



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:25 AM UTC

PDB ID : 9XZZ / pdb_00009xzz
Title : Human prolyl endopeptidase (PREP) - complex with KYP2047
Authors : Fucci, I.J.; Thakur, K.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-28
Resolution : 1.58 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

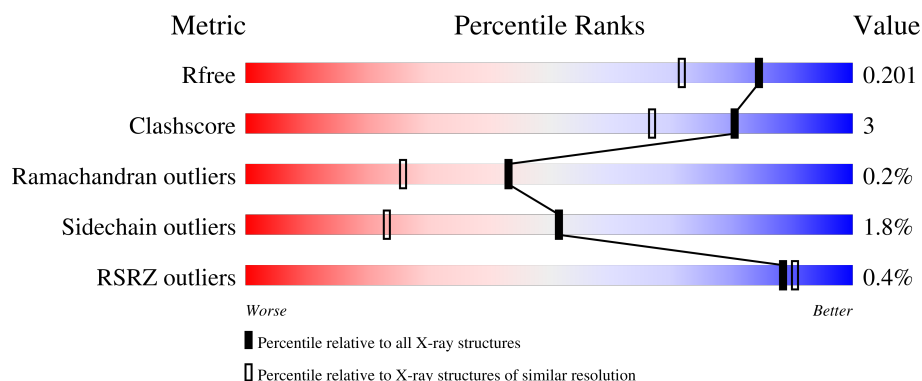
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	91% 8% .
1	B	711	89% 9% .
1	C	711	88% 10% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 36305 atoms, of which 16921 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.

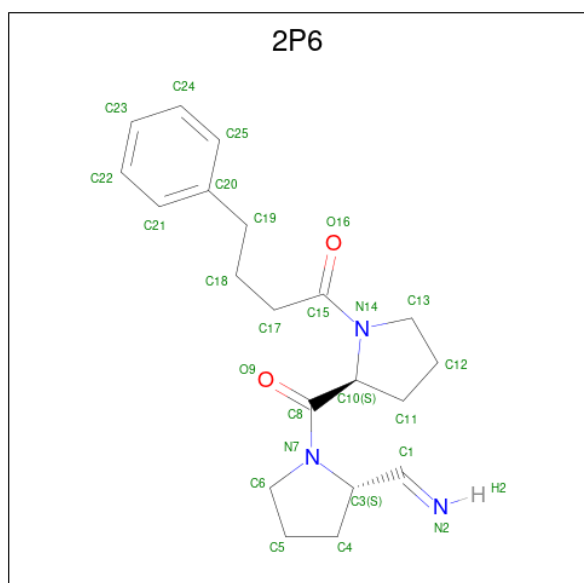
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	708	Total	C	H	N	O	S	180	7	0
			11284	3665	5573	947	1071	28			
1	B	708	Total	C	H	N	O	S	179	8	0
			11291	3668	5574	947	1074	28			
1	C	707	Total	C	H	N	O	S	177	2	0
			11206	3645	5524	941	1068	28			

There are 3 discrepancies between the modelled and reference sequences:

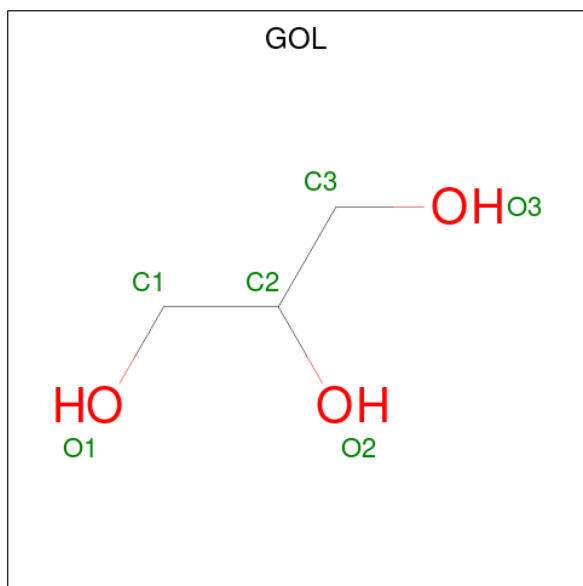
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147
C	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is (2S)-1-[1-(4-phenylbutanoyl)-L-prolyl]pyrrolidine-2-carbonitrile (CCD ID: 2P6) (formula: C₂₀H₂₇N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	1	0
			51	20	26	3	2		
2	B	1	Total	C	H	N	O	1	0
			51	20	26	3	2		
2	C	1	Total	C	H	N	O	1	0
			51	20	26	3	2		

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



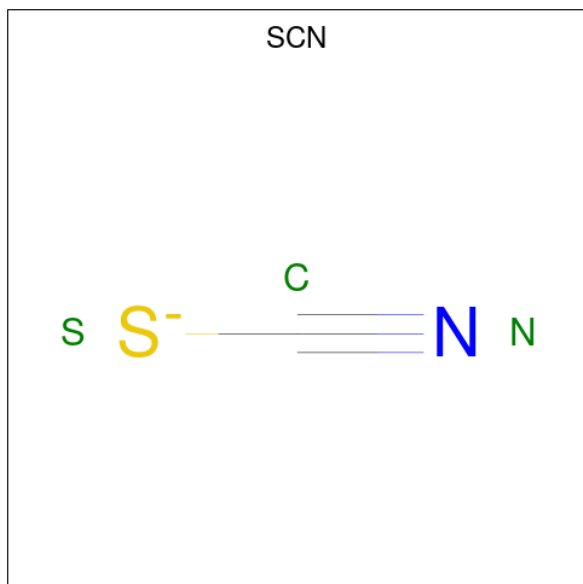
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	C	1	Total	C	H	O	3	0
			14	3	8	3		

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



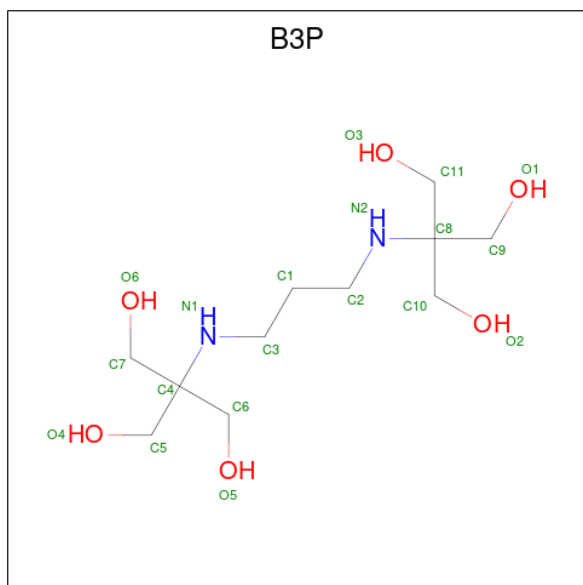
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		
4	C	1	Total	C	N	S	0	0
			3	1	1	1		
4	C	1	Total	C	N	S	0	0
			3	1	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 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
5	A	1	Total	C	H	N	O	8	0
			45	11	26	2	6		
5	C	1	Total	C	H	N	O	8	0
			45	11	26	2	6		

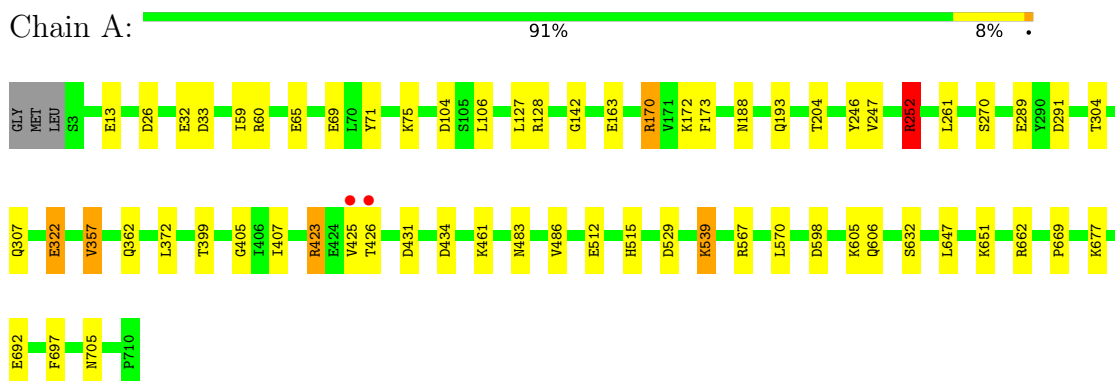
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	719	Total	O	0	1
			720	720		
6	B	762	Total	O	0	0
			762	762		
6	C	570	Total	O	0	1
			571	571		

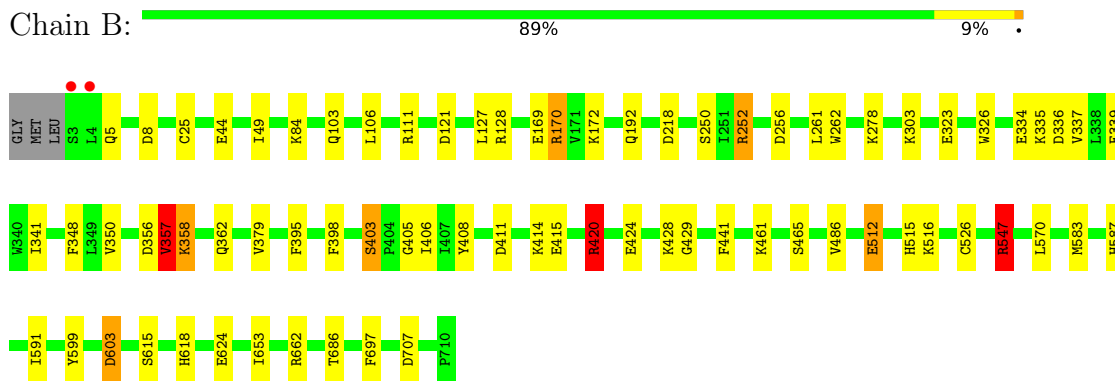
3 Residue-property plots [i](#)

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.

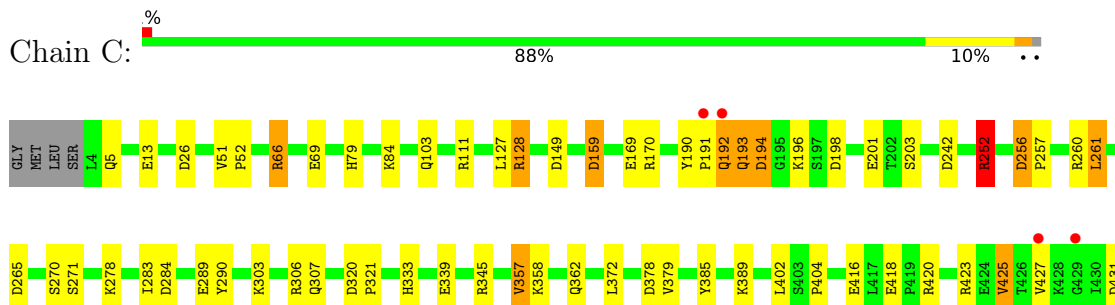
- Molecule 1: Prolyl endopeptidase

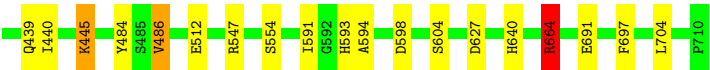


- Molecule 1: Prolyl endopeptidase



- Molecule 1: Prolyl endopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.58Å 66.23Å 156.43Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	34.50 – 1.58 34.50 – 1.58	Depositor EDS
% Data completeness (in resolution range)	66.3 (34.50-1.58) 66.8 (34.50-1.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.150 , 0.200 0.150 , 0.201	Depositor DCC
R_{free} test set	9492 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36305	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, B3P, SCN, 2P6

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	1.02	1/5886 (0.0%)	1.40	38/7981 (0.5%)
1	B	1.05	5/5893 (0.1%)	1.44	40/7988 (0.5%)
1	C	0.96	1/5840 (0.0%)	1.41	36/7917 (0.5%)
All	All	1.01	7/17619 (0.0%)	1.42	114/23886 (0.5%)

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	3
1	B	0	6
1	C	0	8
All	All	0	17

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	SER	CA-CB	-7.60	1.43	1.53
1	B	512	GLU	CD-OE1	6.10	1.36	1.25
1	B	252	ARG	NE-CZ	5.67	1.39	1.33
1	A	515	HIS	ND1-CE1	5.49	1.38	1.32
1	B	515	HIS	ND1-CE1	5.44	1.38	1.32
1	B	587	HIS	ND1-CE1	5.28	1.37	1.32
1	C	664	ARG	NE-CZ	5.04	1.38	1.33

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASP	CB-CA-C	-12.13	85.63	110.38
1	B	8	ASP	CB-CA-C	-10.28	93.44	109.89
1	A	322	GLU	CB-CG-CD	8.76	127.48	112.60
1	C	194	ASP	CA-CB-CG	8.37	120.97	112.60
1	A	170	ARG	CD-NE-CZ	8.13	135.78	124.40
1	B	128	ARG	NE-CZ-NH1	-8.11	113.39	121.50
1	C	627	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	512	GLU	CB-CG-CD	8.10	126.36	112.60
1	A	705	ASN	CA-CB-CG	-8.03	104.57	112.60
1	A	252	ARG	CB-CG-CD	7.89	129.44	111.30
1	A	252	ARG	CA-CB-CG	-7.81	98.49	114.10
1	A	13	GLU	CB-CG-CD	7.74	125.75	112.60
1	B	707	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	539	LYS	N-CA-CB	7.61	121.31	110.12
1	B	103	GLN	N-CA-CB	-7.37	97.93	111.13
1	C	201	GLU	CB-CG-CD	7.24	124.91	112.60
1	C	256	ASP	CA-CB-CG	7.14	119.74	112.60
1	B	624	GLU	CB-CA-C	-7.08	98.81	110.85
1	B	420	ARG	CD-NE-CZ	6.99	134.18	124.40
1	C	512	GLU	CB-CG-CD	6.98	124.46	112.60
1	A	170	ARG	NE-CZ-NH1	-6.97	114.53	121.50
1	C	190	TYR	CB-CA-C	6.91	118.29	108.68
1	C	339	GLU	CB-CA-C	-6.90	98.08	110.70
1	C	192	GLN	CB-CA-C	6.86	119.60	110.06
1	A	170	ARG	NE-CZ-NH2	6.85	125.36	119.20
1	C	252	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	B	603[A]	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	603[B]	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	423	ARG	NE-CZ-NH1	-6.72	114.78	121.50
1	B	335	LYS	CB-CG-CD	6.70	126.72	111.30
1	B	618	HIS	CA-CB-CG	-6.67	107.13	113.80
1	A	252	ARG	NE-CZ-NH2	-6.63	113.23	119.20
1	B	547	ARG	CA-CB-CG	6.63	127.35	114.10
1	A	662	ARG	CD-NE-CZ	6.55	133.57	124.40
1	B	428	LYS	CB-CA-C	6.54	120.83	109.65
1	C	697	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	252	ARG	CG-CD-NE	-6.39	97.94	112.00
1	C	418	GLU	CB-CA-C	6.37	116.48	110.17
1	A	539	LYS	CB-CA-C	-6.31	100.32	110.79
1	A	163	GLU	CB-CA-C	-6.30	100.08	109.90
1	C	664	ARG	CD-NE-CZ	6.30	133.22	124.40
1	A	697	PHE	CA-CB-CG	-6.28	107.52	113.80
1	C	69	GLU	CB-CA-C	6.16	120.45	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	LYS	CB-CA-C	6.16	123.06	109.94
1	C	385	TYR	CA-C-O	-6.16	114.12	120.89
1	C	111	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	B	570	LEU	N-CA-CB	-6.09	100.89	110.46
1	C	149	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	420	ARG	CA-CB-CG	5.99	126.07	114.10
1	B	512	GLU	CG-CD-OE2	-5.96	104.69	118.40
1	A	705	ASN	CB-CA-C	-5.94	103.45	111.89
1	A	128	ARG	CA-CB-CG	-5.92	102.27	114.10
1	C	265	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	252	ARG	CD-NE-CZ	5.90	132.66	124.40
1	A	246	TYR	CA-C-N	-5.88	115.52	122.93
1	A	246	TYR	C-N-CA	-5.88	115.52	122.93
1	B	686	THR	OG1-CB-CG2	5.87	121.04	109.30
1	C	26	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	256	ASP	N-CA-CB	5.84	118.64	110.11
1	A	291	ASP	CB-CA-C	5.84	120.31	110.79
1	B	461	LYS	CB-CA-C	-5.81	99.94	109.53
1	C	193	GLN	CB-CA-C	5.81	120.47	109.37
1	B	526[A]	CYS	CB-CA-C	-5.81	101.76	110.88
1	B	526[B]	CYS	CB-CA-C	-5.81	101.76	110.88
1	B	127	LEU	N-CA-CB	-5.80	101.44	109.97
1	B	348	PHE	CA-CB-CG	5.79	119.59	113.80
1	C	416	GLU	N-CA-C	5.71	117.31	111.14
1	B	429	GLY	N-CA-C	-5.71	107.50	114.92
1	B	420	ARG	CG-CD-NE	5.70	124.53	112.00
1	B	339	GLU	CB-CA-C	-5.63	101.33	110.79
1	C	378	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	60	ARG	CA-C-N	5.59	126.15	120.00
1	A	60	ARG	C-N-CA	5.59	126.15	120.00
1	B	441	PHE	CA-CB-CG	-5.58	108.22	113.80
1	C	159	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	252	ARG	CB-CG-CD	5.55	124.07	111.30
1	C	284	ASP	CB-CA-C	5.54	121.45	110.42
1	C	333	HIS	CB-CA-C	5.49	119.57	109.46
1	C	691	GLU	CB-CG-CD	5.48	121.92	112.60
1	A	252	ARG	CD-NE-CZ	5.44	132.02	124.40
1	C	431	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	529	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	33	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	697	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	425	VAL	N-CA-CB	-5.38	104.86	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	C	289	GLU	CG-CD-OE2	-5.31	106.19	118.40
1	C	416	GLU	CB-CA-C	-5.31	102.51	110.90
1	B	5	GLN	N-CA-CB	-5.31	101.62	110.80
1	B	516	LYS	CB-CG-CD	-5.30	99.10	111.30
1	A	252	ARG	NH1-CZ-NH2	5.30	126.19	119.30
1	B	169	GLU	CB-CG-CD	5.26	121.55	112.60
1	B	515	HIS	N-CA-C	-5.25	105.47	111.14
1	A	26	ASP	CB-CA-C	5.25	118.08	111.21
1	B	303	LYS	CG-CD-CE	5.24	123.36	111.30
1	B	362	GLN	CG-CD-NE2	-5.24	108.54	116.40
1	B	172	LYS	N-CA-CB	-5.23	101.80	111.52
1	A	486	VAL	N-CA-CB	-5.21	103.46	110.54
1	A	372	LEU	N-CA-C	-5.20	107.48	113.88
1	A	69	GLU	N-CA-CB	-5.20	102.53	110.07
1	A	65	GLU	CB-CA-C	5.17	120.60	110.67
1	A	128	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	60	ARG	N-CA-CB	5.14	117.60	109.94
1	B	624	GLU	N-CA-CB	5.12	117.74	110.16
1	C	372	LEU	N-CA-C	-5.12	106.72	113.12
1	C	170	ARG	CD-NE-CZ	5.12	131.57	124.40
1	C	303	LYS	CB-CG-CD	5.10	123.03	111.30
1	B	403	SER	O-C-N	-5.10	118.26	121.88
1	C	362	GLN	CG-CD-NE2	-5.09	108.76	116.40
1	A	605	LYS	N-CA-CB	5.08	117.51	109.94
1	C	593	HIS	CA-CB-CG	5.05	118.85	113.80
1	B	461	LYS	N-CA-CB	5.05	118.41	110.23
1	B	111	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	A	692	GLU	CB-CG-CD	-5.02	104.07	112.60

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain
1	A	188	ASN	Mainchain
1	A	252	ARG	Sidechain
1	B	170[A]	ARG	Sidechain
1	B	170[B]	ARG	Sidechain
1	B	252	ARG	Sidechain
1	B	420	ARG	Sidechain
1	B	547	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	662	ARG	Sidechain
1	C	128	ARG	Sidechain
1	C	252	ARG	Sidechain
1	C	260	ARG	Sidechain
1	C	345	ARG	Sidechain
1	C	423	ARG	Sidechain
1	C	594	ALA	Mainchain
1	C	66	ARG	Sidechain
1	C	664	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	5711	5573	5545	25	0
1	B	5717	5574	5545	33	1
1	C	5682	5524	5501	26	1
2	A	25	26	25	0	0
2	B	25	26	25	1	0
2	C	25	26	25	0	0
3	A	42	56	56	4	0
3	B	30	40	40	2	0
3	C	18	24	24	0	0
4	A	6	0	0	0	0
4	B	3	0	0	0	0
4	C	9	0	0	1	0
5	A	19	26	26	3	0
5	C	19	26	26	0	0
6	A	720	0	0	8	2
6	B	762	0	0	13	0
6	C	571	0	0	3	1
All	All	19384	16921	16838	88	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (88) 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:193:GLN:OE1	3:A:811:GOL:H11	1.80	0.82
1:C:79:HIS:NE2	1:C:103:GLN:NE2	2.30	0.78
1:B:334:GLU:OE2	6:B:901:HOH:O	2.04	0.76
1:B:334:GLU:HB3	6:B:1336:HOH:O	1.90	0.72
1:C:484:TYR:CE2	1:C:486:VAL:HG23	2.24	0.71
1:B:218:ASP:OD2	6:B:902:HOH:O	2.09	0.70
1:B:603[A]:ASP:OD1	6:B:903:HOH:O	2.11	0.69
1:B:25:CYS:HB3	6:B:1427:HOH:O	1.93	0.67
1:B:547:ARG:HD2	6:B:1517:HOH:O	1.95	0.67
1:A:252:ARG:HD2	6:A:1438:HOH:O	1.95	0.66
1:C:5:GLN:HA	1:C:5:GLN:OE1	1.95	0.66
1:B:44:GLU:OE2	6:B:904:HOH:O	2.14	0.64
1:C:420:ARG:HG3	1:C:420:ARG:HH11	1.65	0.62
1:B:358:LYS:HG2	1:B:379:VAL:HG13	1.84	0.60
1:B:262:TRP:HZ3	3:B:803:GOL:H2	1.67	0.59
1:A:362:GLN:NE2	3:A:808:GOL:O2	2.34	0.59
1:B:420:ARG:CD	6:B:1509:HOH:O	2.50	0.59
1:B:411:ASP:OD2	1:B:414:LYS:HE2	2.06	0.56
1:B:420:ARG:CG	6:B:1509:HOH:O	2.54	0.56
1:C:242:ASP:OD2	1:C:389:LYS:HD2	2.06	0.56
1:A:567:ARG:NH2	1:A:570[B]:LEU:HD21	2.23	0.54
1:C:440:ILE:C	1:C:440:ILE:HD12	2.33	0.54
1:A:193:GLN:OE1	3:A:811:GOL:C1	2.56	0.52
1:C:306:ARG:HG3	1:C:307:GLN:HG3	1.92	0.52
1:C:404:PRO:HB2	1:C:425:VAL:HG22	1.92	0.52
1:B:420:ARG:HG2	6:B:1509:HOH:O	2.10	0.51
1:A:606:GLN:H	1:A:606:GLN:CD	2.20	0.50
1:A:539:LYS:HG3	6:A:1106:HOH:O	2.11	0.50
5:A:806:B3P:H52	6:A:1272:HOH:O	2.13	0.48
5:A:806:B3P:H112	6:A:1037:HOH:O	2.13	0.48
1:A:431:ASP:HB3	1:A:434:ASP:OD2	2.14	0.48
1:B:420:ARG:HD3	6:B:1509:HOH:O	2.11	0.48
1:C:402:LEU:O	1:C:427:VAL:CG2	2.62	0.48
1:B:395:PHE:HA	1:B:408:TYR:O	2.14	0.47
1:A:307:GLN:HA	1:A:307:GLN:OE1	2.14	0.47
1:A:204:THR:O	3:A:811:GOL:H12	2.15	0.46
1:A:322:GLU:HG3	6:A:903:HOH:O	2.15	0.46
1:A:399[B]:THR:HG22	1:A:405:GLY:HA2	1.96	0.46
1:A:483:ASN:ND2	6:A:928:HOH:O	2.49	0.46
1:B:336:ASP:OD2	3:B:806:GOL:O3	2.26	0.46
1:A:127:LEU:HD12	1:A:142:GLY:O	2.16	0.46
1:B:278:LYS:HE2	6:B:1228:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ARG:NH1	1:C:256:ASP:O	2.49	0.46
1:A:632:SER:OG	1:A:669:PRO:HD2	2.16	0.45
1:B:337:VAL:HG23	6:B:1208:HOH:O	2.15	0.45
1:B:341:ILE:HA	1:B:350:VAL:O	2.16	0.45
1:A:606:GLN:CD	1:A:606:GLN:N	2.75	0.45
1:A:172:LYS:HD3	1:A:173:PHE:CE2	2.52	0.44
1:C:283:ILE:HG21	1:C:290:TYR:CE2	2.52	0.44
1:B:358:LYS:HE2	1:B:358:LYS:HB2	1.76	0.44
5:A:806:B3P:H31	5:A:806:B3P:H61	1.69	0.44
1:B:583:MET:HE1	1:B:599:TYR:CD2	2.52	0.44
1:C:66:ARG:HA	1:C:66:ARG:HD2	1.68	0.44
1:A:71:TYR:CZ	1:A:75:LYS:HE2	2.52	0.44
1:C:445:LYS:HB2	1:C:445:LYS:HE2	1.42	0.44
1:C:547:ARG:HA	1:C:704:LEU:HD13	1.99	0.44
1:C:13:GLU:HB2	6:C:1292:HOH:O	2.17	0.43
1:C:193:GLN:O	1:C:194:ASP:C	2.62	0.43
1:C:261:LEU:C	1:C:261:LEU:HD13	2.44	0.43
1:B:49:ILE:HD13	1:B:49:ILE:HG21	1.76	0.43
1:C:664:ARG:HD3	6:C:978:HOH:O	2.18	0.43
1:B:170[A]:ARG:HD3	1:B:192:GLN:NE2	2.34	0.42
1:B:170[B]:ARG:HD3	1:B:192:GLN:NE2	2.34	0.42
4:C:804:SCN:S	6:C:1320:HOH:O	2.62	0.42
1:A:407:ILE:HD12	1:A:423:ARG:HG2	2.00	0.42
1:C:196:LYS:HB2	1:C:196:LYS:HE3	1.92	0.42
1:C:51:VAL:HB	1:C:52:PRO:HD3	2.00	0.42
1:A:289:GLU:O	1:A:304:THR:HA	2.19	0.42
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.84	0.42
1:B:323:GLU:HA	1:B:326:TRP:CE2	2.55	0.42
1:C:320:ASP:N	1:C:321:PRO:HD3	2.35	0.42
1:B:591:ILE:HG12	2:B:802:2P6:H19	2.01	0.42
1:C:198:ASP:O	1:C:640:HIS:HD2	2.02	0.41
1:B:583:MET:HB2	1:B:615:SER:HB2	2.02	0.41
1:C:358:LYS:NZ	1:C:439:GLN:OE1	2.53	0.41
1:B:465:SER:O	1:B:547:ARG:HD3	2.21	0.41
1:A:399[A]:THR:HG21	6:A:1310:HOH:O	2.19	0.41
1:A:32:GLU:OE2	1:A:651[A]:LYS:NZ	2.45	0.41
1:A:677:LYS:HE2	1:A:677:LYS:HB3	1.81	0.41
1:B:356:ASP:C	1:B:357:VAL:HG23	2.45	0.41
1:B:398:PHE:O	1:B:405:GLY:HA3	2.21	0.41
1:B:653:ILE:HD12	1:B:653:ILE:HA	1.95	0.41
1:A:461:LYS:HE2	6:A:1494:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ILE:HG12	1:B:424:GLU:HG3	2.04	0.40
1:C:358:LYS:HG2	1:C:379:VAL:HG13	2.02	0.40
1:C:191:PRO:O	1:C:192:GLN:C	2.64	0.40
1:A:647:LEU:HD12	1:A:647:LEU:C	2.46	0.40
1:C:591:ILE:HD12	1:C:591:ILE:HA	1.95	0.40

All (3) 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:408:TYR:HH	1:C:84:LYS:HE2[2_545]	1.02	0.58
6:A:991:HOH:O	6:C:1109:HOH:O[2_555]	1.96	0.24
6:A:1319:HOH:O	6:A:1368:HOH:O[2_556]	2.12	0.08

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	713/711 (100%)	694 (97%)	18 (2%)	1 (0%)	48	28
1	B	714/711 (100%)	695 (97%)	18 (2%)	1 (0%)	48	28
1	C	707/711 (99%)	682 (96%)	23 (3%)	2 (0%)	36	20
All	All	2134/2133 (100%)	2071 (97%)	59 (3%)	4 (0%)	43	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	554	SER
1	C	357	VAL
1	B	357	VAL
1	A	357	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/617 (101%)	613 (99%)	9 (1%)	59	34
1	B	623/617 (101%)	615 (99%)	8 (1%)	61	37
1	C	616/617 (100%)	600 (97%)	16 (3%)	40	11
All	All	1861/1851 (100%)	1828 (98%)	33 (2%)	51	23

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	104	ASP
1	A	106	LEU
1	A	247	VAL
1	A	261	LEU
1	A	270	SER
1	A	357	VAL
1	A	426	THR
1	A	598	ASP
1	B	84	LYS
1	B	261	LEU
1	B	357	VAL
1	B	358	LYS
1	B	403	SER
1	B	415	GLU
1	B	486	VAL
1	B	512	GLU
1	C	127	LEU
1	C	159	ASP
1	C	169	GLU
1	C	203	SER
1	C	257	PRO
1	C	261	LEU
1	C	270	SER
1	C	271	SER
1	C	278	LYS

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Mol	Chain	Res	Type
1	C	357	VAL
1	C	425	VAL
1	C	445	LYS
1	C	486	VAL
1	C	598	ASP
1	C	604	SER
1	C	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	GLN
1	A	397	GLN
1	A	483	ASN
1	A	524	GLN
1	A	531	GLN
1	A	566	GLN
1	B	17	GLN
1	B	103	GLN
1	B	307	GLN
1	B	362	GLN
1	B	483	ASN
1	B	524	GLN
1	B	531	GLN
1	B	551	ASN
1	B	566	GLN
1	B	577	GLN
1	C	103	GLN
1	C	205	ASN
1	C	267	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	SCN	C	807	-	1,2,2	1.06	0	0,1,1	-	-
3	GOL	A	803	-	5,5,5	0.48	0	5,5,5	1.12	1 (20%)
3	GOL	B	803	-	5,5,5	0.35	0	5,5,5	1.31	0
4	SCN	C	804	-	1,2,2	0.78	0	0,1,1	-	-
2	2P6	A	801	1	25,27,27	1.29	1 (4%)	31,36,36	1.00	1 (3%)
5	B3P	A	806	-	18,18,18	0.86	1 (5%)	23,23,23	1.65	6 (26%)
3	GOL	C	806	-	5,5,5	0.16	0	5,5,5	0.48	0
3	GOL	A	811	-	5,5,5	0.21	0	5,5,5	1.05	0
3	GOL	A	810	-	5,5,5	0.19	0	5,5,5	0.37	0
3	GOL	B	801	-	5,5,5	0.65	0	5,5,5	1.22	1 (20%)
3	GOL	A	802	-	5,5,5	0.40	0	5,5,5	0.55	0
3	GOL	A	807	-	5,5,5	0.27	0	5,5,5	0.31	0
5	B3P	C	801	-	18,18,18	0.70	0	23,23,23	1.47	5 (21%)
3	GOL	A	804	-	5,5,5	0.56	0	5,5,5	1.21	0
3	GOL	B	805	-	5,5,5	0.13	0	5,5,5	0.35	0
4	SCN	B	807	-	1,2,2	0.86	0	0,1,1	-	-
3	GOL	C	805	-	5,5,5	0.29	0	5,5,5	0.77	0
3	GOL	C	808	-	5,5,5	0.16	0	5,5,5	0.63	0
4	SCN	A	809	-	1,2,2	0.44	0	0,1,1	-	-
4	SCN	A	805	-	1,2,2	1.19	0	0,1,1	-	-
2	2P6	B	802	1	25,27,27	1.44	2 (8%)	31,36,36	1.05	2 (6%)
4	SCN	C	803	-	1,2,2	0.73	0	0,1,1	-	-
2	2P6	C	802	1	25,27,27	1.16	1 (4%)	31,36,36	0.88	0
3	GOL	B	804	-	5,5,5	0.18	0	5,5,5	0.76	0
3	GOL	B	806	-	5,5,5	0.46	0	5,5,5	1.10	0
3	GOL	A	808	-	5,5,5	0.26	0	5,5,5	0.62	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	GOL	A	803	-	-	0/4/4/4	-
3	GOL	B	803	-	-	3/4/4/4	-
2	2P6	A	801	1	-	0/18/40/40	0/3/3/3
5	B3P	A	806	-	-	12/28/28/28	-
3	GOL	C	806	-	-	2/4/4/4	-
3	GOL	A	811	-	-	3/4/4/4	-
3	GOL	A	810	-	-	4/4/4/4	-
3	GOL	B	801	-	-	2/4/4/4	-
3	GOL	A	802	-	-	3/4/4/4	-
3	GOL	A	807	-	-	0/4/4/4	-
5	B3P	C	801	-	-	3/28/28/28	-
3	GOL	A	804	-	-	2/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	C	805	-	-	2/4/4/4	-
3	GOL	C	808	-	-	4/4/4/4	-
2	2P6	B	802	1	-	2/18/40/40	0/3/3/3
2	2P6	C	802	1	-	1/18/40/40	0/3/3/3
3	GOL	B	804	-	-	4/4/4/4	-
3	GOL	B	806	-	-	0/4/4/4	-
3	GOL	A	808	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	2P6	C3-N7	-5.81	1.42	1.48
2	A	801	2P6	C3-N7	-5.74	1.43	1.48
2	C	802	2P6	C3-N7	-4.80	1.43	1.48
2	B	802	2P6	O16-C15	2.94	1.29	1.23
5	A	806	B3P	C6-C4	2.49	1.56	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	806	B3P	C11-C8-N2	3.31	118.89	109.02
5	A	806	B3P	O5-C6-C4	3.21	118.21	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	801	B3P	C2-N2-C8	-2.84	112.00	116.17
5	A	806	B3P	C3-N1-C4	2.73	120.16	116.17
5	A	806	B3P	C6-C4-N1	2.72	117.14	109.02
5	C	801	B3P	C1-C2-N2	2.61	117.30	110.98
5	A	806	B3P	O3-C11-C8	2.60	116.97	111.68
5	A	806	B3P	C10-C8-N2	-2.57	101.34	109.02
5	C	801	B3P	C11-C8-C10	-2.55	104.44	110.02
2	B	802	2P6	O9-C8-C10	2.20	124.89	120.28
5	C	801	B3P	O5-C6-C4	-2.15	107.32	111.68
2	B	802	2P6	C11-C12-C13	2.08	110.69	104.90
2	A	801	2P6	C18-C17-C15	-2.08	107.28	112.66
3	B	801	GOL	O2-C2-C1	2.07	117.75	109.18
5	C	801	B3P	C7-C4-C6	-2.03	105.57	110.02
3	A	803	GOL	C3-C2-C1	2.02	119.22	111.80

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	GOL	O1-C1-C2-C3
3	A	804	GOL	O1-C1-C2-C3
3	A	810	GOL	O1-C1-C2-C3
3	B	801	GOL	O1-C1-C2-C3
3	B	803	GOL	C1-C2-C3-O3
3	B	804	GOL	C1-C2-C3-O3
3	B	804	GOL	O2-C2-C3-O3
3	B	805	GOL	C1-C2-C3-O3
3	C	805	GOL	C1-C2-C3-O3
3	C	806	GOL	O1-C1-C2-C3
3	C	808	GOL	O1-C1-C2-C3
5	A	806	B3P	C5-C4-N1-C3
5	A	806	B3P	C6-C4-N1-C3
5	A	806	B3P	C7-C4-N1-C3
5	A	806	B3P	N1-C4-C6-O5
5	A	806	B3P	C5-C4-C6-O5
5	A	806	B3P	C7-C4-C6-O5
5	A	806	B3P	C3-C1-C2-N2
5	A	806	B3P	C2-C1-C3-N1
3	C	806	GOL	O1-C1-C2-O2
3	A	808	GOL	O1-C1-C2-C3
3	A	811	GOL	O1-C1-C2-C3
3	B	804	GOL	O1-C1-C2-C3

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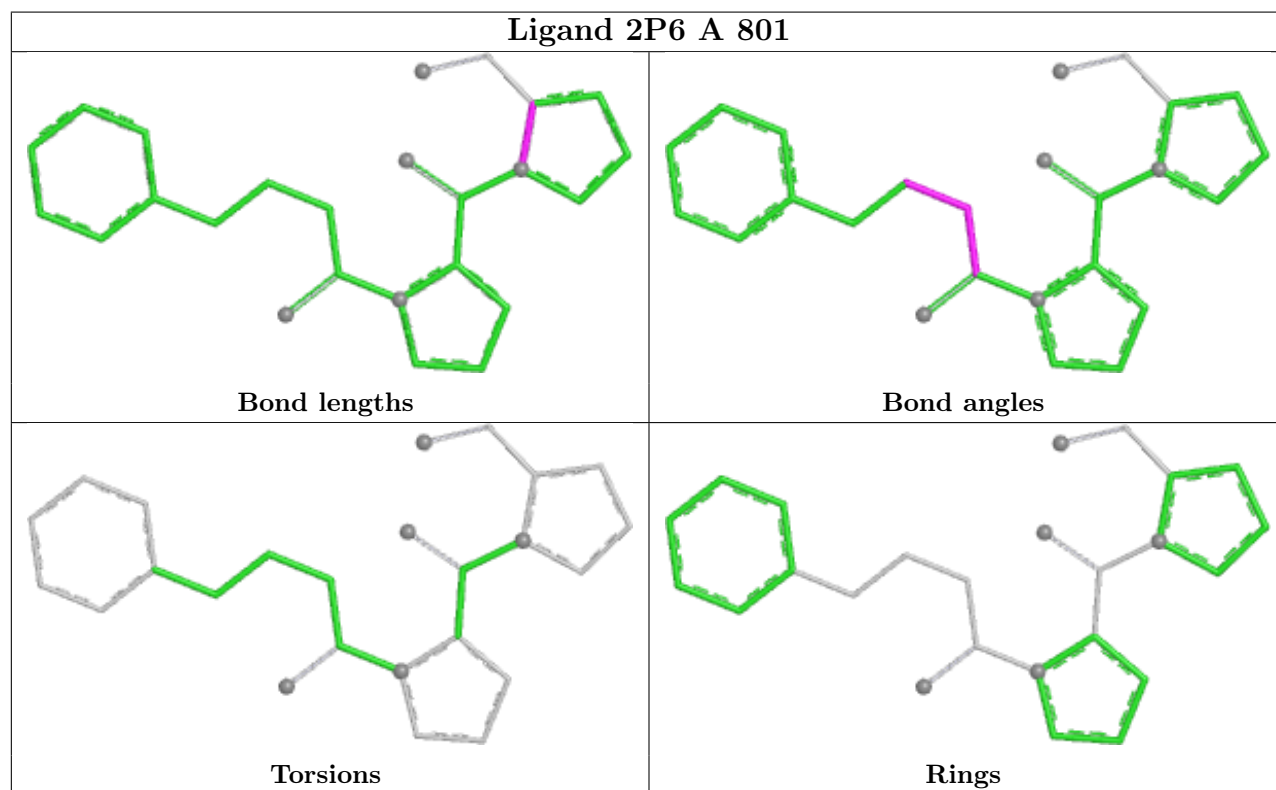
Mol	Chain	Res	Type	Atoms
3	C	808	GOL	C1-C2-C3-O3
3	A	804	GOL	O1-C1-C2-O2
3	A	810	GOL	O1-C1-C2-O2
3	B	801	GOL	O1-C1-C2-O2
3	B	803	GOL	O2-C2-C3-O3
3	B	805	GOL	O2-C2-C3-O3
3	C	808	GOL	O2-C2-C3-O3
3	A	810	GOL	O2-C2-C3-O3
3	B	804	GOL	O1-C1-C2-O2
3	C	808	GOL	O1-C1-C2-O2
5	A	806	B3P	C1-C2-N2-C8
5	A	806	B3P	C1-C3-N1-C4
3	A	811	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-O2
3	A	808	GOL	O2-C2-C3-O3
3	A	811	GOL	O2-C2-C3-O3
3	B	803	GOL	O1-C1-C2-O2
3	A	810	GOL	C1-C2-C3-O3
3	A	808	GOL	O1-C1-C2-O2
3	C	805	GOL	O2-C2-C3-O3
5	A	806	B3P	C10-C8-C9-O1
5	C	801	B3P	O2-C10-C8-C9
2	B	802	2P6	C18-C19-C20-C25
2	C	802	2P6	C15-C17-C18-C19
2	B	802	2P6	C18-C19-C20-C21
5	A	806	B3P	N1-C4-C7-O6
5	C	801	B3P	O2-C10-C8-N2
3	A	802	GOL	O2-C2-C3-O3
5	C	801	B3P	C5-C4-C7-O6

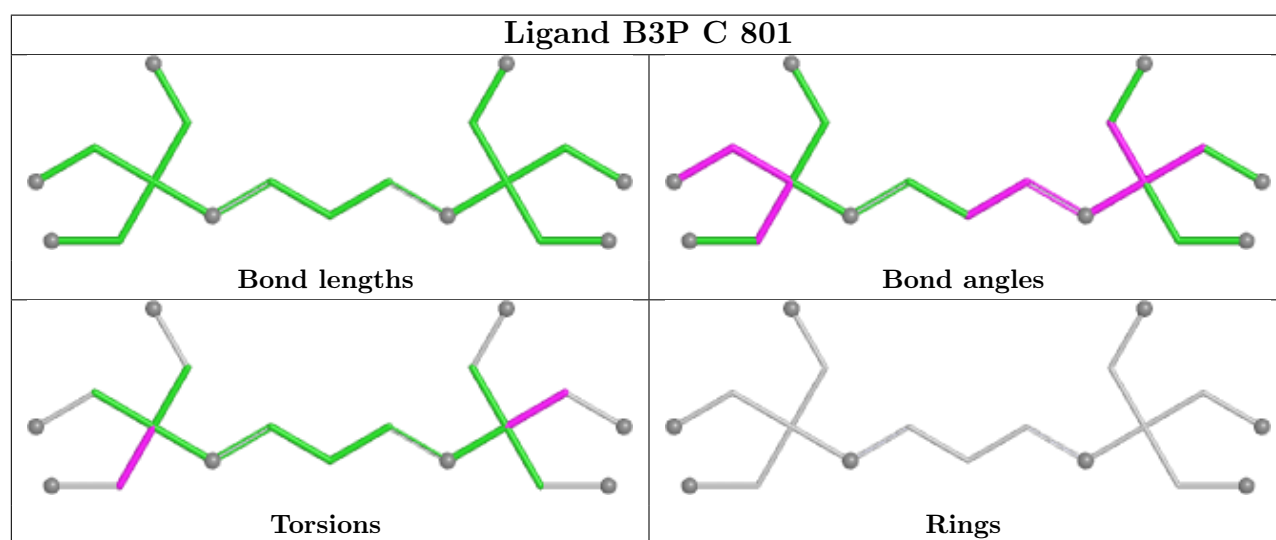
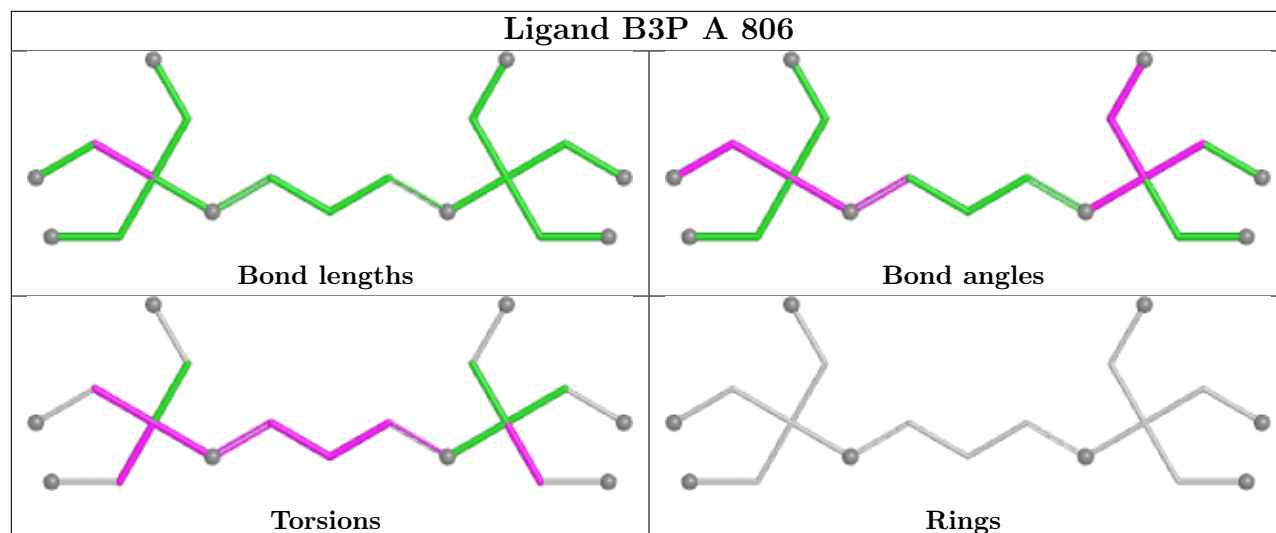
There are no ring outliers.

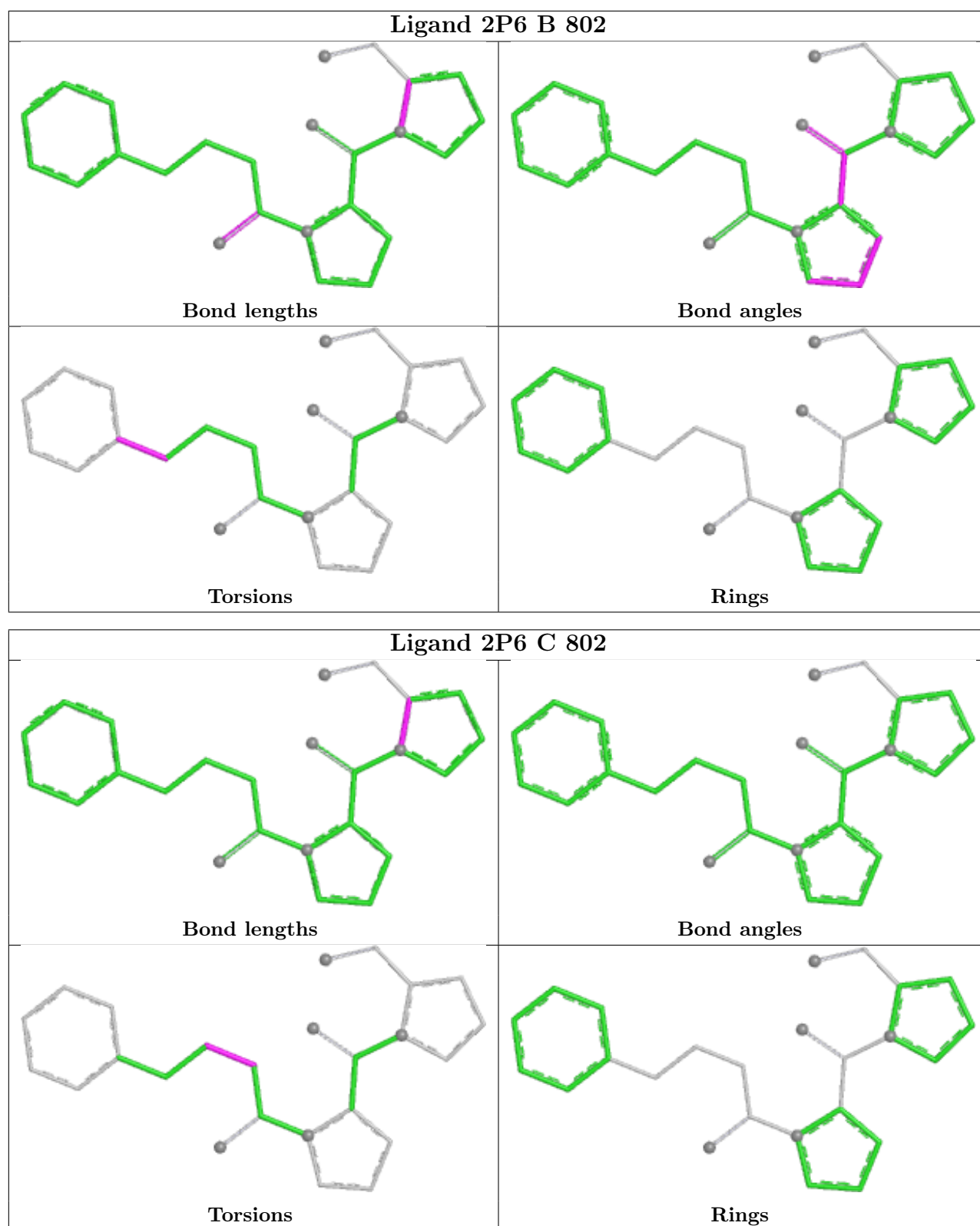
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	GOL	1	0
4	C	804	SCN	1	0
5	A	806	B3P	3	0
3	A	811	GOL	3	0
2	B	802	2P6	1	0
3	B	806	GOL	1	0
3	A	808	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.







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 [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	708/711 (99%)	-0.72	2 (0%)	90 91	6, 17, 36, 62	6 (0%)
1	B	708/711 (99%)	-0.81	2 (0%)	90 91	6, 14, 30, 56	7 (0%)
1	C	707/711 (99%)	-0.51	4 (0%)	85 89	7, 21, 42, 71	2 (0%)
All	All	2123/2133 (99%)	-0.68	8 (0%)	88 90	6, 17, 37, 71	15 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	THR	2.6
1	B	4	LEU	2.6
1	C	427	VAL	2.5
1	A	425	VAL	2.5
1	C	429	GLY	2.2
1	C	192	GLN	2.1
1	B	3	SER	2.1
1	C	191	PRO	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,

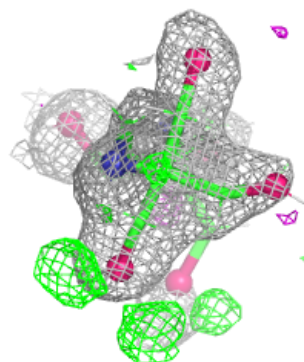
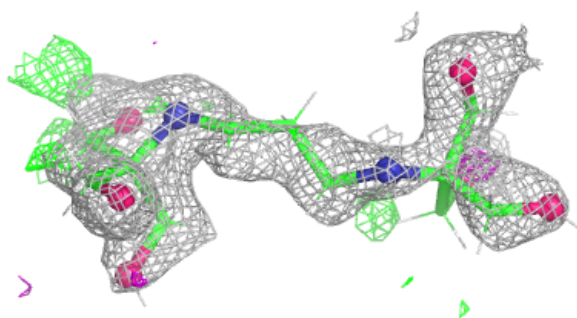
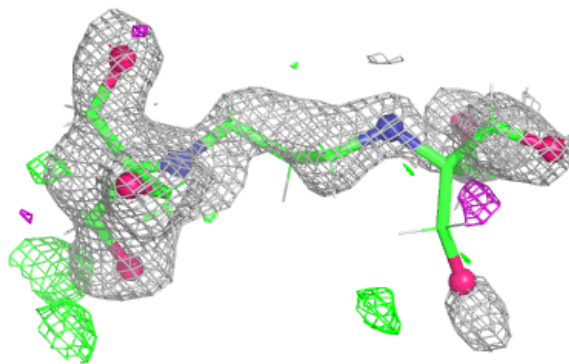
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	B3P	A	806	19/19	0.84	0.14	34,47,62,67	8
3	GOL	A	808	6/6	0.87	0.12	31,32,38,45	3
3	GOL	C	806	6/6	0.88	0.12	38,44,49,50	3
4	SCN	A	809	3/3	0.88	0.14	38,38,41,46	0
3	GOL	B	804	6/6	0.88	0.11	28,38,53,54	3
4	SCN	C	807	3/3	0.90	0.11	35,35,47,58	0
3	GOL	C	808	6/6	0.90	0.11	34,38,39,45	14
3	GOL	A	803	6/6	0.91	0.12	19,38,51,52	3
3	GOL	B	806	6/6	0.92	0.08	24,28,38,38	3
3	GOL	A	811	6/6	0.92	0.09	19,28,38,38	3
3	GOL	A	810	6/6	0.93	0.07	32,37,39,47	3
3	GOL	B	805	6/6	0.93	0.07	38,43,44,47	3
3	GOL	B	801	6/6	0.93	0.09	18,30,38,38	3
3	GOL	B	803	6/6	0.93	0.08	21,29,38,38	3
4	SCN	C	803	3/3	0.94	0.10	34,34,42,44	0
3	GOL	A	804	6/6	0.94	0.08	23,28,38,41	3
3	GOL	A	802	6/6	0.94	0.07	22,31,38,38	3
4	SCN	B	807	3/3	0.95	0.07	28,28,42,44	0
4	SCN	C	804	3/3	0.95	0.07	28,28,31,46	0
3	GOL	A	807	6/6	0.97	0.05	21,24,38,38	3
3	GOL	C	805	6/6	0.97	0.05	23,27,38,38	3
4	SCN	A	805	3/3	0.97	0.09	28,28,31,33	0
5	B3P	C	801	19/19	0.97	0.04	14,19,38,38	8
2	2P6	C	802	25/25	0.98	0.04	12,16,28,38	1
2	2P6	A	801	25/25	0.98	0.04	10,14,25,38	1
2	2P6	B	802	25/25	0.98	0.05	9,12,28,38	1

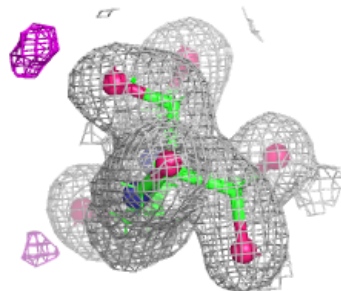
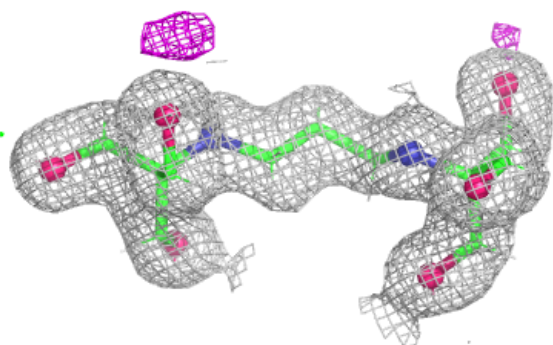
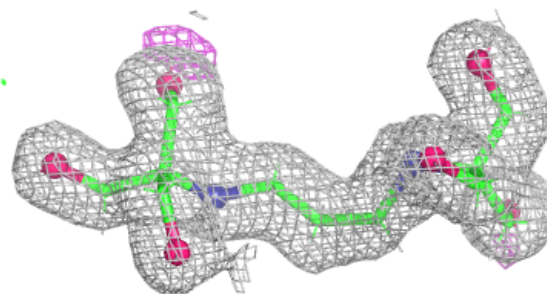
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P A 806:

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

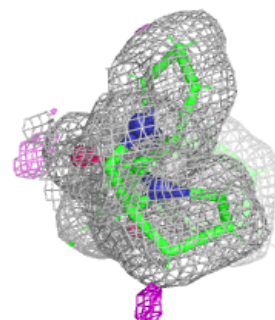
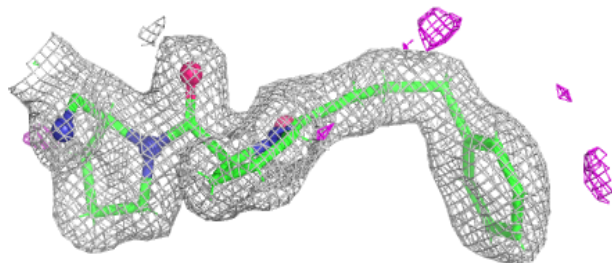
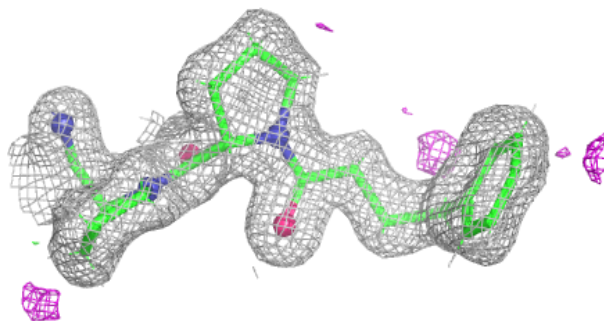
**Electron density around B3P C 801:**

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

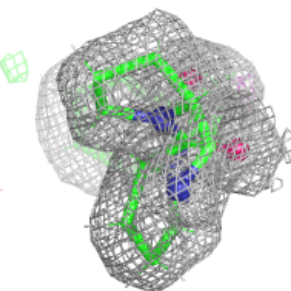
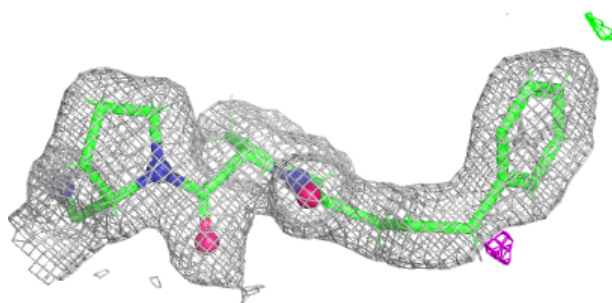
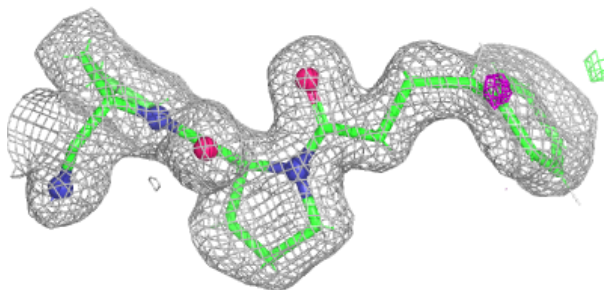


Electron density around 2P6 C 802:

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

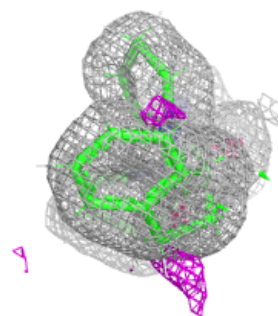
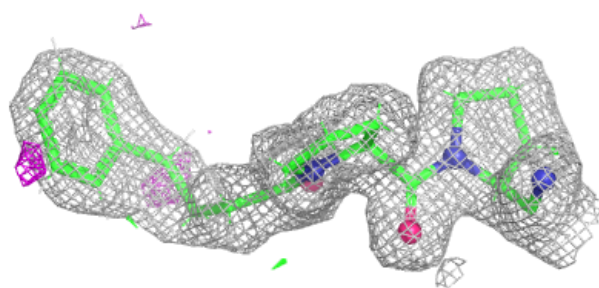
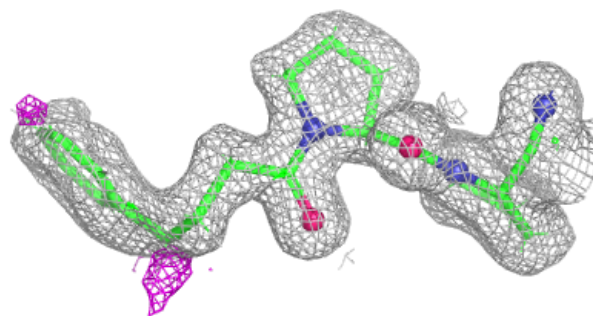
**Electron density around 2P6 A 801:**

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



Electron density around 2P6 B 802:

$2mF_o-DF_c$ (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.