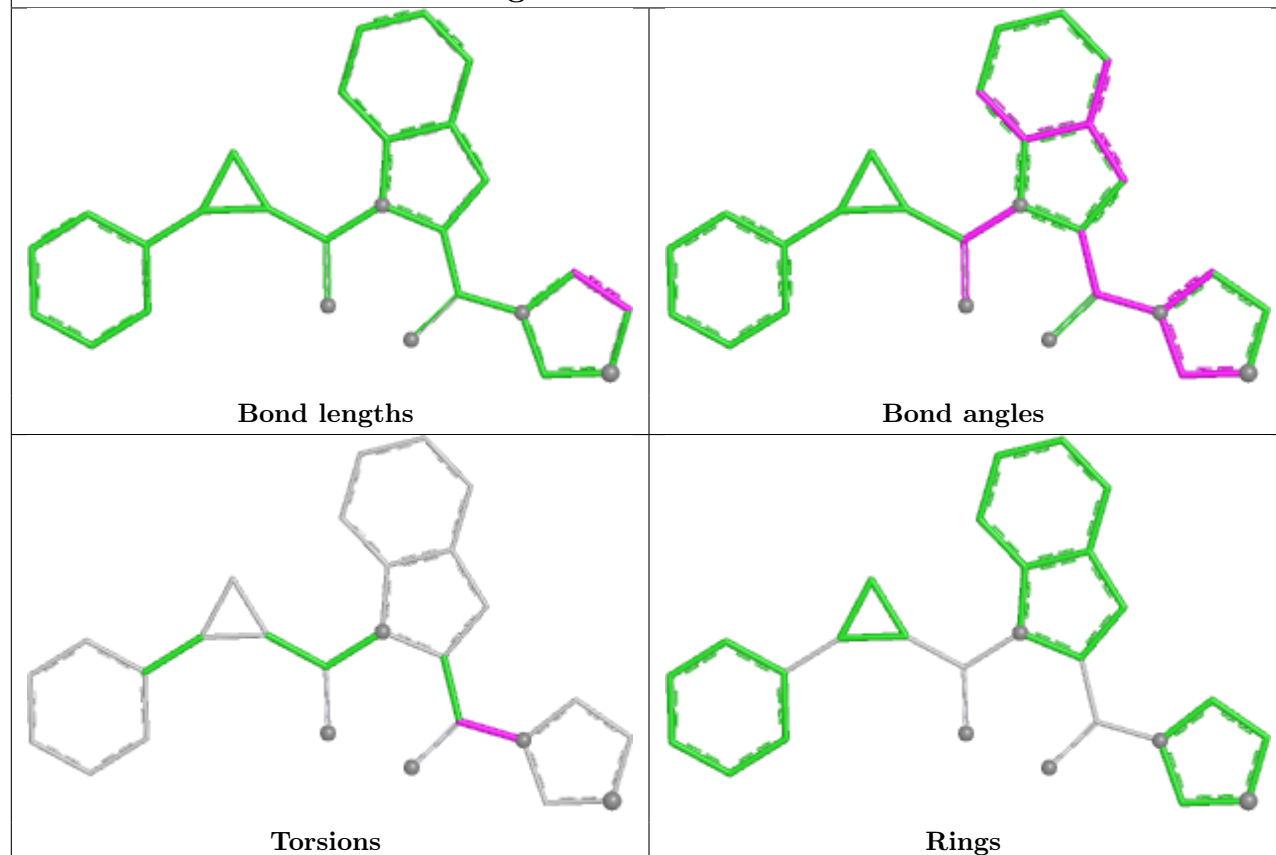
Ligand A1CRK D 801



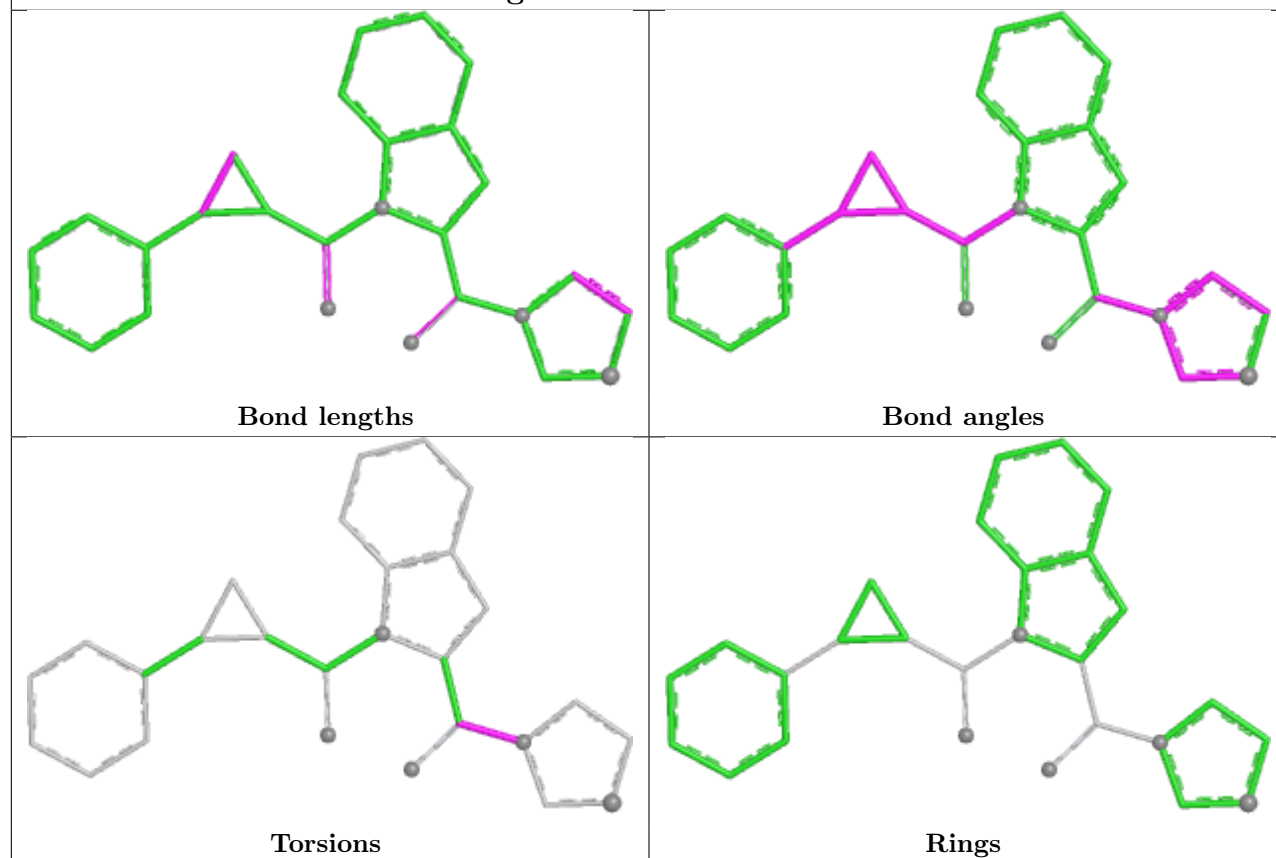
Ligand B3P C 801

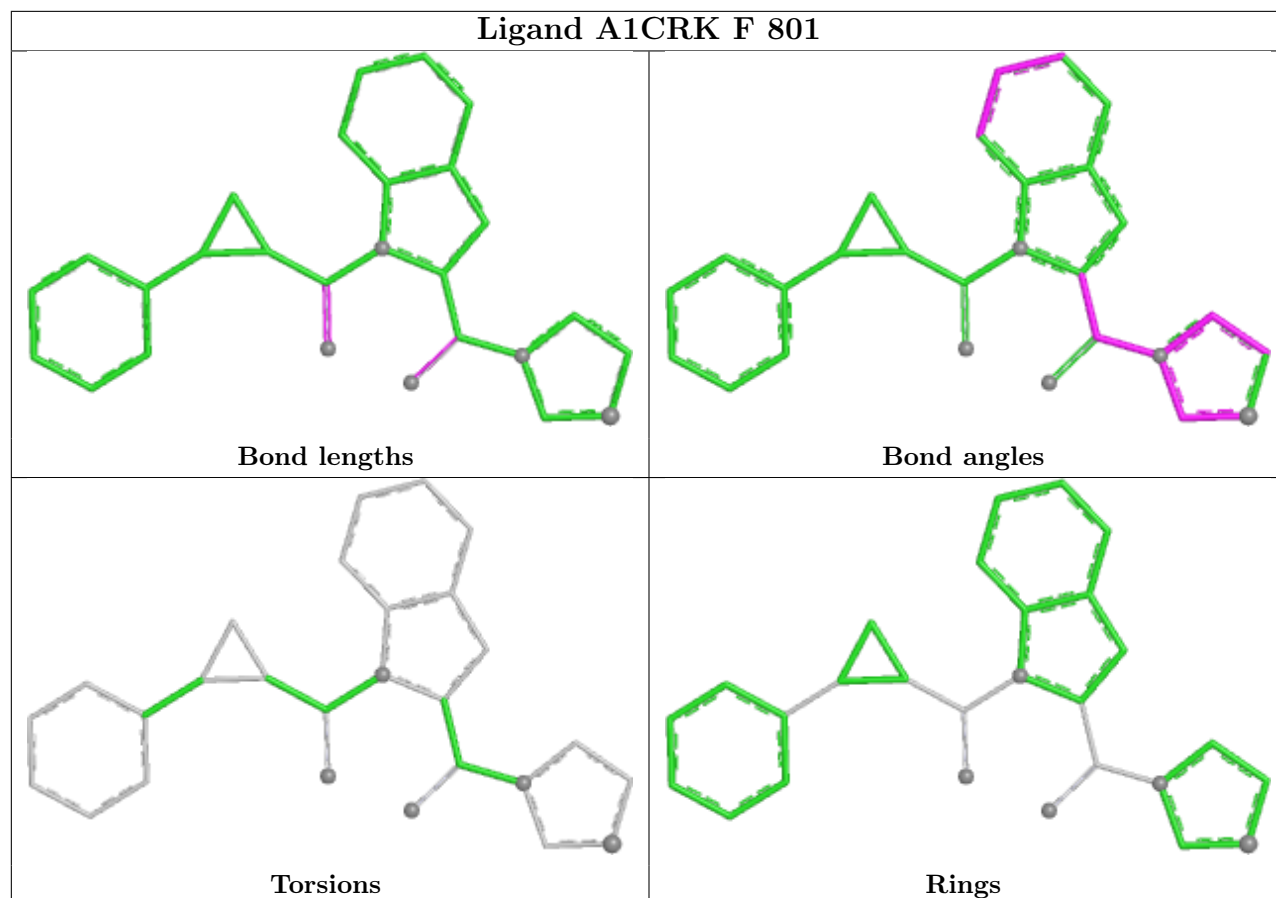


Ligand A1CRK E 801



Ligand A1CRK C 802





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, 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	707/711 (99%)	-1.38	0 100 100	10, 21, 34, 50	3 (0%)
1	B	707/711 (99%)	-1.38	0 100 100	12, 21, 36, 57	0
1	C	707/711 (99%)	-1.36	0 100 100	13, 22, 37, 57	0
1	D	707/711 (99%)	-1.28	0 100 100	16, 26, 43, 65	1 (0%)
1	E	707/711 (99%)	-1.25	0 100 100	17, 27, 46, 71	0
1	F	707/711 (99%)	-1.32	0 100 100	15, 24, 41, 63	0
All	All	4242/4266 (99%)	-1.33	0 100 100	10, 24, 40, 71	4 (0%)

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 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(Å ²)	Q<0.9
3	GOL	B	802	6/6	0.98	0.04	27,32,39,42	3

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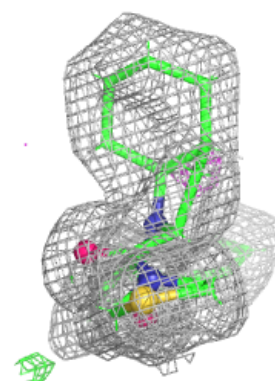
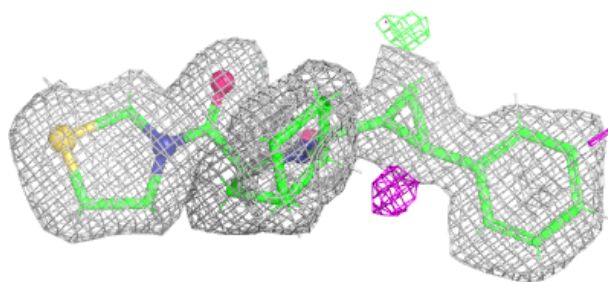
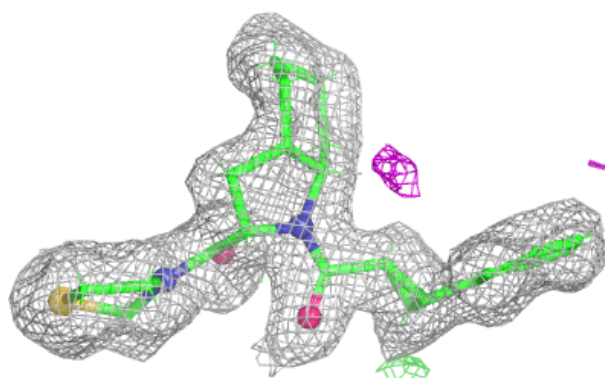
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	804	6/6	0.98	0.04	22,31,39,43	3
3	GOL	B	805	6/6	0.98	0.11	15,19,39,39	14
3	GOL	C	804	6/6	0.98	0.04	18,22,39,39	3
3	GOL	D	802	6/6	0.98	0.04	27,35,39,39	3
3	GOL	E	805	6/6	0.98	0.10	16,20,39,39	14
4	SCN	C	805	3/3	0.98	0.06	36,36,41,46	0
4	SCN	D	803	3/3	0.98	0.07	35,35,41,49	0
4	SCN	E	802	3/3	0.98	0.04	26,26,40,56	0
5	PEG	A	807	7/7	0.98	0.05	25,36,41,41	2
2	A1CRK	A	801	27/27	0.99	0.03	14,19,25,28	0
2	A1CRK	B	801	27/27	0.99	0.03	12,17,31,32	0
2	A1CRK	C	802	27/27	0.99	0.03	16,20,25,29	0
3	GOL	C	803	6/6	0.99	0.03	21,28,39,39	3
2	A1CRK	D	801	27/27	0.99	0.04	17,21,28,31	0
2	A1CRK	E	801	27/27	0.99	0.03	17,24,28,31	0
3	GOL	E	804	6/6	0.99	0.04	21,32,39,41	3
2	A1CRK	F	801	27/27	0.99	0.03	16,22,26,29	0
4	SCN	A	805	3/3	0.99	0.03	24,24,25,45	0
4	SCN	B	803	3/3	0.99	0.04	17,17,27,38	0
3	GOL	A	802	6/6	0.99	0.03	21,25,39,39	3
4	SCN	C	806	3/3	0.99	0.03	33,33,39,44	0
3	GOL	A	803	6/6	0.99	0.04	30,39,43,45	3
3	GOL	A	804	6/6	0.99	0.04	27,33,39,39	3
4	SCN	E	803	3/3	0.99	0.04	48,48,51,53	0
3	GOL	A	806	6/6	0.99	0.04	24,39,41,46	3
6	B3P	C	801	19/19	0.99	0.03	14,21,39,39	8

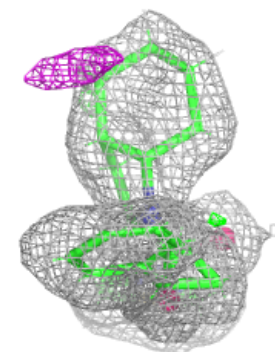
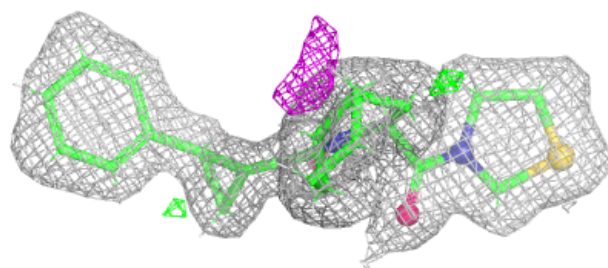
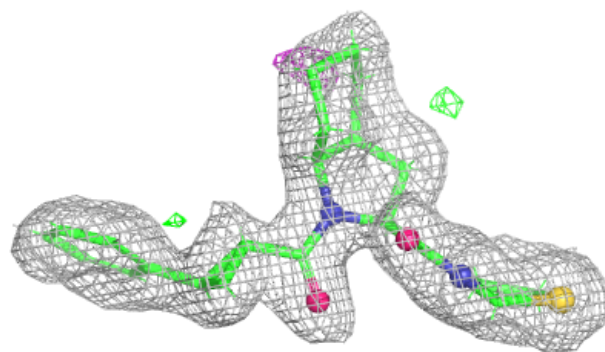
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CRK A 801:

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

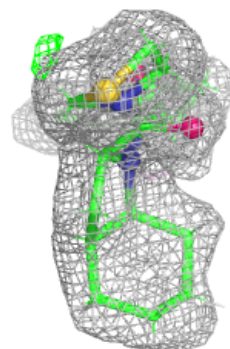
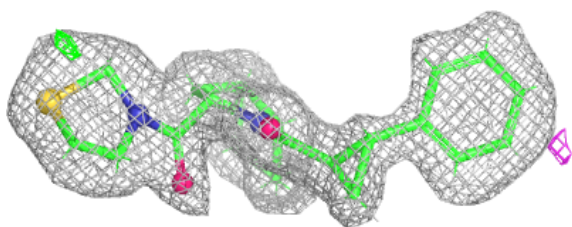
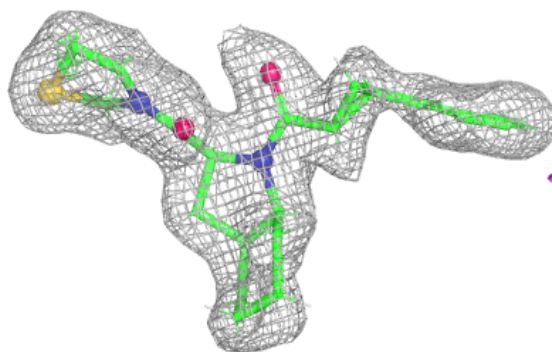
**Electron density around A1CRK B 801:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

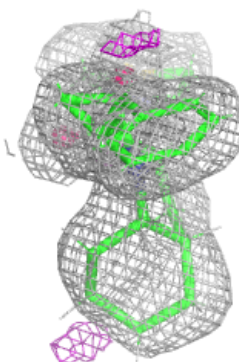
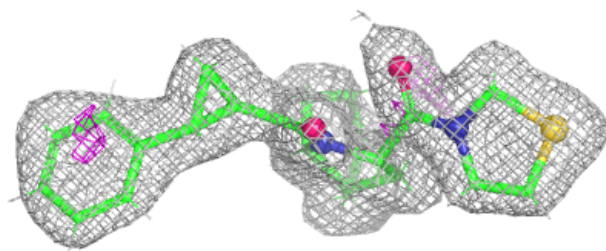
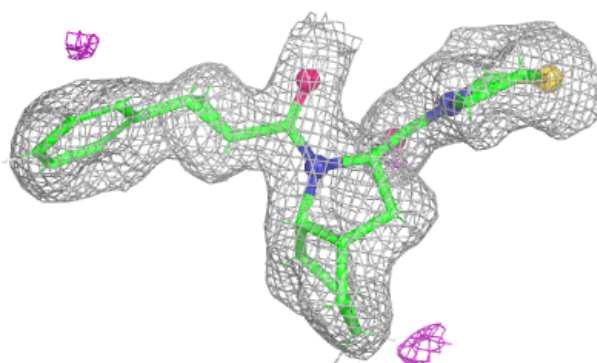


Electron density around A1CRK C 802:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

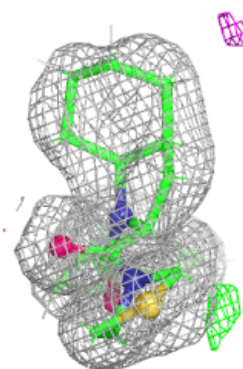
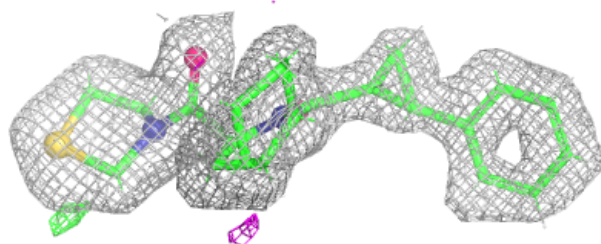
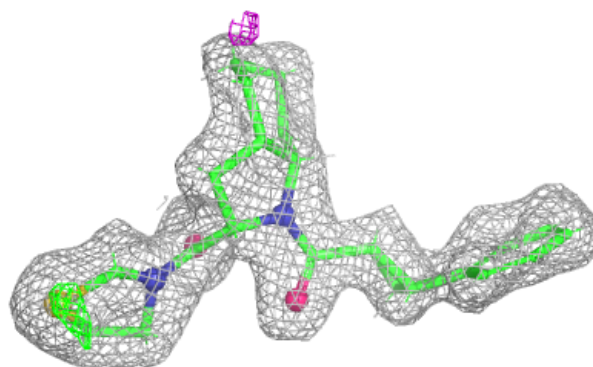
**Electron density around A1CRK D 801:**

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and green (positive)

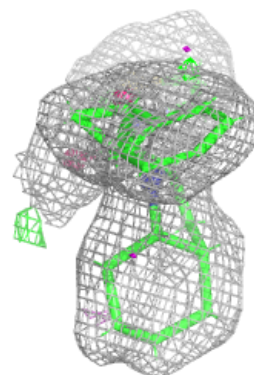
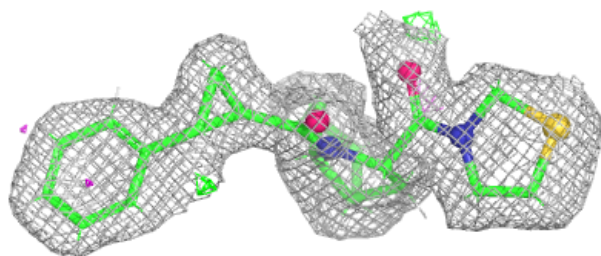
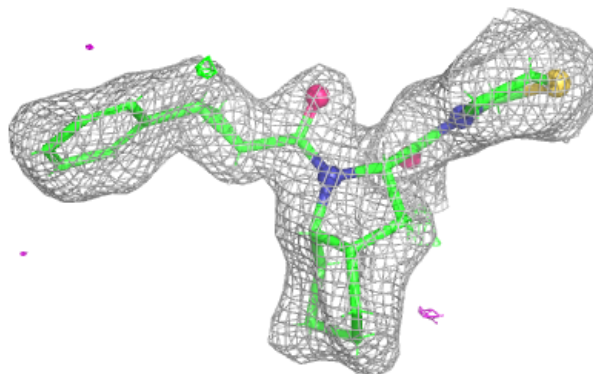


Electron density around A1CRK E 801:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

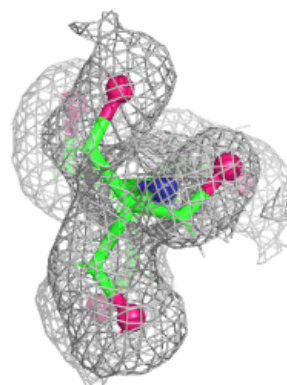
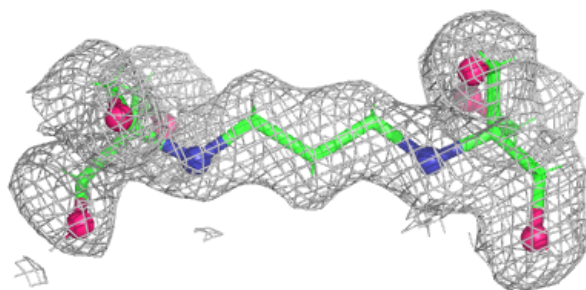
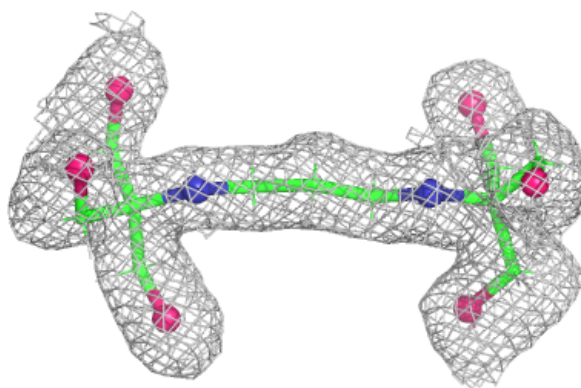
**Electron density around A1CRK F 801:**

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



Electron density around B3P C 801:

$2mF_o-DF_c$ (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.